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First 4-Pyridylidene Carboxylate Complexes of Ruthenium and their Water Oxidation Catalysis; Origin of High (*E*)-selectivity in Alkene Isomerization by a CpRu(PN) Catalyst

A dissertation submitted in partial satisfaction of the requirements for a Doctor of Philosophy

in

Chemistry

by

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2021

The dissertation of Thomas Chi Cao is approved, and it is acceptable in quality and form for publication on microfilm and electronically:

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Chair

University of California San Diego

San Diego State University

2021

DEDICATION

Dedicated to my parents, brother, and sister.

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PUBLICATIONS

"Origin of High Kinetic (E)-selectivity in a CpRu(PN) Catalyst for Alkene Isomerization; a Combined Computational and Experimental Approach"
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"Increasing Ligand Denticity for Water Oxidation Catalysis using P^V as Connecting Element"
Saeedifard, Farzaneh; Cao, Thomas C.; Kamdar, Jayneil M.; Smith, Diane K.; Cooksy, Andrew L.; Rheingold, Arnold L.; Moore, Curtis E.; Grotjahn, Douglas B.
Submission planned **2021**.

"X-ray crystallography and electrochemistry reveal electronic and steric effects of phosphine and phosphite ligands in complexes $Ru^{II}(\kappa^4\text{-bda})(PR_3)_2$ and $Ru^{II}(\kappa^3\text{-bda})(PR_3)_3$ (bda = 2,2'-bipyridine-6,6'-dicarboxylato)"
Yazdani, Sima; Silva, Braden E.; Cao, Thomas C.; Rheingold, Arnold L.; Grotjahn, Douglas B.
Polyhedron **2019**, *161*, 63-70. doi.org/10.1016/j.poly.2018.12.033

PRESENTATIONS

"Origin of Selectivity in CpRu Catalyst for Alkene Isomerization"
Thomas Chi Cao, Erik Paulson, Andrew L. Cooksy, Douglas B. Grotjahn
April 2018. Organic Reactions Catalysis Society, 27th Biannual Meeting, San Diego, CA

"Novel mesoionic/remote N-heterocyclic carbene ligands and their ruthenium(II) aqua complexes"
Thomas Chi Cao, Douglas B. Grotjahn
April 2017. 253rd ACS National Meeting & Exposition, San Francisco, CA; *presented at Sci-Mix*
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"Ruthenium(II) coordination to pyridylidene remote N-heterocyclic carbenes: A complex story"
Thomas Chi Cao, David Marelius, Jayneil Kamdar, Arnold Rheingold, Curtis Moore, Douglas Grotjahn
April 2016. ACS San Diego Section 75th Anniversary Symposium/Poster Session, San Diego, CA

"Ruthenium(II) coordination to pyridylidene remote N-heterocyclic carbenes: A complex story"
Thomas Chi Cao, David Marelius, Jayneil Kamdar, Arnold Rheingold, Curtis Moore, Douglas Grotjahn
April 2016. SoCal Organometallics Meeting XVI; Irvine, CA

"Ruthenium(II) coordination to pyridylidene remote N-heterocyclic carbenes: A complex story"
Thomas Chi Cao, David Marelius, Jayneil Kamdar, Arnold Rheingold, Curtis Moore, Douglas Grotjahn
March 2016. 251st ACS National Meeting & Exposition, San Diego, CA; INOR-358

"Measurement of Trace Amounts of Carbon Dioxide in Water by MS - How Hard Can That Be?"
June 2020. ASMS Meeting
Dale A. Chatfield, Colton Breyer, Aaron G. Nash, Thomas Chi Cao, Douglas B. Grotjahn, Diane K. Smith.

"Kinetics analysis of selective organometallic catalysts for alkene isomerization"
Andrew L. Cooksy, Erik R. Paulson, Thomas Chi Cao, Douglas Grotjahn
August 2019. 258th ACS National Meeting & Exposition, San Diego, CA; CATL-0429.

"Toward more stable water oxidation catalysts: progress in measurement and synthesis"
Aaron G. Nash, Colton Breyer, Brett D. Vincenzini, Thomas Chi Cao, Dale Chatfield, Diane K. Smith, Douglas B. Grotjahn
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"Measuring and increasing water oxidation catalyst viability"
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ABSTRACT OF THE DISSERTATION

First 4-Pyridylidene Carboxylate Complexes of Ruthenium and their Water Oxidation Catalysis; Origin of High (*E*)-selectivity in Alkene Isomerization by a CpRu(PN) Catalyst

by

Thomas Chi Cao

Doctor of Philosophy in Chemistry

University of California San Diego, 2021
San Diego State University, 2021

Professor Douglas Grotjahn, chair

Part 1 of this dissertation entails the synthesis and characterization of a new family of ruthenium complexes bearing remote NHC, 4-pyridylidene ligands for water oxidation. Catalytic water oxidation is important for the development of cost-effective and carbon-neutral methods to produce hydrogen fuel from water. We describe the Zincke pyridine synthesis of ligand precursors OC^{R}, where OC = 3-carboxypyridinium and the nitrogen atom of the pyridinium has been quaternized has been functionalized such that R = methyl (Me), adamantyl (Ad), and 2,6-dimethylphenyl (Ar). All three ligand precursors were successfully cyclometallated to yield coordination complexes of the formula $[Ru^{II}(OC^{R})(tpy)(L)]^{+}[PF_6]^{-}$ (tpy = 2,2';6',2"-terpyridine, L = CH_3CN or H_2O). The 4-pyridylidene coordination of the OC^{R} ligand was confirmed by NMR and x-ray diffraction studies. $Ru(OC^{Ad})$ exhibited a reversible Ru^{II}/Ru^{III} with an $E_{1/2}$ of 0.441 V at pH 1. Combined UV-vis, QTOF-MS, and TDDFT were used

to study the stability of the complexes in solution. During catalytic screening for water oxidation activity with ceric ammonium nitrate as the sacrificial oxidant, Ru(OC^{R}) appeared to exhibit an initial burst of O_2 production followed by a plateau after 40-100 turnovers.

Part 2 of this dissertation examines an alkene isomerization catalyst Ru(acn), that was previously reported by the Grotjahn lab to exhibit high activity for isomerizing terminal alkenes to their internal isomers. The catalyst was noteworthy for its fast reaction times, mild reaction conditions, and significantly, its unprecedented kinetic (*E*)-selectivity. We conduct the first combined experimental and theoretical study to unveil the mechanism of isomerization and the origin of the high (*E*)-selectivity exhibited by the catalyst. In-situ NMR reaction monitoring were used to acquire time-dependent kinetics data for the Ru(acn)-mediated isomerization of but-1-ene into its (*E*)-and (*Z*)-but-2-ene isomers, the latter of which required special reaction conditions. An extensive computational model was developed, and lowest energy pathways validated by experimental Arrhenius activation energies derived from the experimental data. The experimental activation energies compared well to the DFT energies for the isomerization pathway featuring an exo-coordinated η^3-allyl, and the structures of key intermediates reveal inner-sphere steric interactions that favor the (*E*)-allyl intermediate over the (*Z*)-isomer.

Part 1. First 4-Pyridylidene Carboxylate Remote N-Heterocyclic Carbene Complexes of Ruthenium and their Water Oxidation Catalysis

Thomas Chi Cao, Arnold L. Rheingold, and Douglas B. Grotjahn

1.1. Background

Replacing hydrocarbon-based fossil fuels with carbon-neutral alternatives is a constructive step towards addressing the threat of climate change. One such alternative is molecular hydrogen, which has a gravimetric energy density comparable to that of traditional fossil fuels such as gasoline. While hydrogen can be consumed for energy without the emission of carbon byproducts, carbon-neutral production of hydrogen remains a challenge. As of 2017, 96% of global hydrogen reserves were produced from the steam reforming of hydrocarbons (**Eqn 1**), a process which generates carbon emissions.[1]

Eqn 1. Steam reforming $CH_4 + H_2O \rightarrow CO + 3H_2$

Molecular hydrogen is unavailable as a planetary resource and must be produced from compounds that contain it. Of such compounds, water is the most abundant and readily available, and is thus highly desirable as a potential feedstock for producing hydrogen. One way to extract hydrogen from water is via electrolysis, which splits the water molecule into hydrogen and oxygen (**Eqn 2**). However, water electrolysis is not cost-effective for the industrial-scale production of hydrogen, and suffers from low overall efficiency compared to other methods.[1,2] For this reason, significant scientific attention has been devoted to discovering ways to increase the efficiency of water splitting.

Eqn 2. Water splitting $2H_2O \rightarrow 2H_2 + O_2$

Eqn 3. Oxidation half reaction $2H_2O \rightarrow 4H^+ + 4e^- + O_2\,(g)$ $\Delta G° = 1.23$ V

Eqn 4. Reduction half reaction $4H^+ + 4e^- \rightarrow 2H_2\,(g)$ $\Delta G° = 0.00$ V

Water splitting is an oxidation-reduction (redox) reaction that can be divided into two half reactions (**Eqns 3** and **4**). The oxidation half reaction requires a minimum potential difference of 1.23 V (114 kcal/mol) to overcome just the unfavorable thermodynamic difference between reactants and products (**Figure 1**). In addition, the high activation energy required for the concerted $4H^+/4e^-$ WOX reaction contributes to the large

overpotentials typically associated with the reaction. Reducing the overpotential for WOX is the bottleneck in the practical application of water splitting to hydrogen production.[3]

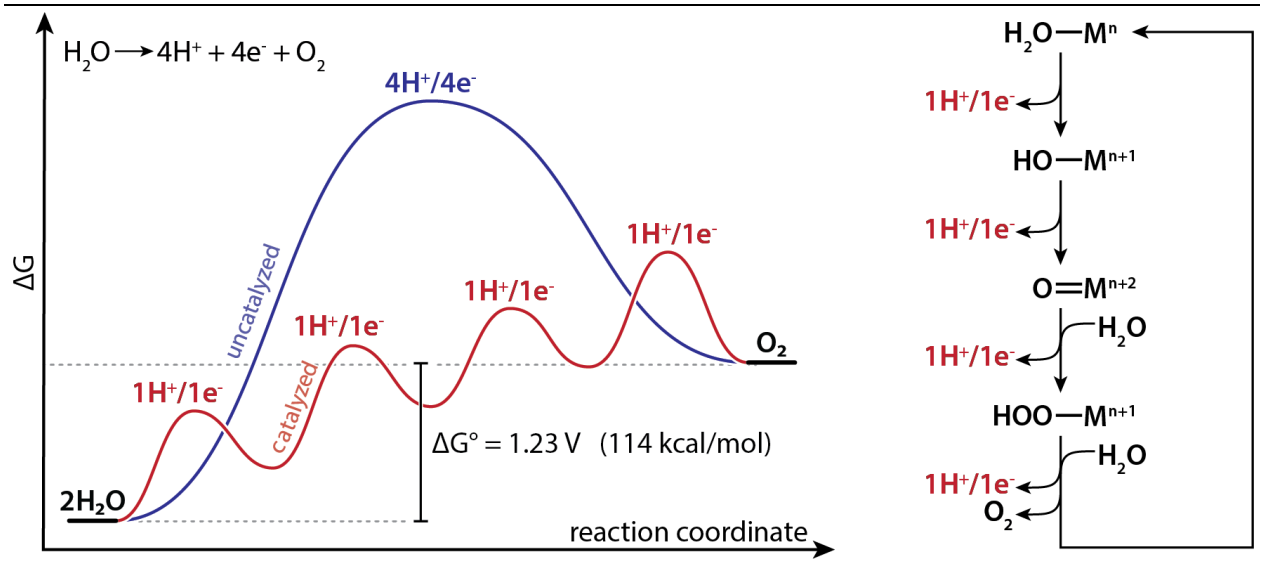
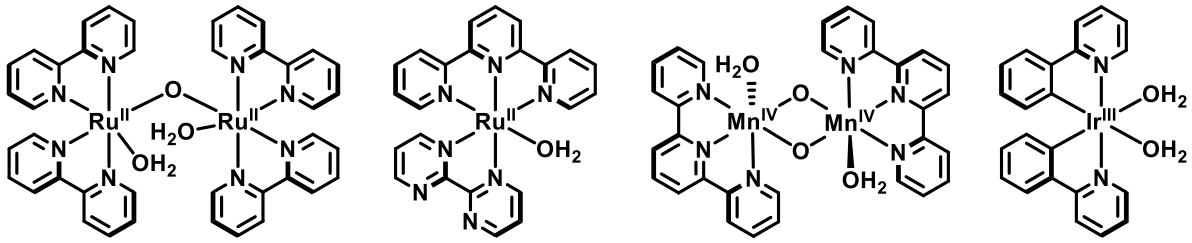


Figure 1. Left, generic energy diagram for water oxidation. Right, one mechanism for water oxidation by a transition metal; note that in some cases, proton transfer and electron transfer are not concurrent.

A water oxidation catalyst (WOC) can reduce the energy needed for the WOX reaction by breaking up the concerted $4H^+/4e^-$ process into a series of smaller, stepwise oxidations (**Figure 1**, left, red curve). These steps may be simultaneous H^+ and e^- transfers (proton coupled electron transfers, PCET) or sequential H^+ or e^- transfer followed by e^- or H^+ transfer, where the PCET is thought to result in lower barriers than sequential transfers.[4,5] Either PCET or sequential proton and electron transfers can be mediated by transition metal complexes. A water oxidation complex (WOC) can coordinate to water to forming a complex that, when oxidized, causes water to shed protons until O-O bond formation (**Figure 1**, right).

An example of WOX catalysis takes place within the chloroplasts of photosynthetic plants.[6] Chloroplasts have proteins that direct sunlight to the Oxygen Evolving Center (OEC) of Photosystem II to drive the oxidation of water into protons, electrons, and O_2. The protons and electrons generated in this process are passed to downstream processes driving the biosynthesis of energy carrier molecules ATP and NADPH.[7]



A. Meyer (JACS/1983) **B.** Meyer (JACS/2008) **C.** Brudvig (Science/1999) **D.** Bernhard (JACS/2008)

Figure 2. Examples of WOCs. A[8], B[9], C, D[10]

The photosynthetic apparatus of plants has inspired humans to create synthetic WOCs. Since 1983, considerable academic effort has been expended towards the synthesis, discovery, and study of both heterogeneous and homogeneous WOCs. At the present time, a vast array of homogeneous WOCs have been reported for many transition metal complexes of ruthenium,[8,9,11–16] iridium,[10,17,18] cobalt,[19,20] and others[21] (**Figure 2**). The proliferation of known WOCs, however, has unfortunately shown that most synthetic WOCs were only capable of modest catalytic activity (see ref[21] for WOC review).

It was not until 2012 that the field saw the introduction of a WOC capable of a turnover frequency of 303 s^{-1}, elevating artificial WOCs to the level of the OEC.[15] The WOC reported by Sun et al., a Ru^{II} complex bearing a tetradentate, 2,2′-bipyridine-6,6′-dicarboxylate ligand (bda) (Figure 3, at left), was said to be two orders of magnitude faster than the existing WOCs at the time.[15]

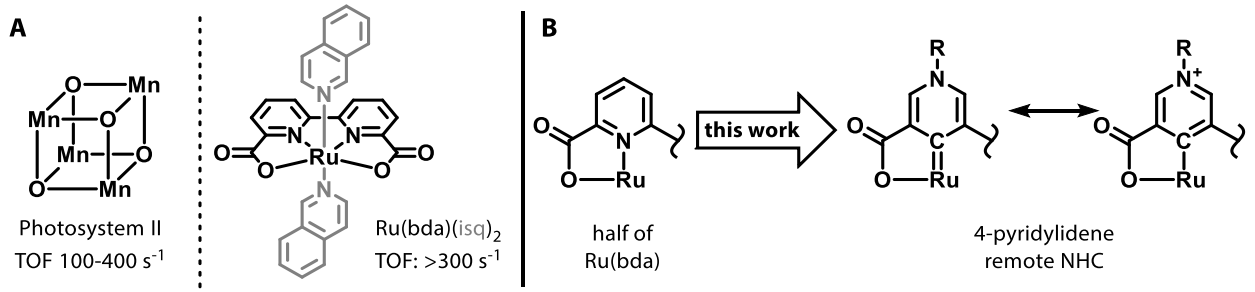


Figure 3. Left, OEC and bda. Right, general aim of this work.

Prior to Ru(bda), a majority of mainstream homogeneous WOCs were supported by neutral polypyridyl ligands (see ref [21] for a review on WOCs). Ru(bda) represented a paradigm shift towards anionic ligand scaffolds. Transition metal complexes bearing anionic ligands such as carboxylates exhibit decreased redox potentials compared to analogues that only have neutral polypyridyl ligands.[22] The lowered potentials promote the

formation of high-valent intermediates during water oxidation.[13,14] In addition, the tetradentate dicarboxylate bipyridyl chelating nature of bda promote an unusual distorted octahedral coordination geometry that allow substrate waters to coordinate Ru(bda) as a seventh ligand instead of undergoing a costly bond-breaking step.[13]

Inspired by the remarkable WOX ability exhibited by Ru(bda), we envisioned strategies to upgrade the bda scaffold to increase its electron donor ability, which we believed would result in further lowering of redox potentials in the resulting complexes.[17] One modification consistent with this goal is the replacement of one or more pyridyl rings of bda with a 4-pyridylidene motif (**Figure 4**, right). The literature precedent for this idea can be found in 3- and 4-pyridylidene complexes reported by Tanaka et al., where the pyridylidene complexes exhibited $E_{1/2}$ potentials about 400 mV lower than that of their pyridyl analogues (Figure 4).[23,24] Perhaps the pyridylidene analogue of a pyridyl WOC would result in improved catalytic parameters in a similar vein to the effect achieved through the carboxylate ligands on Ru(bda).

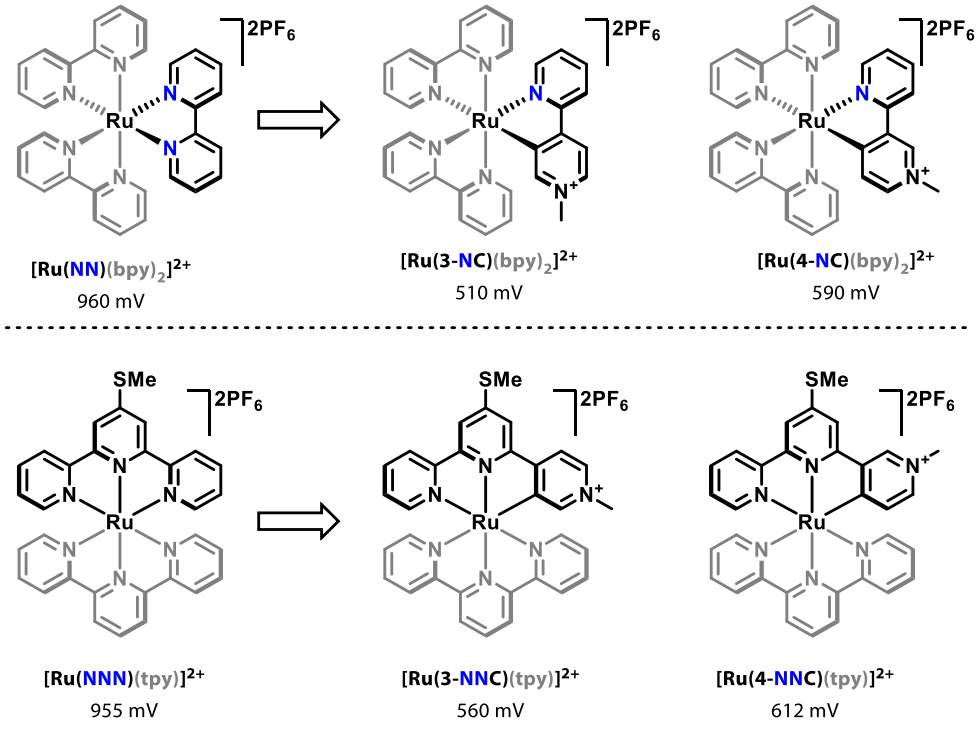


Figure 4. Comparison of NN and NC complexes reported by Tanaka et al.[23,24] Reported E1/2 for Ru(III)/Ru(II) couple shown in millivolts.

While five-membered N-heterocyclic carbene (NHC) complexes are well known as water oxidation catalysts, reports of pyridylidene complexes are comparatively rare.[25] Compared to their five-membered

imidazoylidene and triazoylidene cousins, pyridylidenes have fewer heteroatoms to stabilize the carbene (**Figure 5**), which causes them to form more robust metal-carbene bonds and act as better donors.[26] Unfortunately, only a handful of examples[27,28] of other ruthenium complexes bearing pyridylidene exist in the literature, and none so far have been reported to exhibit water oxidation ability.

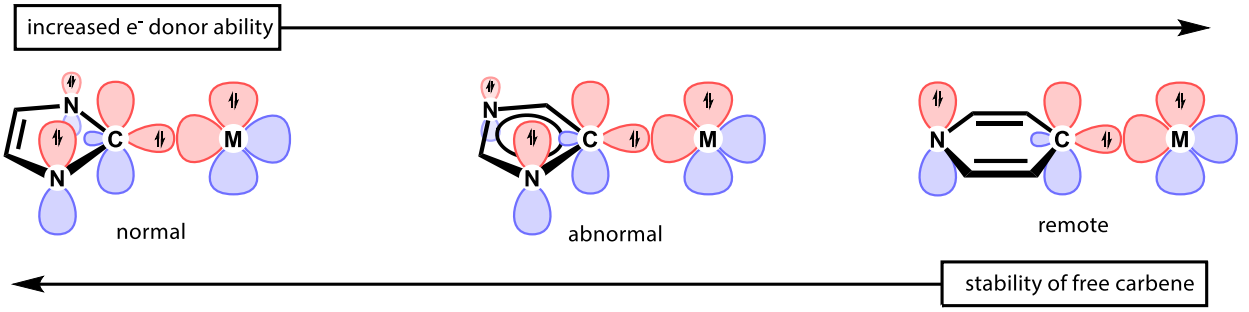


Figure 5. NHC stability. 'Normal': Arduengo[29] NHC with two heteroatom adjacent to carbene. 'Abnormal': less stabilized abnormal NHC with heteroatoms displaced. 'Remote': 4-pyridylidene as an example.

Our initial synthetic target was a direct Ru(bda) analogue wherein one or both pyridine rings in the bda ligand are replaced with a pyridylidene moiety (**Figure 6**, at left). Three such bda-like ligand precursors were synthesized (section 1.4.1.3-5). We expected that the carboxylate and/or pyridyl groups on the precursors serve as a directing group for a ruthenium atom to insert into the pyridinium ring at the position *para* to the quaternary nitrogen, thus coordinating in a pyridylidene fashion. However, early metallation attempts gave intractable reaction mixtures whose ^{1}H NMR showed forests of peaks in the aromatic region, suggesting the formation of multiple products.

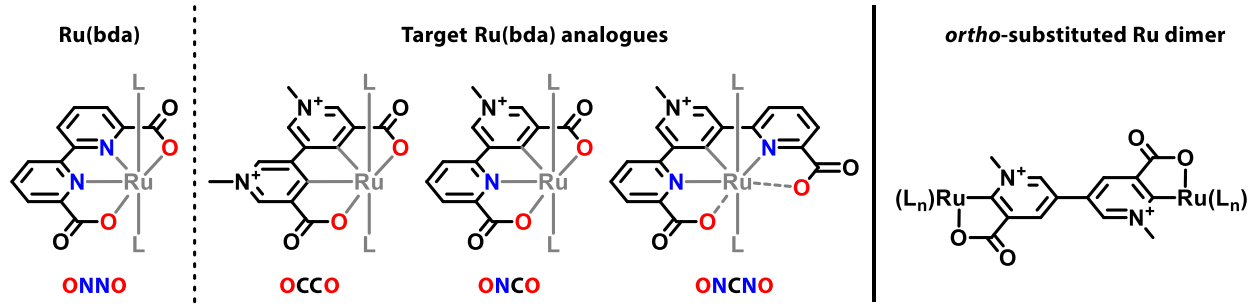


Figure 6. *Left*: Ru(bda) and comparison to analogues targeted in the initial stages of this work. *Right*: XRD structure of *ortho*-substituted OCCO dimer. Each ruthenium atom has 3 acetonitrile ligands and a 4-methylpyridine *trans* to the carbene.

A crystal structure (**Figure 6**, *at right*; see also 1.6.5.2) obtained from a reaction of the OCCO precursor revealed an *ortho*-substituted Ru dimer wherein each ruthenium atom is coordinated in a bidentate fashion to the OCCO ligand. The ruthenium atoms were additionally coordinated to three acetonitrile ligands, which suggests a mechanism for the formation of multiple products due to ligand exchange. For this reason, we decided to shift our focus towards installing bulkier functional groups on the quaternary nitrogen of the pyridinium ring to sterically disfavor *ortho*-substitution. To develop synthetic methodology, a simpler 3-carboxylate system was used as a model substrate in place of more complex polypyridyl systems. Three ligand **OC^{R}** ligand precursors (where R = methyl, adamantyl, and 2,6-dimethylphenyl) were synthesized. Upon reaction with $[Cl_2Ru(tpy)]_2$, all three precursors gave coordination complexes wherein the ruthenium atom is coordinated in a pyridylidene fashion at *para*-position of the ligand.

1.2. Synthesis

1.2.1. N-(alkyl/aryl)pyridinium ligand precursors

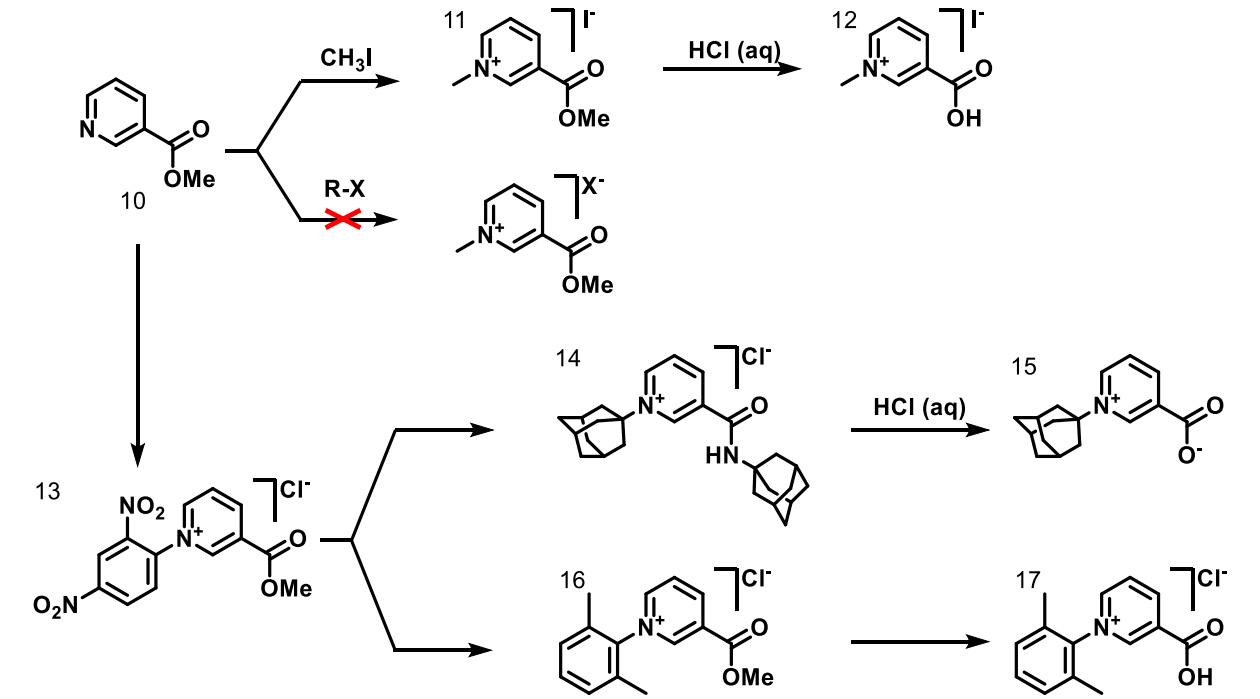


Figure 7. Synthetic sequences for OC ligand precursors.

Detailed procedures for the preparation of Ru(OC^{R}) complexes and OC^{R} ligand precursors are presented in section 1.4.1. Ligand precursors **12**, **15**, and **17** (**Figure 7**) were synthesized as bidentate, OC analogues to the NC precursor ligands reported by Tanaka et al,[24] with precursor **12** a direct analogue in terms of the methyl functionality on the pyridine quaternary nitrogen. We expected that upon exchange with a suitable source of ruthenium, the carboxylate groups will serve to direct the metal to substitute at the *para* position of the pyridinium ring. However, our preliminary experiments with polypyridyl ligand precursors (1.4.1.3, 1.4.1.4, and 1.4.1.5) indicated the possibility of *ortho* substitution (see 1.6.5.2), and therefore compounds **15** and **17** were conceived as sterically bulky analogues of **12** to block approach of the metal towards both *ortho* positions of the pyridinium ring.

N-functionalization was the crux of the synthetic sequence because the electron-withdrawing methoxycarbonyl reduces the nucleophilicity of the pyridyl nitrogen. While N-alkylation of **10** occurred readily

with methyl iodide, **10** did not react with more hindered haloalkanes such as 2-bromopropane and 1-bromoadamantane.

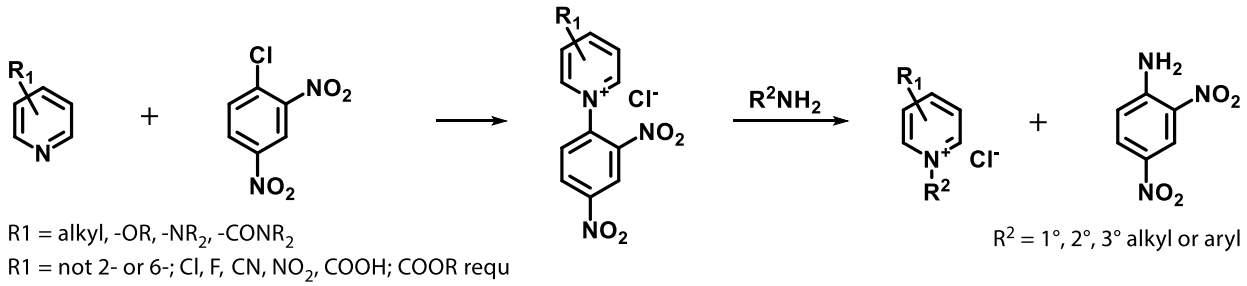


Figure 8. General reaction scheme of Zincke reaction

The challenging reactivity of **10** prompted us to search for an alternative procedure to effect quaternization of the nitrogen of **10.** To accomplish, this, we turned to the Zincke reaction, where 1° and 2° amines react N-(2,4-dinitrophenyl)pyridinium chloride to obtain the corresponding N-(alkyl/aryl)pyridinium salt.[30] The mechanism of this reaction is thought to involve ring opening and recyclization steps (**Figure 9**) that we hoped would circumvent the poor nucleophilicity of **10**.

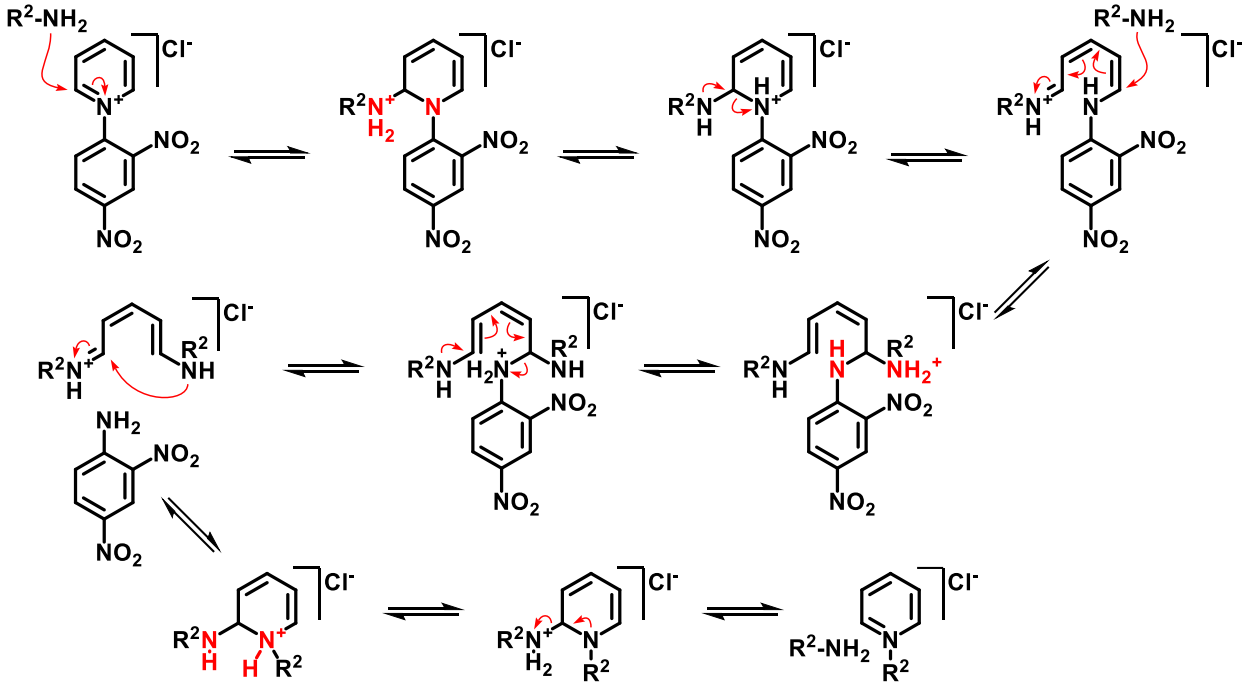


Figure 9. Scheme of possible mechanistic steps in ring-opening and re-aromatization of the Zincke pyridine.

To utilize the Zincke reaction, **10** must first be reacted with 2,4-dinitrochlorobenzene (dnpCl) to synthesize the N-(2,4-dinitrophenyl)pyridinium salt **13**. Literature reports indicate that in this step, pyridines bearing electron withdrawing substituents require high temperatures or do not react at all.[30] Despite significant effort, formation of **13** was not observed under the attempted conditions. This was the case even when **10** was reacted with dnpCl neat at 130 °C (**Figure 10**).

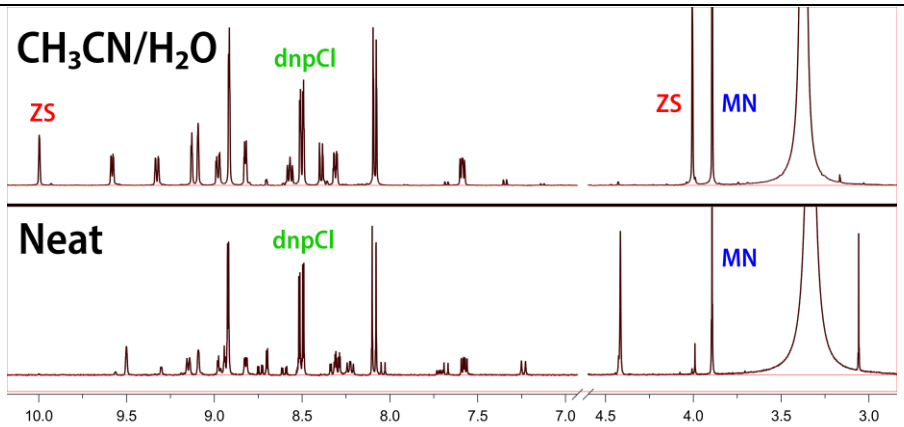


Figure 10. ^{1}H NMR for reactions with **10** and 2,4-dinitrochlorobenzene in mixed solvent (top) and neat (bottom). Diagnostic peaks are labeled ZS = Zincke salt **15**, MN = methyl 3-nicotinate **14**, dnpCl = 2,4-dinitrochlorobezene.

This synthetic trajectory changed with the serendipitous discovery that the addition of water to a stalled reaction resulted in the formation of a new product that was later identified as **13**. Given that this reaction likely proceeds via an S_NAr mechanism, water likely helps to stabilize the polar transition state formed from the attack of **10** on dnpCl or the charges on the ionic products.The reaction proceeded even under mild conditions, albeit as far as 1:1 unreacted **10** and product **13**, as observed by ^{1}H NMR spectroscopy. While a systematic effort to increase the yield was not attempted, subsequent preparations gave similar ratios of starting material and product, despite variations in water content, molar ratio of dnpCl, and reaction times. This could suggest the presence of an equilibrium between the S_NAr reaction of **10** with dnpCl, and attack by the free chloride ion on the N-C carbon atom on **13** to yield **10** and dnpCl.

The possibility of such an equilibrium would be easy to rule out by simplying dissolving **13** in aqueous acetonitrile and bringing mixture to reaction temperatures used to synthesize **13** in the first place. However, the idea of this experiment was only conceived upon drafting this work.

Pyridinium salt **13** reacted readily with 1° amines 1-aminoadamantane and 2,4-dimethylaniline in the presence of a water-methanol solvent mixture to provide **14** and **16**, respectively. Quantitative conversion was indicated by ^{1}H NMR spectroscopic analysis of the reaction mixtures, and isolated yields were similarly high (see 0 and 0). A slight excess of amine was used to ensure that all **13** had been consumed, which meant that the pyridinium salts **14**/**16** would be the only ionic species in post-reaction mixtures, enabling easy workup since the excess amine and 2,4-dinitroaniline byproduct could be extracted using ether from the concentrated aqueous phases.

During the synthesis of **14**, 1-aminoadamantane attacked the carbonyl 3′ carbonyl of **10**, a fact that was addressed by adding in excess of two equivalents of the amine to ensure reaction completion. The subsequent hydrolysis step gave a product that had the elemental composition consistent with the formula of the zwitterionic species shown as **15**. This indicated that the adamantylamine on the carbonyl formed a soluble hydrochloride salt that was removed during workup.

The aryl ester salt **16** underwent partial hydrolysis under the mixed solvent conditions, and therefore was not isolated. After extractive workup, the aqueous phases containing **16** and **17** was boiled to finish the hydrolysis.

1.2.2. 4-pyridylidene complexes of Ru(R)

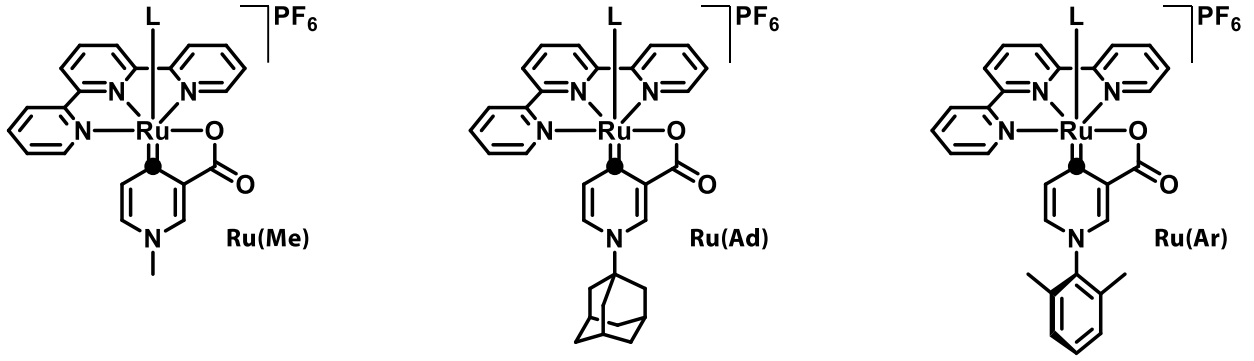


Figure 11. The three 4-pyridylidene complexes synthesized in this work. **Ru** = $Ru^{II}(\kappa^3$-2,2':6',2''-terpyridine)[rNHC(R)](L)$^+$ PF_6^- where rNHC(R) = κ^2-(O,C)-[(**Me**), (**Ad**), and (**Ar**)]; L = CH_3CN or H_2O.

Pyridinium salts **15** and **17** were suitable substrates for cyclometallation with $[Cl_2Ru^{II}(tpy)]_2$ to the obtain title complexes **Ru(Me)**, **Ru(Ad)**, and **Ru(Ar)** in good yields (ca. 47-66%, **Figure 11**). Optimum conditions were found to involve excess (5-6 equivs.) silver acetate in methanolic solutions heated at 70°C for at least two days.

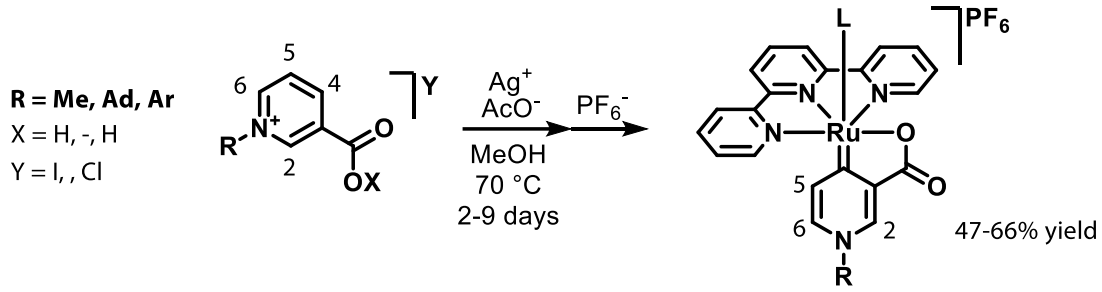


Figure 12. General reaction scheme for the synthesis of **Ru(R)**.

Reaction progress was easily monitored by ^{1}H NMR spectroscopy because the H2 of the **OC^{R}** precursors presents as a doublet near 10 ppm, well clear of any obstructions or trees in the aromatic forest (**Figure 13**). As the reaction proceeds, a new signal whose J-values are consistent with H5 appears at δ 6.5 ppm, indicating a large chemical shift change from δ 8.5 ppm in the free ligand. This represents the first iota of structural information obtainable from the NMR data; the 2 ppm upfield shift in H5 suggests significant shielding from the ring current of the terpyridine π-system, a configuration only expected for the *cis* isomer of **Ru(OC^{R})** shown in **Figure 12**.

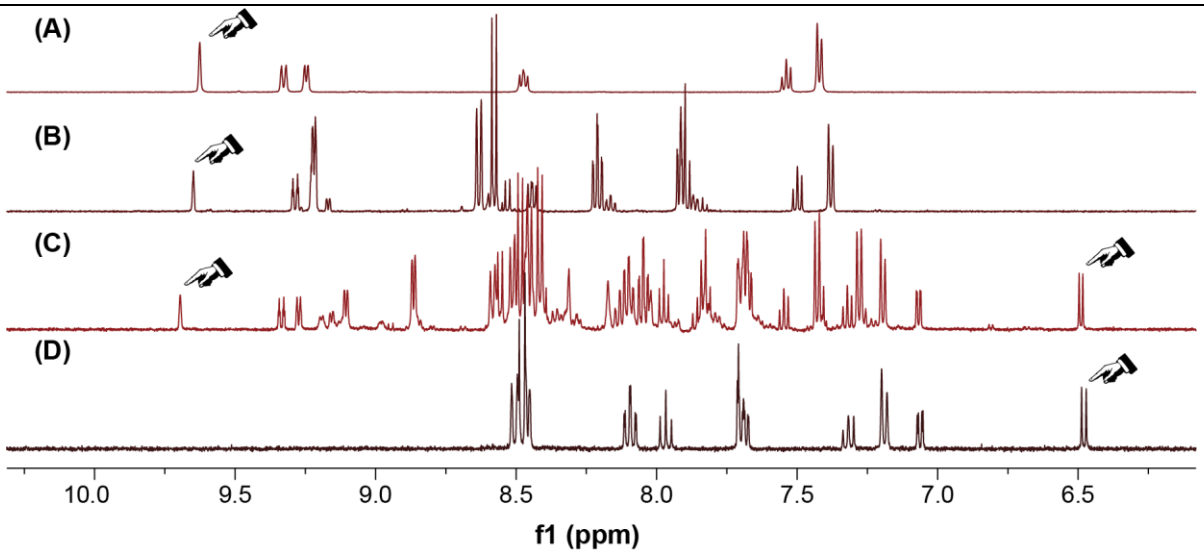


Figure 13. ^{1}H NMR of samples and reaction aliquots taken during a synthesis of **Ru(Ar)** in methanol at 23°C. (A) free ligand; (B) after 4 days at 70°C w/ AgOTf only; (C) after adding KOAc, heating resumed at 70°C for 2 days; (D) product after salt exchange from reaction.

A rigorous attempt to optimize reaction conditions was not attempted owing to good yields, low cost, and simplicity of the procedure. However, samples taken for reaction monitoring suggest that cyclometallation approaches about 50% completion at two days, and that continued heating for up to nine days gave higher yields. Moreover, both a halide abstractor and a Lewis base are needed for cyclometallation to proceed, and thus AgOAc

was chosen as a dual-purpose reagent.[31] During initial survey of metalation conditions, it was found that when KOAc or $AgPF_6$ were used alone, no reaction occurred. However, the reaction can proceed upon addition of the missing component. When acetonitrile was used as the reaction solvent instead of methanol, two major products were seen (**Figure 14**). An attempt was made to isolate the products on alumina column, but a 1:1 mixture of *cis*-**Ru(OC^{Me})** and an unidentified species appeared to co-elute. We speculate that the unidentified species to be an isomer of *cis*-**Ru(OC^{Me})**, perhaps *trans*-**Ru(OC^{Me})**.

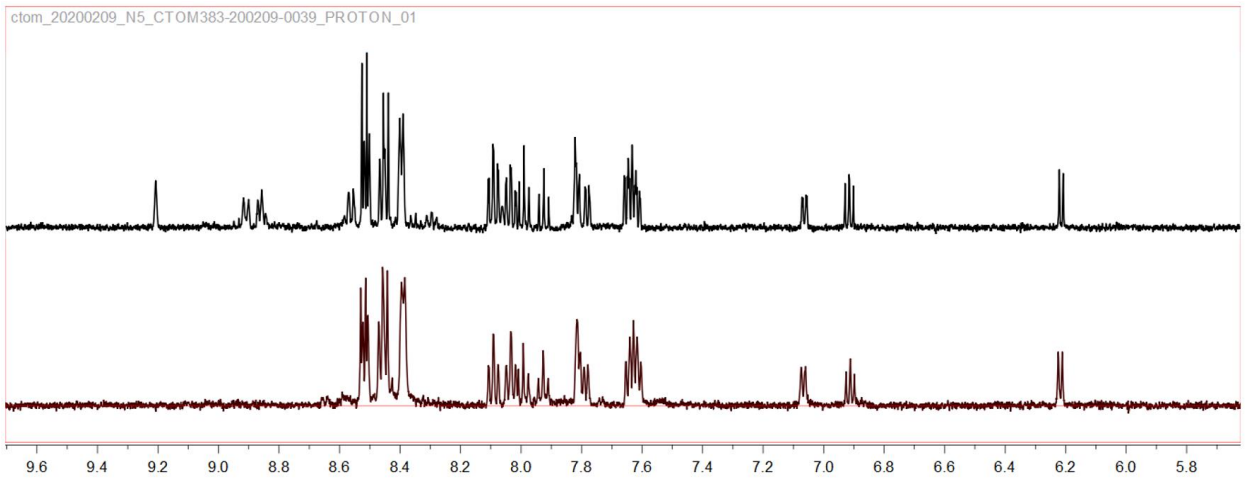


Figure 14. Synthesis of **Ru(Me)** where CH_3CN was used instead of MeOH. Top: reaction mixture prior to workup. Bottom: product obtained after chromatography.

Isolation of **Ru(OC^{R})** was achieved by salt exchange with aqueous KPF_6. First, the reaction mixtures were cooled to room temperature, after which insoluble silver halide salts were filtered off under inert atmosphere. The filtrate was dried on a rotary evaporator; care should be taken at this stage since concentrated solutions of **Ru(OC^{R})** exhibit increased viscosity and exude finger-like projections above the solvent line and are prone to bumping. Upon achieving dried solids, the flask should be taken under inert atmosphere in preparation for salt exchange. The crude material tends to deposit in a thin coating along the walls of the flask and is problematic because it requires prolonged contact with water to become solubilized. Only a minimal amount of water should be added to the flask, and any undissolved solids should be mechanically dislodged into bulk solution. The resultant slurry should then be stirred, violently if necessary, for >30 min until homogeneous (at which point more water can be added if necessary). Addition of KPF_6 results in the rapid appearance of insoluble brown solids that can be collected by filtration. The isolated KPF_6 salts of **Ru(OC^{R})** are readily soluble in polar organic solvents such as

acetonitrile, acetone, and methanol. Aqueous preparations of **Ru(OC^{R})** usually required mechanical agitation, extended periods of stirring, or first dissolving **Ru(OC^{R})** in an organic solvent. The identity of **R** qualitatively correlates to solubility where **R** = **Me** > **Ad** > **Ar** in terms of greater solubility.

1.3. Characterization

1.3.1. NMR Resonances

NMR data is available for all three **Ru(OC^{R})** complexes in section 1.4.1.2. Downfield ^{13}C NMR signals at δ 230.87, δ 231.05, and δ 237.03 ppm were seen for **Ru(OC^{Me})**, **Ru(OC^{Ad})**, and **Ru(OC^{Ar})**, respectively, indicating carbenic character and confirming cyclometallation at the 4-position of the **OC^{R}** ring. The observed resonances show are in good agreement with ruthenium pyridylidene complexes **Ru(4-NC)** and **Ru(4-NNC)**, as well as other other M=C complexes.[23] The observed ranges of ^{13}C chemical shifts for **Ru(OC^{R})** are greater than if the NHC complex had been 3-substituted (**Figure 15**, **Ru(3-NC)** and **Ru(3-NNC)**). The identity of **R** only had a minor effect on the ^{13}C NMR shifts of the carbene and is most pronounced in the case of **Ru(OC^{Ar})**, whose carbene signal has been shifted downfield by 6-7 ppm relative to **Ru(OC^{Me})** or **Ru(OC^{Ad})**.

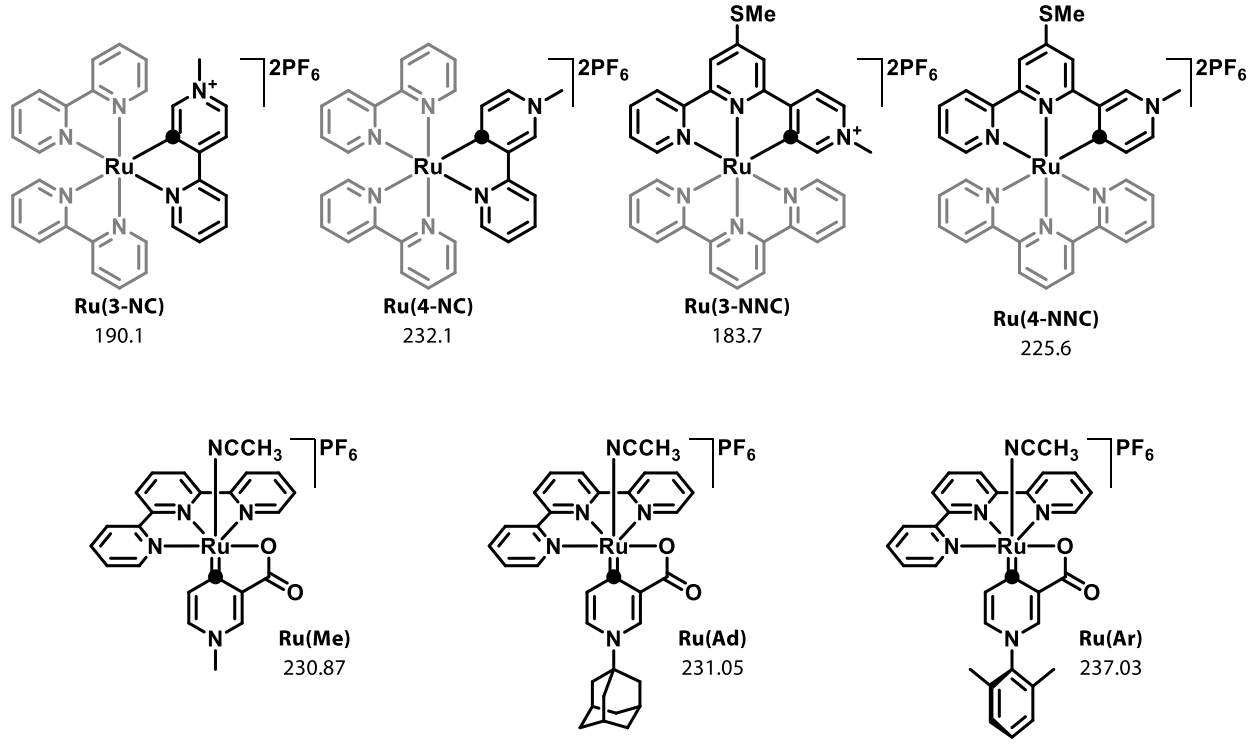


Figure 15. Comparison of ^{13}C NMR peaks of Ru(R) and reference complexes.[23,24]

The ^{1}H NMR spectrum of each complex **Ru(R)** showed the expected number of signals for the structures as drawn in **Figure 11**. The proton signals for the terpyridine ring appeared at relatively constant chemical shifts. A total of 6 signals (2 overlapped) corresponding to 11 protons on terpyridine can be seen in clusters at δ 8.4, δ

7.9, and δ 7.4 ppm (**Figure 16**, orange). Three ^{1}H NMR signals corresponding to protons on **OC^{R}** could be seen. H5 (**Figure 16**, H^{A}) exhibited an upfield shift to δ 6.18, δ 6.21, and δ 6.41 ppm for **Ru(OC^{Me})**, **Ru(OC^{Ad})**, and **Ru(OC^{Ar})**, respectively, consistent with experiencing shielding due to proximity to the π system of the terpyridine ring in the structure of the *cis*-isomer of **Ru(OC^{R})**. Evidence of the electron-withdrawing effects of the aryl substituent on **Ru(OC^{Ar})** can be seen in δ 0.2 ppm downfield shift for H5, as well as in the ^{13}C NMR shifts of the carbene.

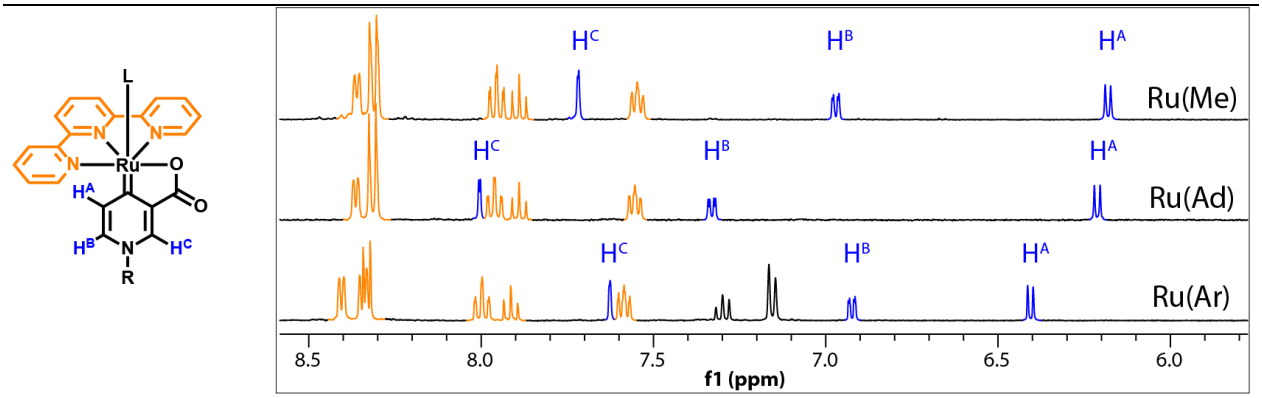


Figure 16. ^{1}H NMR spectra of Ru(R) showing location of the protons signals of terpyridine (orange) and the three proton resonances corresponding to the complexed nicotinate ring (blue).

Somewhat interestingly, H2 and H6 on **Ru(OC^{Ad})** exhibit downfield shifts -0.28 and -0.32 ppm relative to the same protons in **Ru(OC^{Me})** (**Table 1**), suggestive of inductive deshielding due to the stabilized partial positive charge on the quaternary carbon of the adamantyl moiety.[32]

Table 1. ^{1}H NMR shifts of **OC^{R}** (left) and relative differences in chemical shifts (right).

entry	A	B	C	ΔA	ΔB	ΔC
Ru(OC^{Me})	6.18	6.97	7.72	0.00	0.00	0.00
Ru(OC^{Ad})	6.21	7.33	8.00	+0.03	+0.36	+0.28
Ru(OC^{Ar})	6.41	6.92	7.63	+0.23	-0.05	-0.09

1.3.2. Structural Determination by X-ray Diffraction

Crystals of **Ru(OC^{R})** complexes tended to grow as thin needles that were poorly suited to x-ray diffraction studies. However, one fortuitous attempt gave crystals of dimer containing two Ru(Ad) units and 3 PF_6^- ions (**Figure 17**) from the vapor diffusion of ether into acetonitrile solution. The presence of three anions could indicate a mixed-valent species, but due to the crystallographic parameters the possibility of hidden PF_6^- ions could not be ruled out in the solved structure. Both subunits are hexacoordinated; one monomeric unit (labeled **Ru2** in **Figure 17**) had acetonitrile as its sixth ligand, while the other (**Ru2**) was had acetonitrile as its sixth ligand while the sixth ligand for the other (**Ru1**) carboxylate C=O oxygen atom of **Ru2**. The oxidation states of both subunits were unclear. The **Ru1** monomer exhibited longer Ru=C and Ru-terpy bond lengths than **Ru2** by 0.027 Å and 0.026 Å, respectively. Interestingly, this trend is reversed for the Ru-OCO bonds of the carboxylate ligands; the bond in **Ru1** is shorter than **Ru2** by 0.114 Å. Detailed x-ray crystallographic data can be found in section 1.6.5.

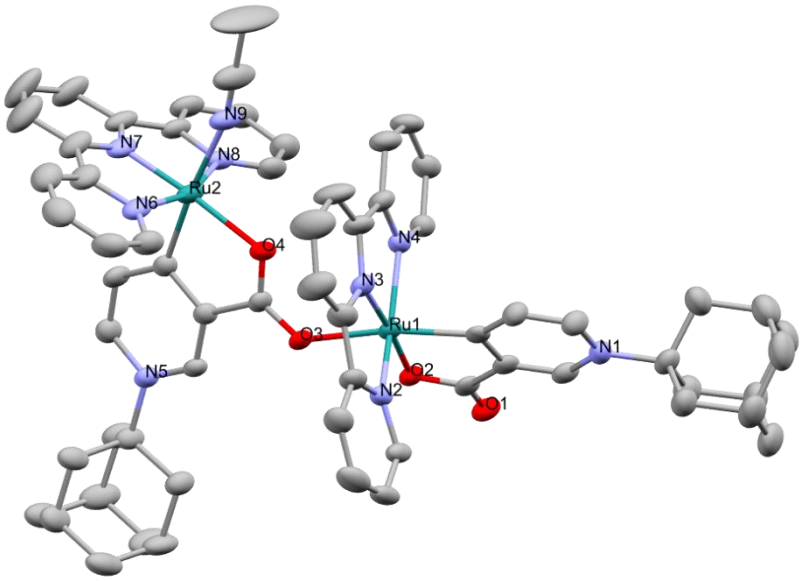


Figure 17. Crystal structure of $[Ru(OC^{Ad})]_2(CH_3CN)]^{3+}$, PF_6 omitted

1.4. Experimental

1.4.1. Preparation of compounds & NMR spectra

1.4.1.1. OC pyridiniums

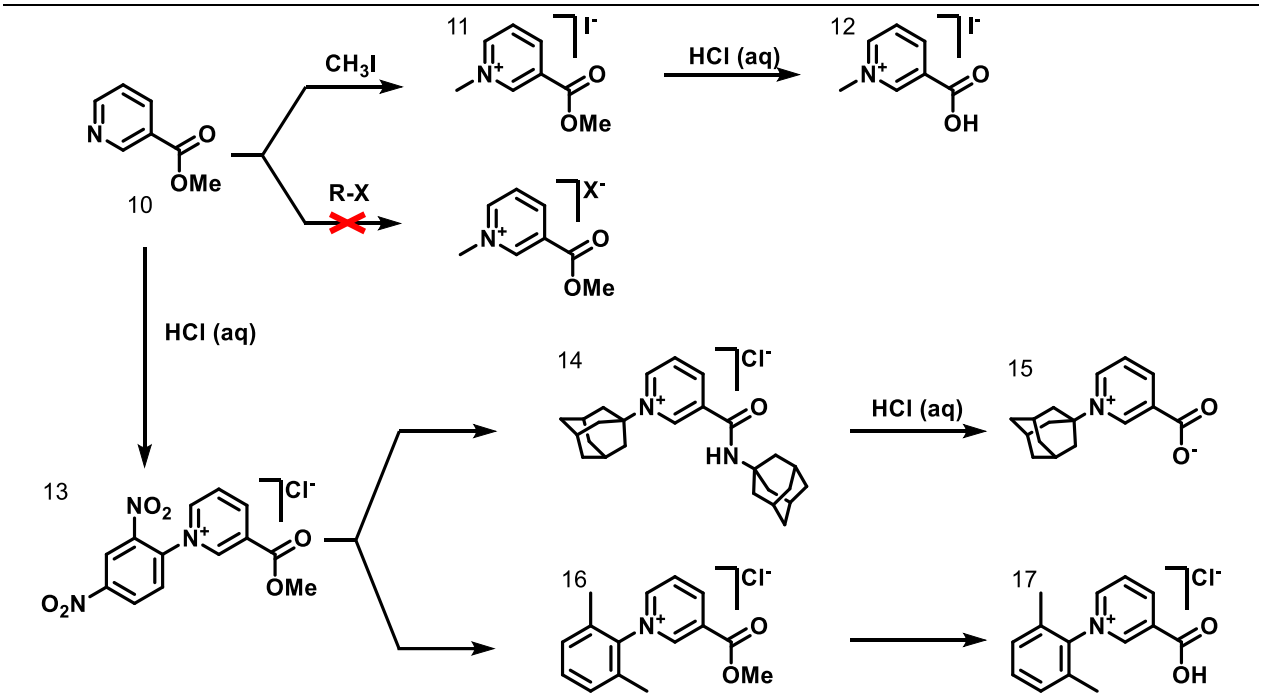
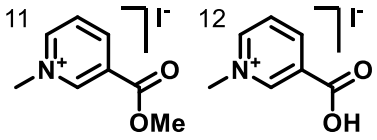


Figure 18. Synthesis of ligand precursors **12**, **15**, **17**.

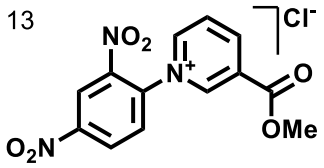
3 -(methoxycarbonyl)-1-methylpyridin-1-ium iodide (11) and 3-carboxy-1-methylpyridin-1-ium iodide (12)



3-(methoxycarbonyl)-1-methylpyridin-1-ium iodide (11)[33] and 3-carboxy-1-methylpyridin-1-ium iodide (12)[34] were synthesized from procedures modified from the literature in 58.7% overall yield.

1-(2,4-dinitrophenyl)-3-(methoxycarbonyl)pyridin-1-ium chloride (13)

13



Methyl nicotinate (5.1978 g) and 2,4-dinitrochlorobenzene (21.7827 g) was suspended in a mixture of deionized water (30 mL) and methanol (50 mL). While under positive nitrogen pressure, the resultant orange slurry was heated and stirred at 65°C for 46 hours. The mixture was cooled to room temperature, after which the solution separated into a clear yellow supernate above a dark red syrup. Rotary evaporation was used to remove most of the methanol from the reaction mixture, after which the resultant aqueous solution was washed with diethyl ether (10 x 50 mL). The aqueous phase was removed in vacuo to yield hygroscopic, pale yellow solids (3.1528 g, 24.5%).

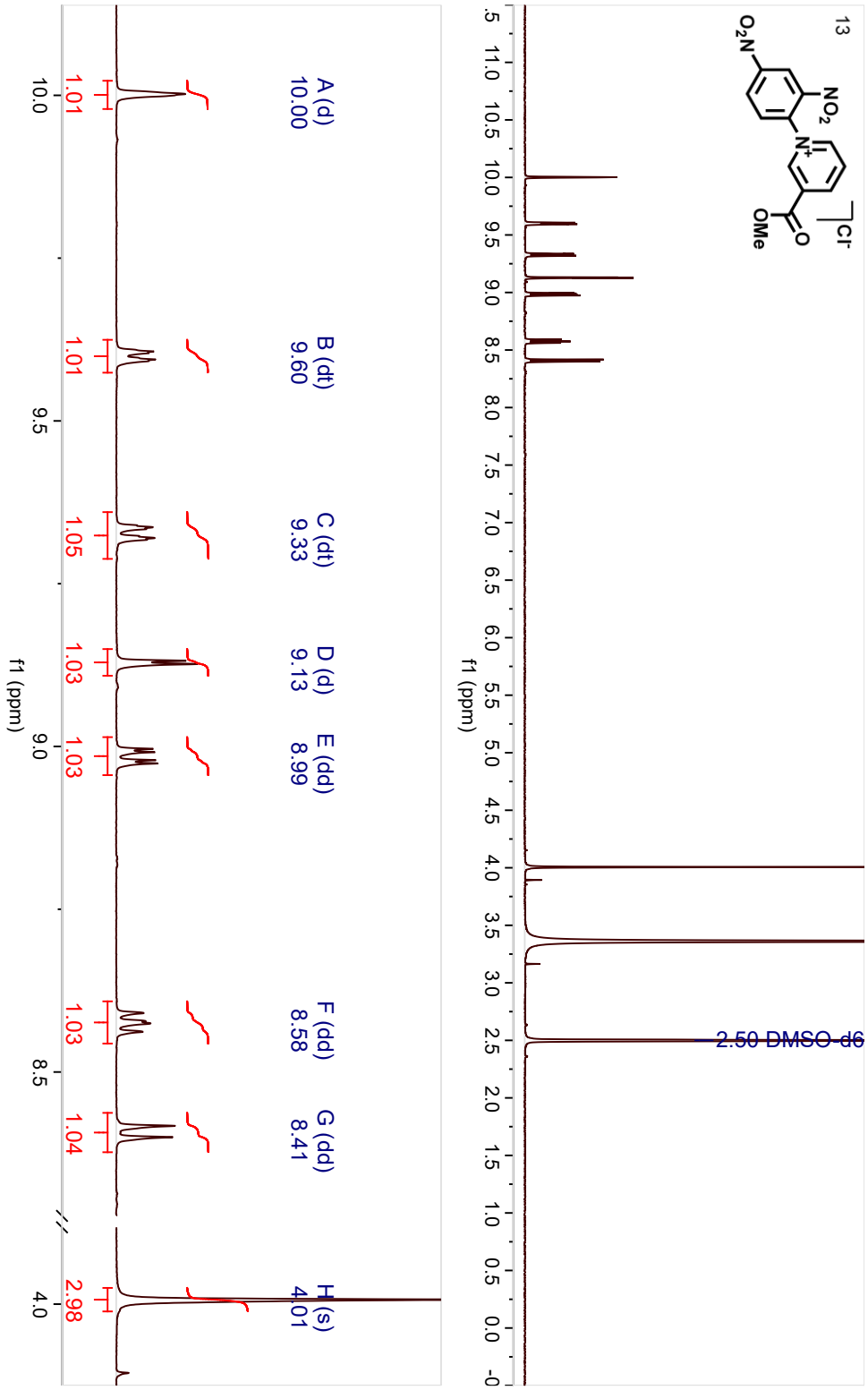
^{1}H NMR (499.95 MHz, DMSO-d_6) δ 10.00 (d, J = 1.7 Hz, 1H), 9.60 (dt, J = 6.1, 1.4 Hz, 1H), 9.33 (dt, J = 8.3, 1.5 Hz, 1H), 9.13 (d, J = 2.5 Hz, 1H), 8.99 (dd, J = 8.7, 2.5 Hz, 1H), 8.58 (dd, J = 8.2, 6.2 Hz, 1H), 8.41 (dd, J = 8.6, 1.6 Hz, 1H), 4.01 (s, 3H).

^{1}H -^{1}H COSY ((499.95, 499.95) MHz, DMSO-d_6) δ (10.01 9.60), (10.01 9.33), (9.60 9.33), (9.60 8.57), (9.60 10.00), (9.33 9.60), (9.33 8.58), (9.33 10.00), (9.13 8.99), (8.99 9.13), (8.99 8.41), (8.58 9.33), (8.58 9.60), (8.41 8.99).

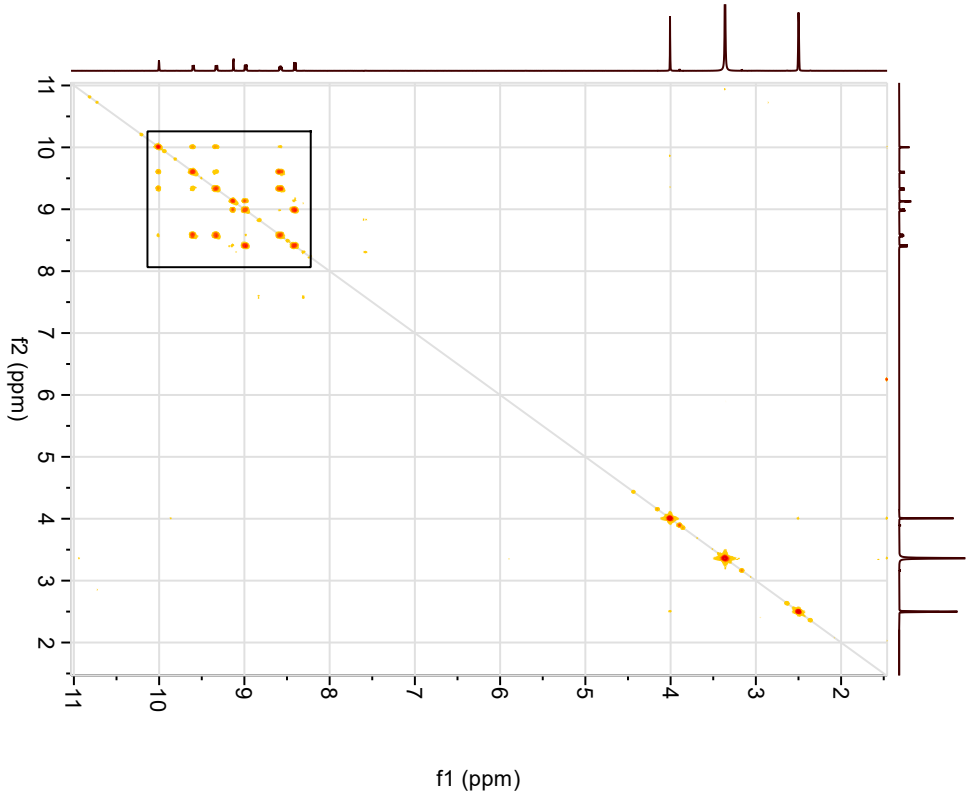
CHN calc'd for $C_{13}H_{10}ClN_3O_6$: C, 45.97; H, 2.97; N, 12.37.

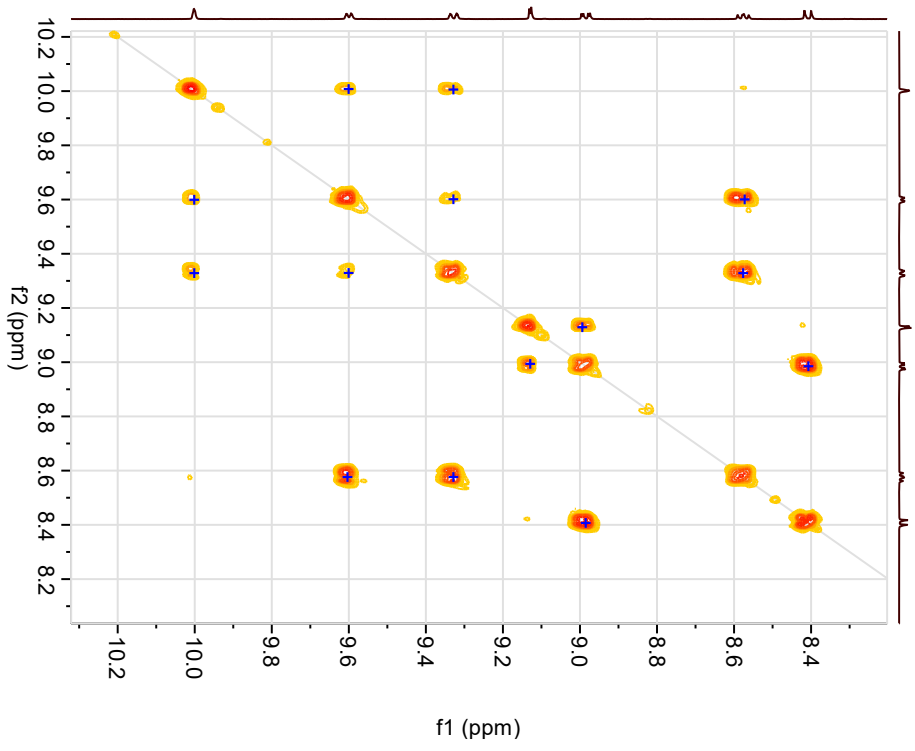
CHN found: C, 44.51; H, 3.45; N, 12.00.

^{1}H NMR, DMSO-d_6



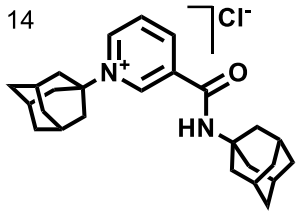
^{1}H-^{1}H COSY, DMSO-d_6





1-adamantanyl-3-((adamantan-1-yl)carbamoyl)pyridin-1-ium chloride (14)

14



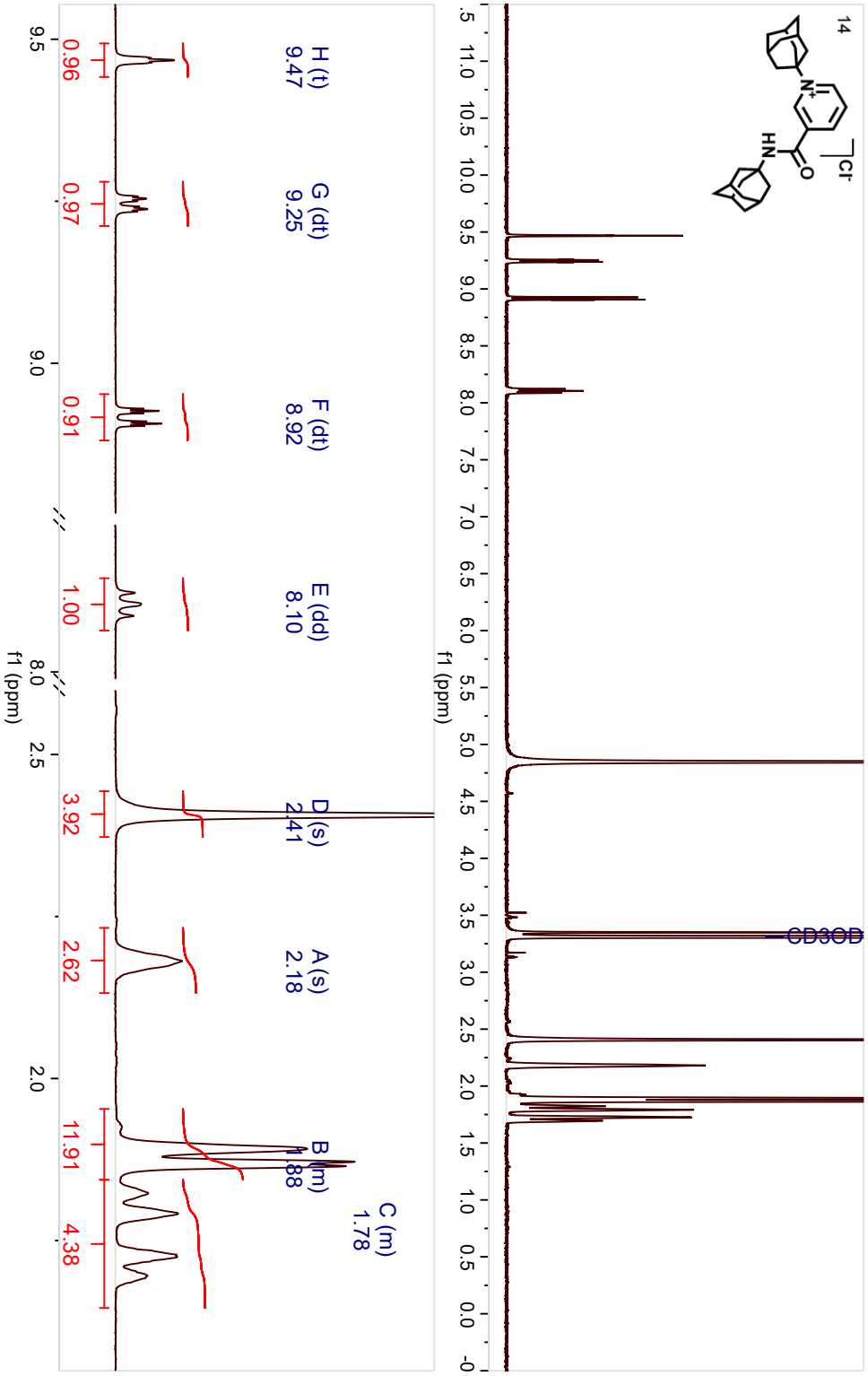
A 20 mL vial was charged with **13** (2.8154 g, 8.3205 mmol), 1-adamantylamine (2.8247 g, 18.642 mmol), and a magnetic stirrer. The solids turned red upon contact. A 9:1 mixture of methanol and water (about 10 mL) was added, which resulted in a blood-red suspension and a warm vial. The vial was sealed, heated, and stirred at 60°C for 48 h, after which the yellow-orange suspension was transferred to a flask where solvent was removed by rotary evaporator. The residual material was resuspended in acetone and the product collected by filtration (3.3417g, 83.5%).

^{1}H NMR (399.75 MHz, CD_3OD) δ 9.47 (t, J = 1.4 Hz, 1H), 9.25 (dt, J = 6.4, 1.5 Hz, 1H), 8.92 (dt, J = 7.8, 1.4 Hz, 1H), 8.10 (dd, J = 7.8, 6.5 Hz, 1H), 2.41 (s, 4H), 2.18 (s, 3H), 1.95 – 1.84 (m, 12H), 1.84 – 1.65 (m, 4H).

CHN calc'd for $C_{26}H_{35}ClN_2O + 3H_2O$: C, 64.91; H, 8.59; N, 5.82.

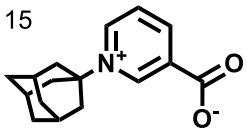
CHN found: C, 65.62; H, 8.07; N, 6.14.

^{1}H NMR, CD_3OD


14
Cl-
HN
O
N+
CD3OD
f1 (ppm)
H (t) 9.47
G (dt) 9.25
F (dt) 8.92
E (dd) 8.10
D (s) 2.41
A (s) 2.18
B (m) 1.88
C (m) 1.78
0.96
0.97
0.91
1.00
3.92
2.62
11.91
4.38

1-(adamantan-1-yl)pyridin-1-ium-3-carboxylate (15)

15



The addition of **14** (680.18 mg, 1.5957 mmol) and aqueous hydrochloric acid (3 M, 8 mL) to a flask resulted in a yellow suspension. The contents of the flask were heated and stirred under reflux for 2 h. Upon cooling, the solvent was removed in vacuo to obtain white solids, to which was added acetone (about 20 mL) and methanol (about 2 mL). The flask was placed on an ultrasonic water bath until a homogeneous suspension resulted. After the precipitate had settled, the supernate was decanted. The crude product was subject to additional washes with acetone (4 x 10 mL), then transferred onto a fritted funnel using fresh acetone washes. The filtrate was collected by vacuum filtration and washed with a 2:1 mixture of acetone and methanol (5 mL) and fresh acetone (5 mL). This washing step was repeated twice until the 1-adamantylamine peaks was no longer detected on ^{1}H NMR of the crude material. The obtained bright white solids were dried in vacuo (250.75 mg, 61%).

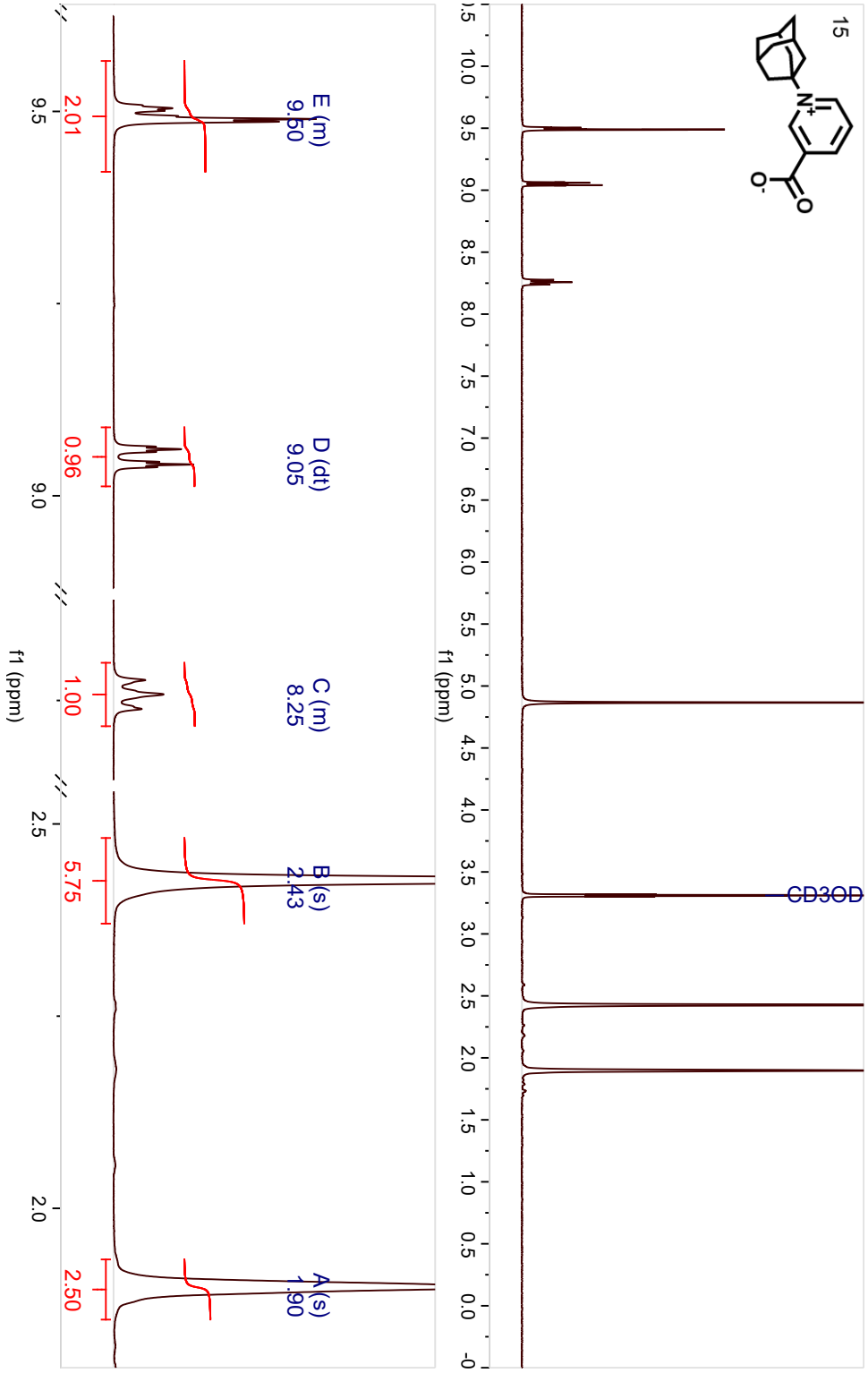
^{1}H NMR (399.75 MHz, CD_3OD) δ 9.57 – 9.42 (m, 2H), 9.05 (dt, J = 7.9, 1.4 Hz, 1H), 8.30 – 8.22 (m, 1H), 2.43 (s, 6H), 1.90 (s, 2H).

^{13}C NMR (100.528 MHz, CD_3OD) δ 164.14, 146.63, 145.64, 143.57, 133.13, 129.52, 72.42, 42.95, 36.01, 31.76.

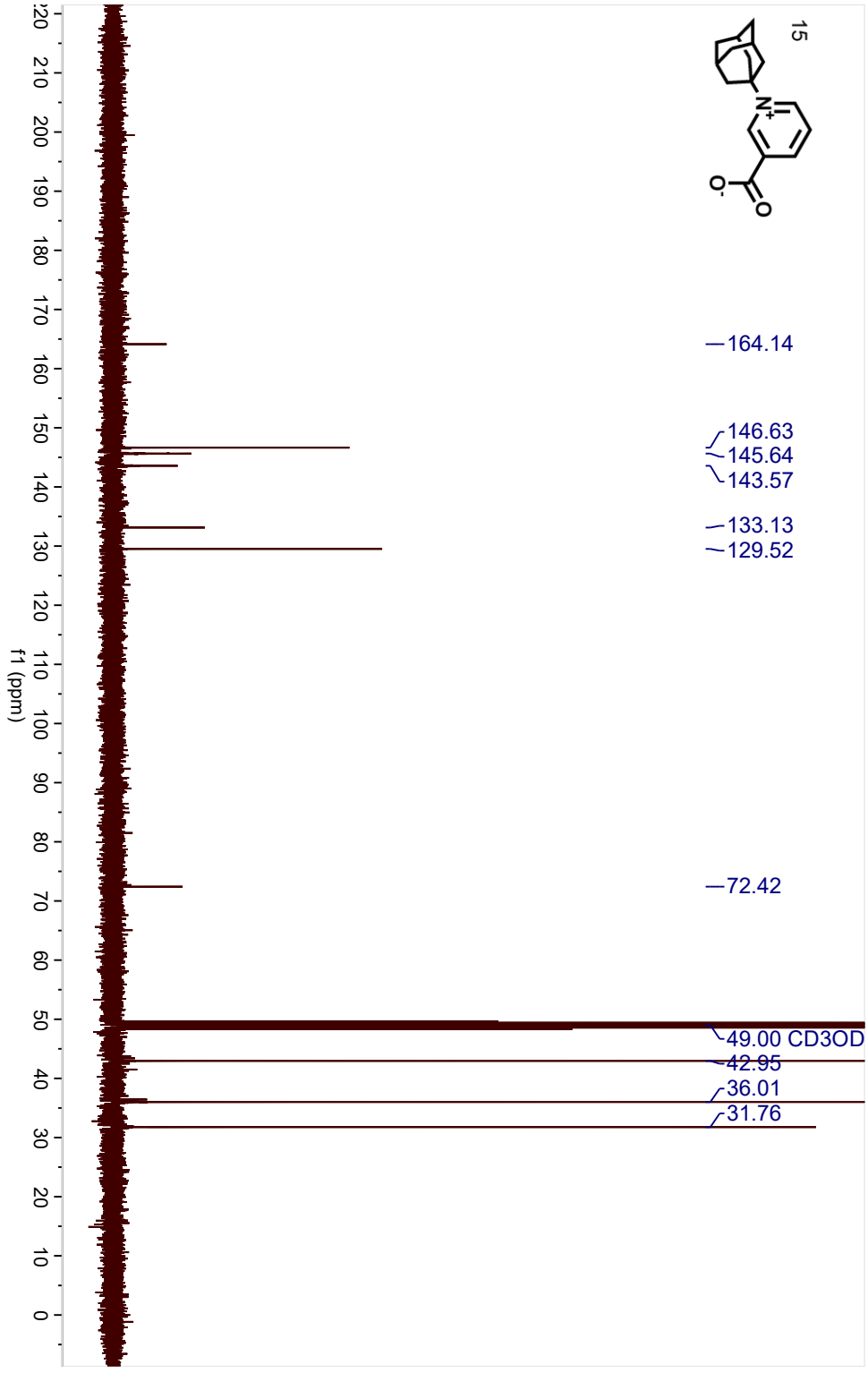
CHN calc'd for $C_{16}H_{19}NO_2 + 3H_2O$: C, 61.72; H, 8.09; N, 4.50.

CHN found: C, 61.59; H, 7.74; N, 4.59.

^{1}H NMR, CD_3OD

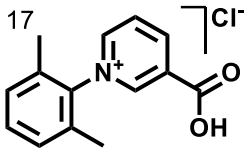

CD3OD
f1 (ppm)
E (m)
9.50
D (dt)
9.05
C (m)
8.25
B (s)
2.43
A (s)
1.90
2.01
0.96
1.00
5.75
2.50

^{13}C NMR, CD_3OD



1-(2,6-dimethylphenyl)pyridin-1-ium-3-carboxylate (17).

17



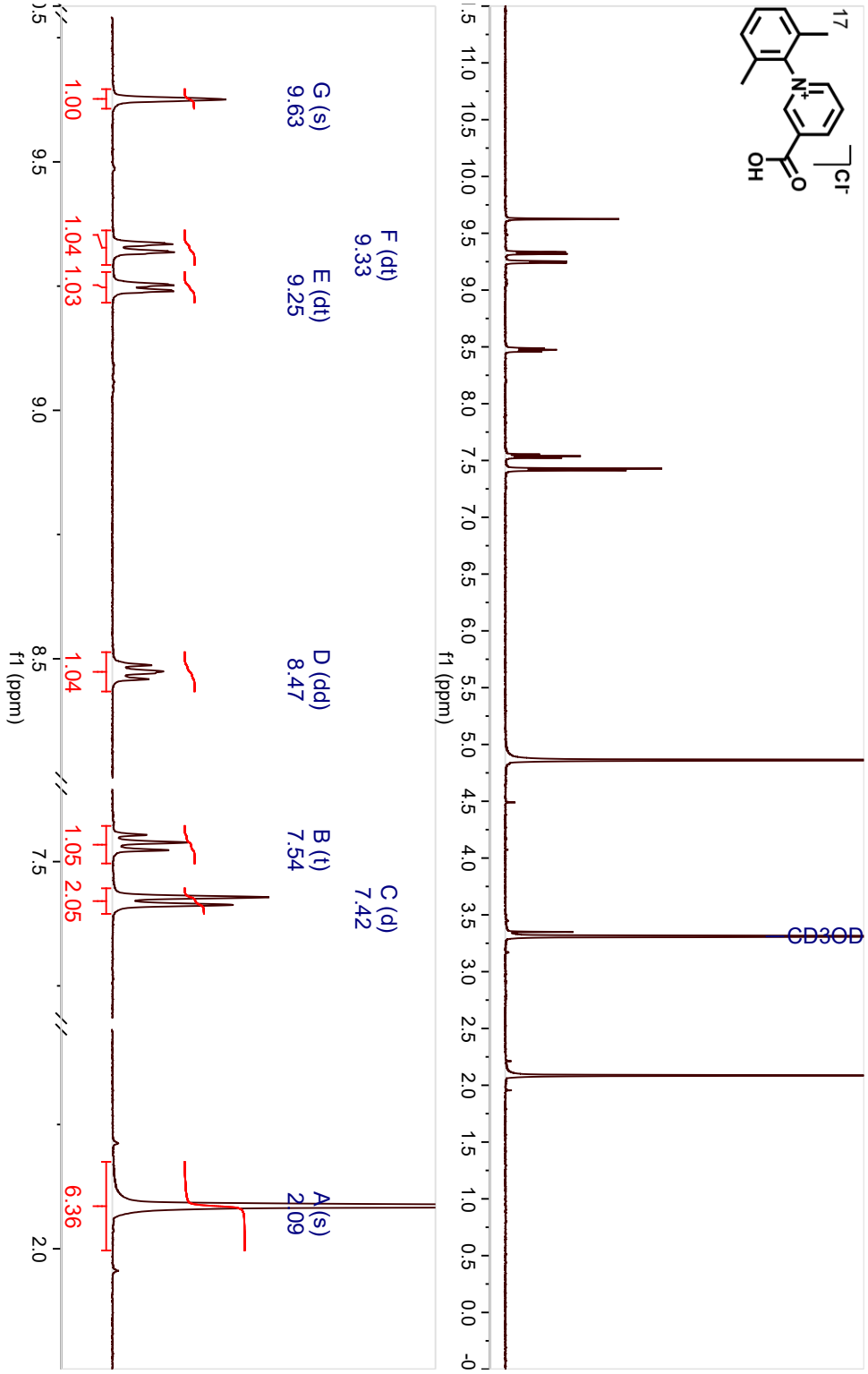
A 20 mL vial was charged with pyridinium salt **13** (0.5119 g, 1.507 mmol), 2,6-dimethylaniline (0.2072 g, 1.7099 mmol), and 10 mL of a 9:1 solution of methanol and water. The vial was sealed, heated, and stirred at 70°C for 23 hours. Upon cooling, 5 mL of deionized water was added to the vial, and the contents of the vial was transferred to a flask using methanol (about 40 mL). The solution was reduced to about 15 mL on rotary evaporator, after which the contents were diluted with 10 mL water and 35 mL diethyl ether. The aqueous layer was extracted and washed with additional diethyl ether (8 x 25 mL). ^{1}H NMR indicated that the crude product is a mixture of **16** and **17**. The aqueous layer was placed on air-cooled reflux for 62 h, after which the aqueous solution was boiled dry. The obtained brown solids were dried in vacuo to remove residual water. Acetonitrile was added to the solids and the mixture was placed on ultrasonic bath until a homogeneous suspension was achieved. The precipitate was filtered and dried to obtain cream-colored solids (0.2840 g, 83%).

^{1}H NMR (499.946 MHz, CD_3OD) δ 9.63 (s, 1H), 9.33 (dt, J = 8.1, 1.5 Hz, 1H), 9.25 (dt, J = 6.0, 1.3 Hz, 1H), 8.47 (dd, J = 8.1, 6.0 Hz, 1H), 7.54 (t, J = 7.7 Hz, 1H), 7.42 (d, J = 7.7 Hz, 2H), 2.09 (s, 6H).

CHN calc'd for $C_{14}H_{14}ClNO_2$: C, 63.76; H, 5.35; N, 5.31

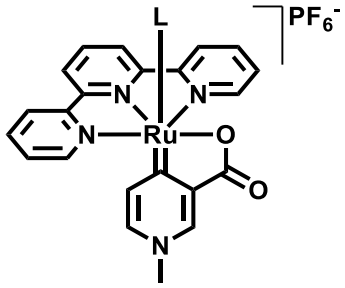
CHN found: C, 62.32; H, 4.72; N, 5.44

^{1}H NMR, CD_3OD


17
Cl⁻
OH
O
CD3OD
f1 (ppm)
A (s) 2.09
B (t) 7.54
C (d) 7.42
D (dd) 8.47
E (dt) 9.25
F (dt) 9.33
G (s) 9.63
1.00
1.04
1.03
1.04
1.05
2.05
6.36

1.4.1.2. 4-pyridylidene complexes

Ru(Me)



Inside N_2 glovebox, charged 20 mL vial with 460.0 mg (0.5676 mmol) $[Cl_2Ru(tpy)]_2$, **12** 318.8 mg (1.142 mmol) **12**, and 1128.6 mg (6.760 mmol) AgOAc, and magnetic stirrer added. The solids were suspended in methanol (about 5 mL) and the vial sealed. The reaction mixture was heated and stirred at 70°C for 92 h, after which the mixture was poured through a fine glass fritted funnel lined with celite remove AgI. The residue on the frit was washed with methanol until elutent became almost colorless. The methanol washes were collected in portions (about 1 L total), after which solvent was removed by rotary evaporation to obtain a reddish solid that coated the interior of the flask. The crude product was taken under N_2 atmosphere, where the solids were mechanically dislodged from the walls of the flask and suspended in about 70 mL deoxygenated deionized water. A stir bar was added to the flask, which was stirred until the aqueous solution appeared to be homogeneous. KPF_6 (1.7890 g) was added to the solution, for which stirring was continued for 27 hours. The precipitate was filtered on a fine frit, and repeat (x 9) washings using the mother liquor was performed to complete the material transfer. The brownish-red solids on the frit were carefully washed with 5% w/v ascorbic acid solution (1 mL x 2), then deoxygenated deionized water (1 mL x 1). The product was dried in vacuo to obtain a brown dust (0.4750 g, 66%).

Notes on NMR spectra: A concentrated sample (7.7 mg in about 0.7 mL CD_3CN) was prepared in N_2 glovebox within an air-tight J-Young NMR tube. Aromatic region peaks were initially broad, and a yellow precipitate could be seen forming in the NMR tube. Inside N_2 glovebox, the supernate was decanted into a fresh NMR tube, and to both supernate and precipitate samples was added a suitable amount of CD_3CN. Both supernate and precipitate samples indicated the same set of broad aromatic peaks. After resting a few days, the supernate sample had sharp peaks and was used to acquire NMR data of the complex.

^{1}H NMR (399.75 MHz, CD_3CN) δ 8.36 (d, J = 5.5 Hz, 2H), 8.34 – 8.28 (m, 4H), 7.96 (ddd, J = 8.1, 7.5, 1.6 Hz, 2H), 7.89 (t, J = 8.1 Hz, 1H), 7.72 (d, J = 1.7 Hz, 1H), 7.55 (ddd, J = 7.2, 5.8, 1.1 Hz, 2H), 6.97 (dd, J = 6.4, 1.7 Hz, 1H), 6.18 (d, J = 6.4 Hz, 1H), 3.66 (s, 3H).

^{13}C NMR (100.53 MHz, CD3CN) δ 230.87, 175.95, 160.13, 159.17, 151.31, 146.85, 137.46, 136.09, 134.85, 133.75, 130.01, 128.35, 123.67, 123.25, 46.85.

^{31}P NMR (161.82 MHz, CD_3CN) δ -144.64 (hept, J = 706.2 Hz).

^{19}F NMR (376.11 MHz, CD_3CN) δ -72.94 (d, J = 706.0 Hz).

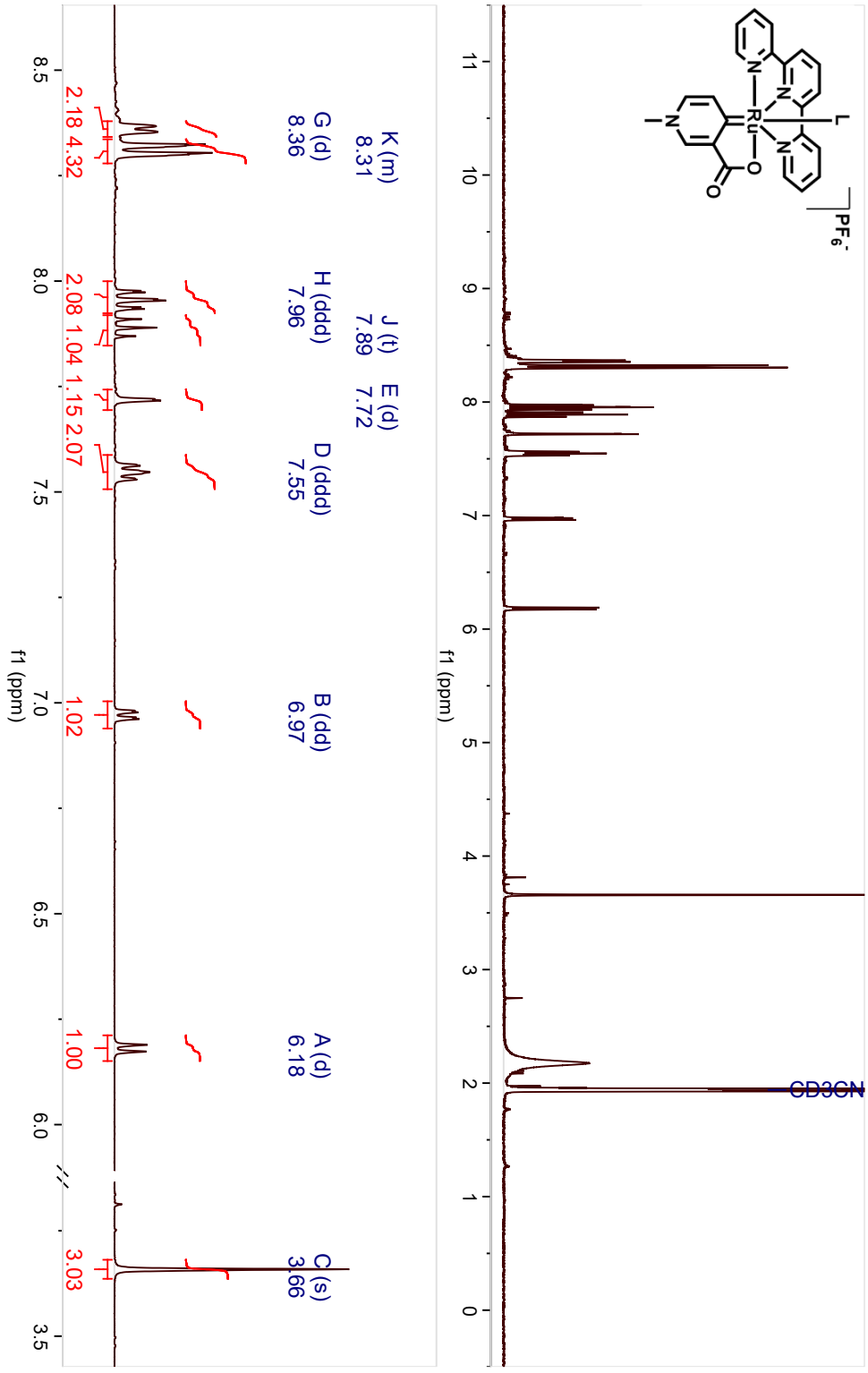
^{1}H-^{1}H COSY ((399.75, 399.75) MHz, CD_3CN) δ (8.37 7.55), (8.32 7.90), (8.31 7.96), (7.96 8.31), (7.95 7.55), (7.90 8.32), (7.71 3.66), (7.71 6.97), (7.55 7.95), (7.55 8.37), (6.97 7.71), (6.97 6.19), (6.97 3.66), (6.19 6.97), (3.66 6.97), (3.66 7.71).

^{1}H-^{13}C HSQC ((400.13, 100.62) MHz, CD_3CN) δ (8.37 151.31), (8.31 123.25), (8.31 123.67), (7.95 137.46), (7.89 130.01), (7.71 134.85), (7.55 128.35), (6.97 136.09), (6.19 133.75), (3.66 46.25).

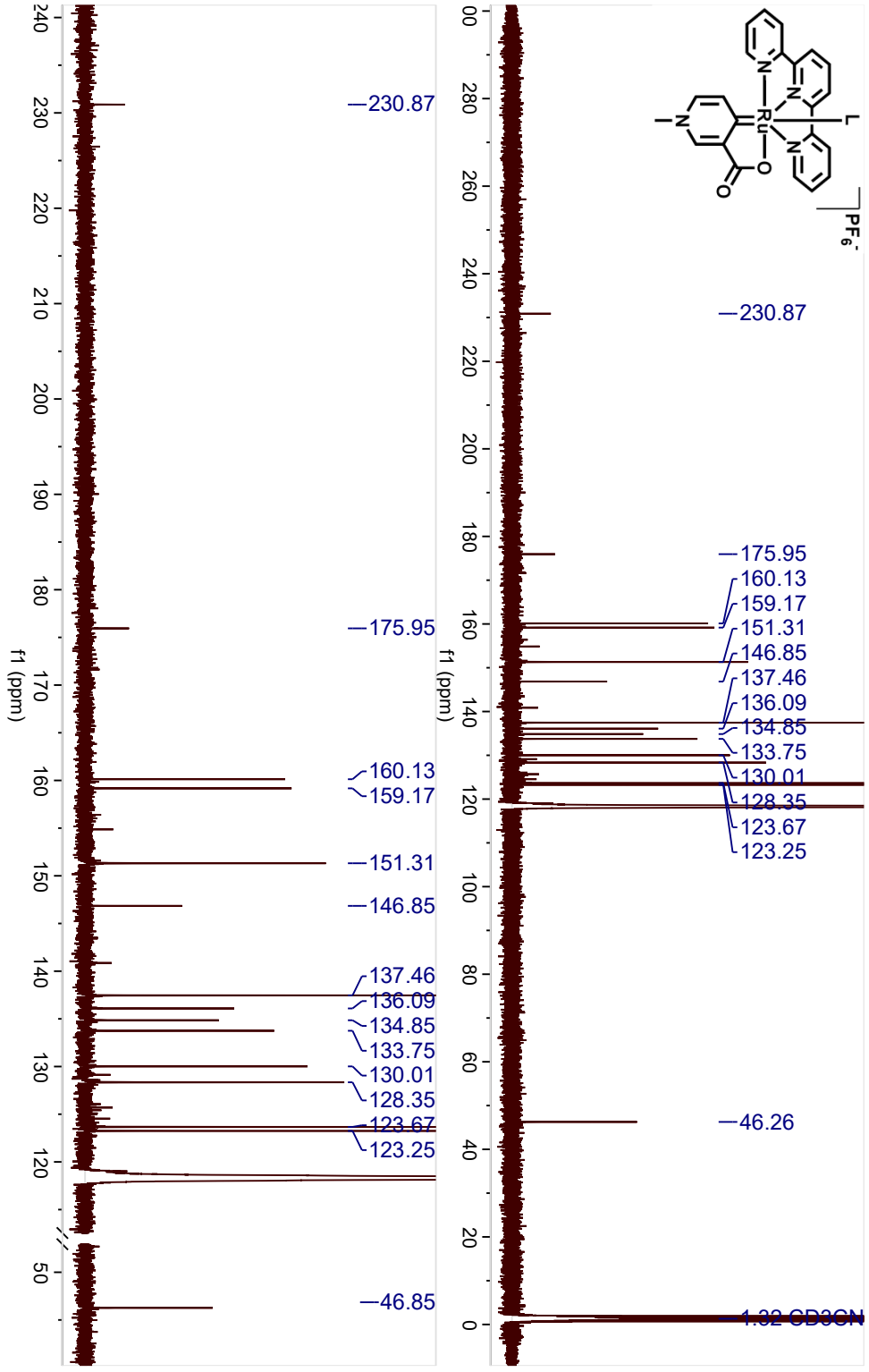
^{1}H-^{13}C HMBC ((400.13, 100.62) MHz, CD_3CN) δ (8.37 128.35), (8.37 137.46), (8.37 159.17), (8.31 123.25), (8.31 128.35), (8.31 159.17), (8.31 160.13), (7.95 151.31), (7.95 159.17), (7.88 160.13), (7.71 46.25), (7.71 136.09), (7.55 123.25), (7.55 151.31), (6.97 134.85), (6.97 46.25), (6.19 136.09), (6.19 146.85), (3.66 133.75), (3.66 134.85), (3.66 136.09).

CHN calc'd for [Ru**(Me)(**κ^1-H_2O**)**]PF_6 ($C_{22}H_{19}F_6N_4O_3PRu$) :	C, 41.71; H, 3.02; N, 8.84.
CHN calc'd for [Ru**(Me)**(κ^1-H_2O)]PF_6 + 2H_2O:	C, 39.47; H, 3.46; N, 8.37.
CHN found:	C, 39.51; H, 3.22; N, 8.49.

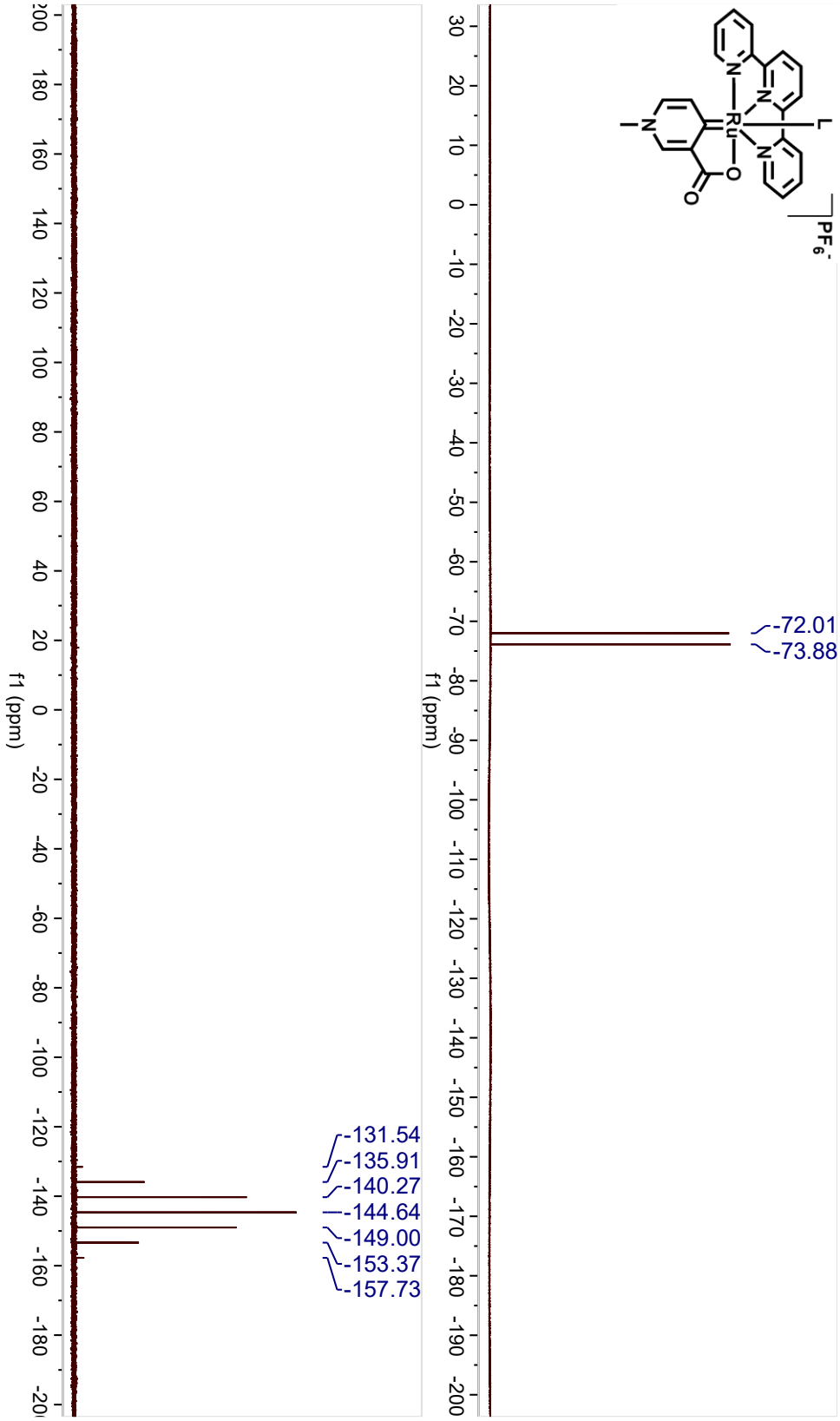
^{1}H NMR, CD_3CN


PF6-
CD3CN
f1 (ppm)
K (m) 8.31
J (t) 7.89
E (d) 7.72
G (d) 8.36
H (ddd) 7.96
D (ddd) 7.55
B (dd) 6.97
A (d) 6.18
C (s) 3.66
2.18 4.32
2.08 1.04 1.15 2.07
1.02
1.00
3.03

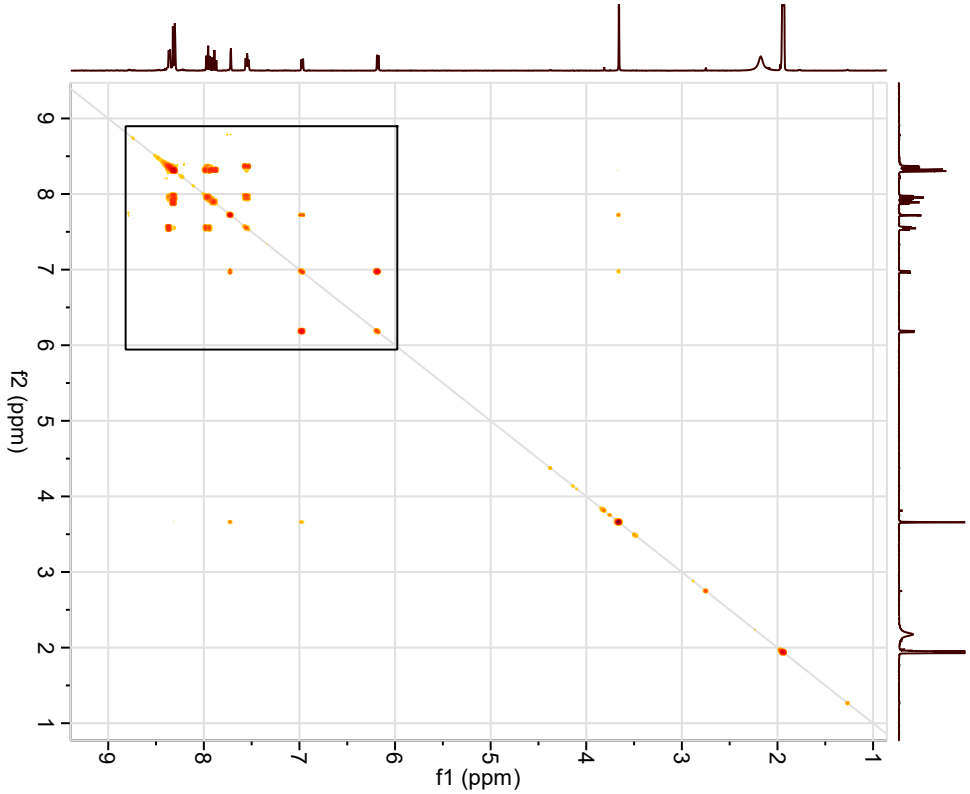
^{13}C NMR, CD3CN

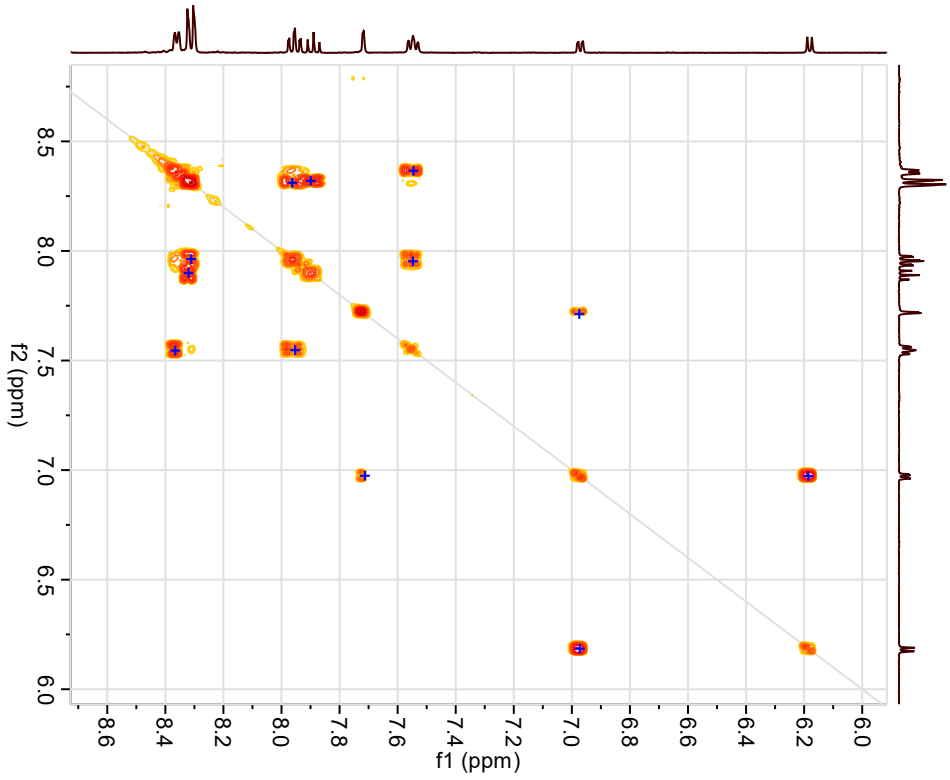


^{31}P & ^{19}F NMR, CD_3CN

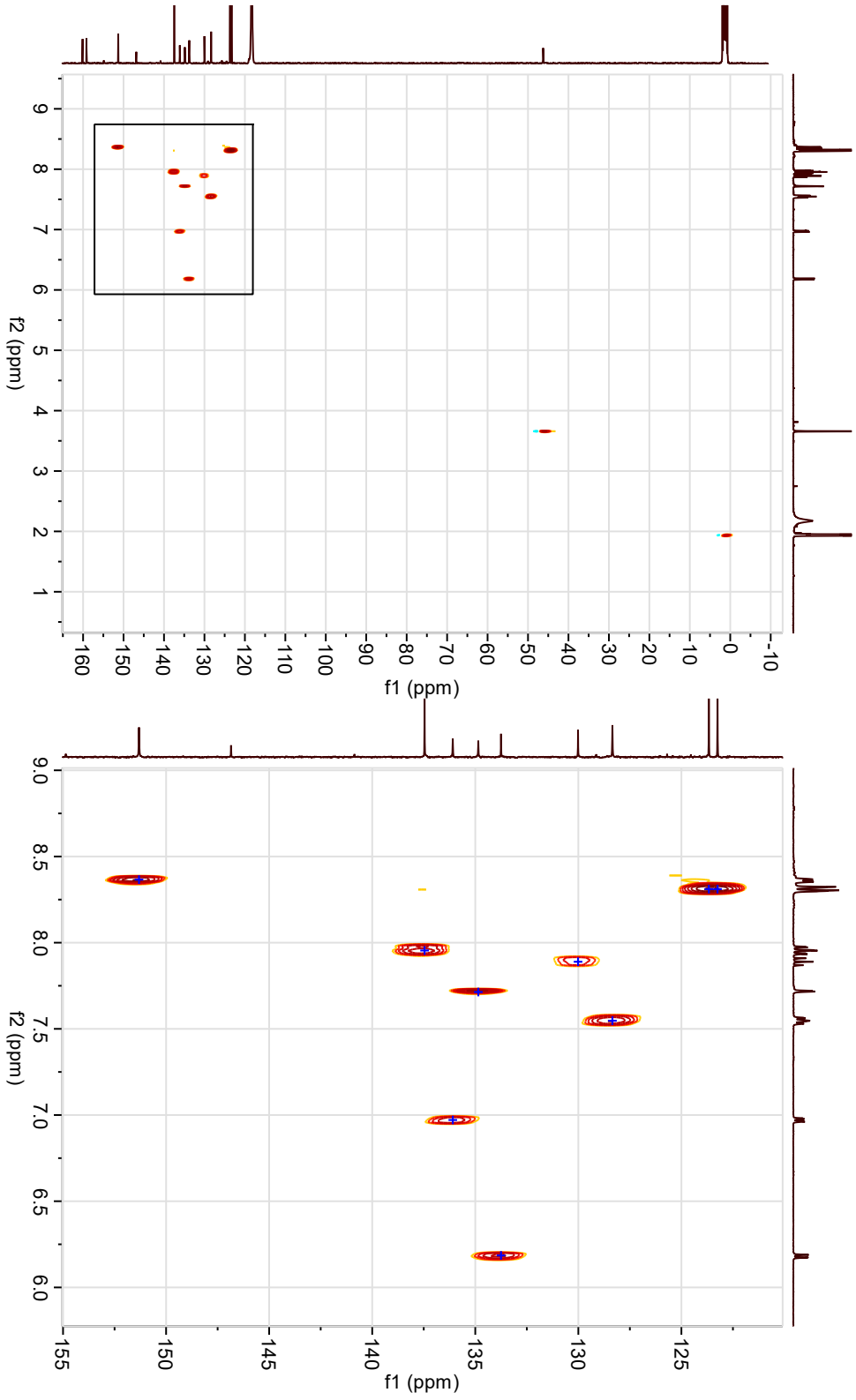


^{1}H-^{1}H COSY, CD_3CN

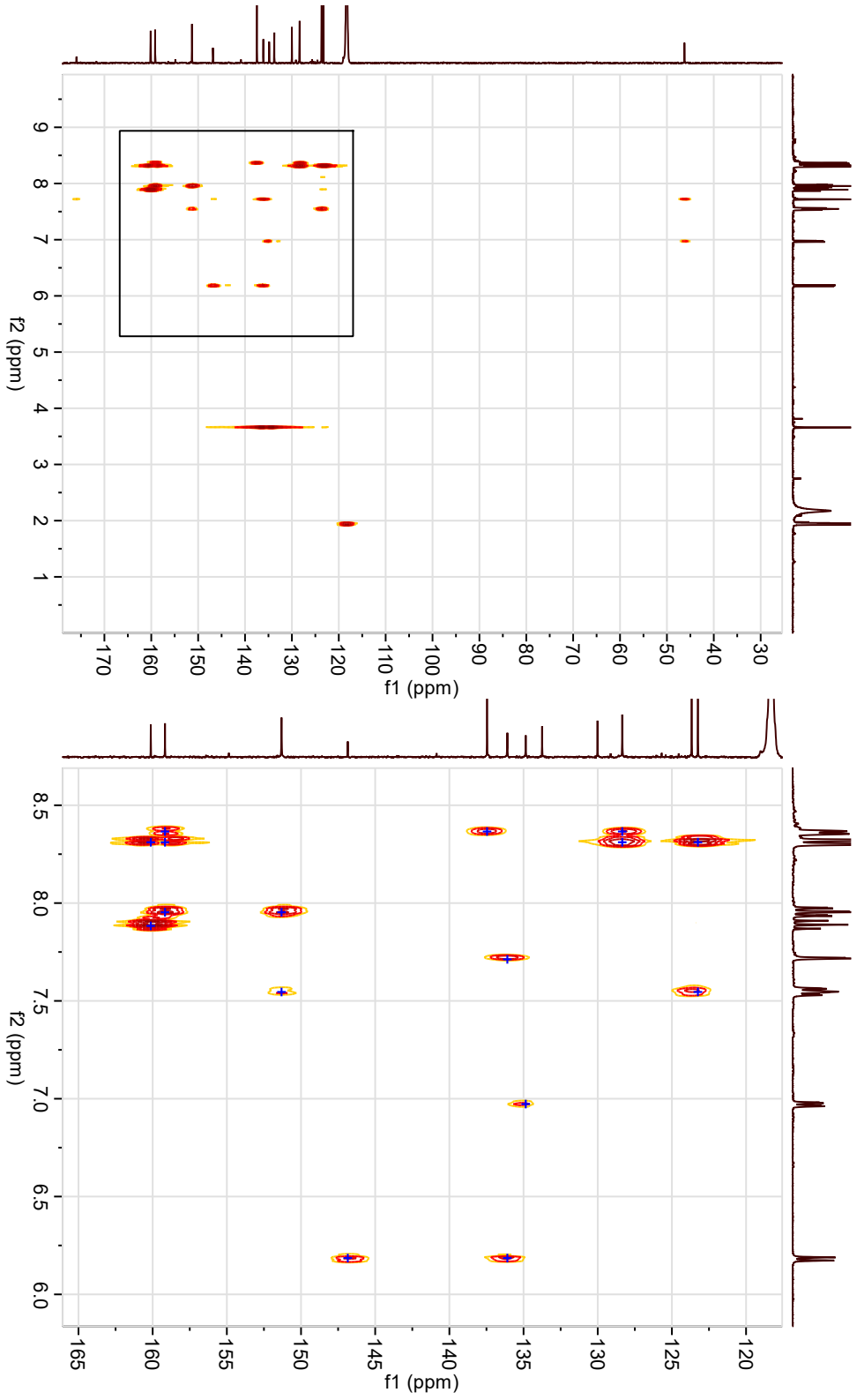




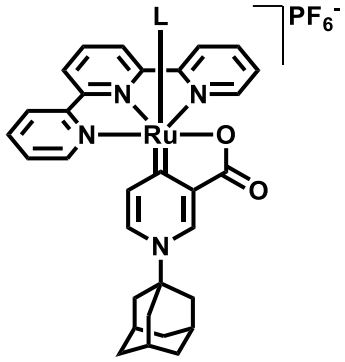
^{1}H-^{13}C HSQC, CD_3CN



^{1}H-^{13}C HMBC, CD_3CN



Ru(Ad)



Inside N_2 glovebox, a 20 mL vial was charged with **15** (805.6 mg, 0.3133 mmol), AgOAc (199.0 mg, 1.1923 mmol), $[Ru(tpy)Cl_2]_2$ (156.4 mg, 0.1930 mmol), and a stir bar added. Methanol (about 10 mL) was added, resulting in a dark purple solution. The vial was sealed, heated, and stirred at 70°C for 39 h. The reaction mixture was filtered through celite and a fine fritted funnel to remove AgCl. The celite pad was washed with methanol (5 x 10 mL) after which the elutent became clear. The crude product was dried by rotary evaporation, and redissolved in methanol (about 3 mL), after which a saturated solution of NH_4PF_6 (aq) was added (8 mL). A purple precipitate appeared, and the solution was carefully placed on rotary evaporator to remove methanol. The solution was diluted with water to (4 mL) and placed on ultrasonic water bath until the precipitate became uniform in size. The precipitate was transferred onto a fine fritted funnel using repeat washes of the mother liquor and vacuum filtered. The dark brown material on the frit was rinsed with saturated NH_4PF_6 (aq) (3 mL) and water (2 mL). Once dried, the solids were washed with ether (10 mL), redissolved in acetonitrile, filtered, and dried in vacuo to obtain red crystals (138.15 mg, 58.5%).

^{1}H NMR (400.13 MHz, CD_3CN) δ 8.36 (d, J = 5.2 Hz, 2H), 8.34 – 8.27 (m, 4H), 8.00 (d, J = 2.0 Hz, 1H), 7.96 (td, J = 7.8, 1.6 Hz, 2H), 7.89 (t, J = 8.0 Hz, 1H), 7.55 (ddd, J = 7.3, 5.5, 1.3 Hz, 2H), 7.33 (dd, J = 6.7, 2.0 Hz, 1H), 6.21 (d, J = 6.7 Hz, 1H), 1.97 (d, J = 3.0 Hz, 6H), 1.67 (q, J = 12.5 Hz, 6H).

^{13}C NMR (100.53 MHz, CD_3CN) δ 176.10, 160.14, 159.15, 151.41, 146.79, 137.45, 133.79, 131.38, 129.91, 129.86, 128.36, 123.64, 123.21, 65.73, 42.41, 35.72, 30.88. Note: ^{13}C signal for carbene carbon not seen.

^{13}C NMR (100.532 MHz, CD_3OD) δ 234.28, 161.36, 159.94, 151.42, 146.69, 138.27, 134.91, 131.13, 130.69, 130.35, 128.74, 123.91, 123.53, 65.92, 42.75, 36.21, 31.38.

^{31}P NMR (161.822 MHz, CD_3OD) δ -144.61 (p, J = 708.0, 708.0, 707.4 Hz).

^{19}F NMR (376.109 MHz, CD_3OD) δ -74.86 (d, J = 707.7).

^{1}H-^{1}H COSY ((399.75, 399.75) MHz, CD_3CN) δ (8.36 7.56), (8.31 7.89), (8.31 7.96), (8.01 7.33), (7.96 7.54), (7.96 8.31), (7.89 8.31), (7.56 8.36), (7.54 7.96), (7.33 6.22), (7.33 8.01), (6.22 7.33), (2.17 1.67), (1.98 1.67), (1.67 1.98), (1.67 2.17).

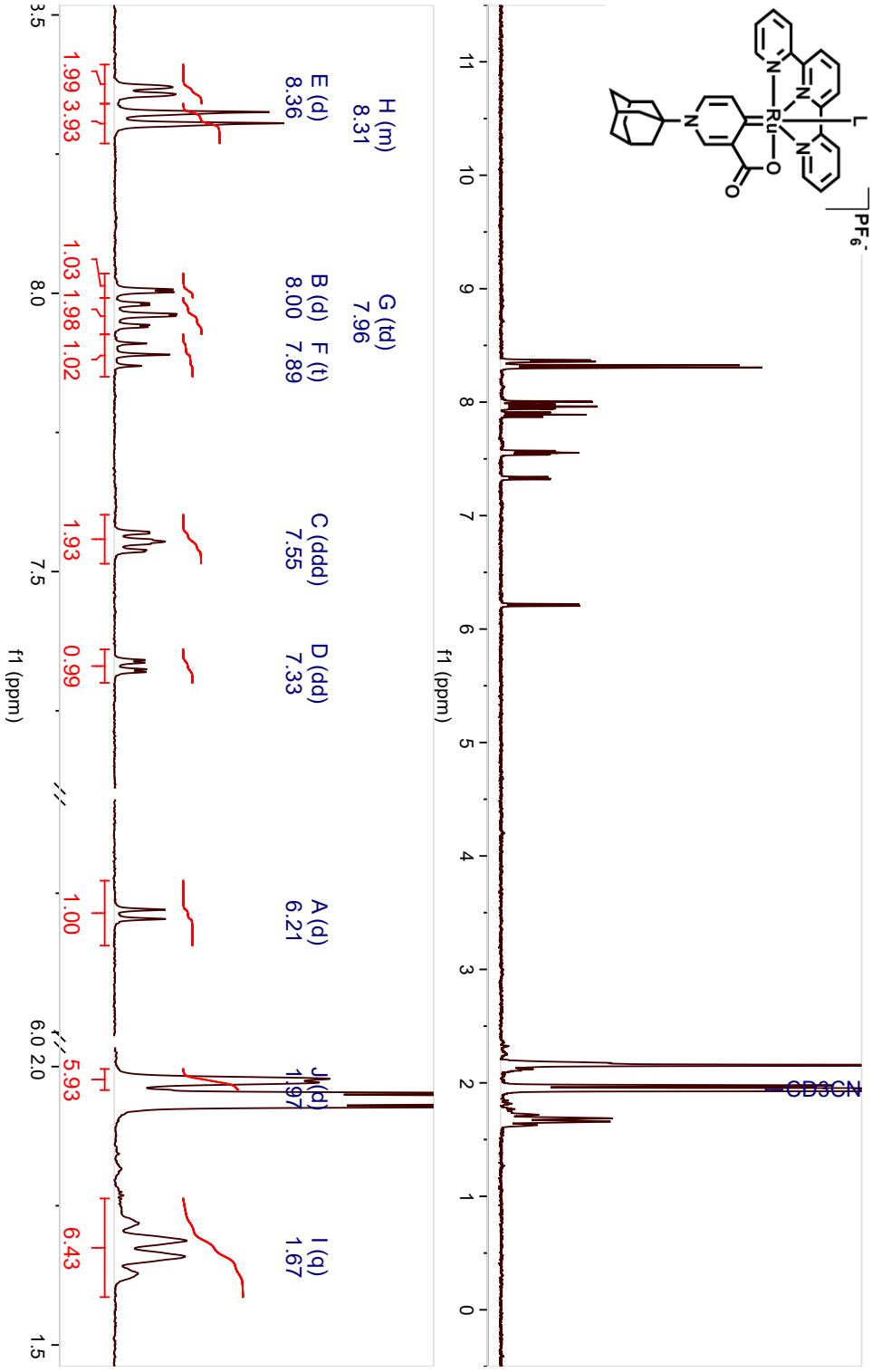
^{1}H-^{13}C HSQC ((400.13, 100.62) MHz, CD_3CN) δ (8.36 151.35), (8.31 123.62), (8.31 123.19), (8.01 129.90), (7.96 137.44), (7.89 129.90), (7.56 128.33), (7.33 131.38), (6.22 133.77), (2.17 30.83), (1.98 42.35), (1.67 35.67).

^{1}H-^{13}C HMBC ((400.13, 100.62) MHz, CD_3CN) δ (8.36 128.33), (8.36 137.44), (8.36 159.10), (8.31 123.19), (8.31 128.33), (8.31 160.08), (8.01 131.38), (7.96 151.35), (7.96 159.10), (7.89 123.21), (7.89 160.08), (7.56 123.62), (7.54 151.41), (7.33 129.90), (6.22 131.38), (6.22 146.67), (1.98 30.88), (1.98 35.72), (1.98 42.41), (1.98 65.73).

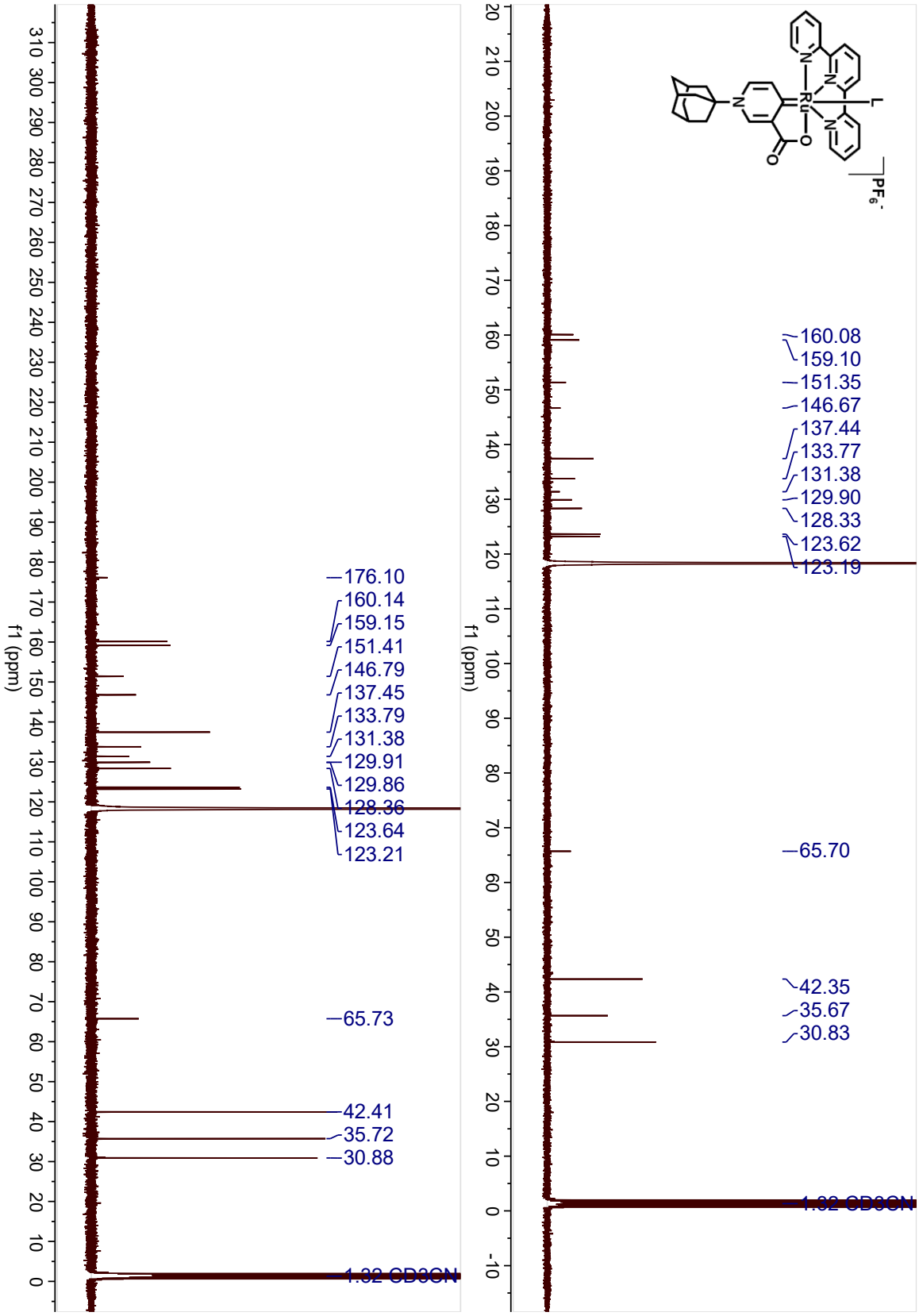
CHN calc'd: for [Ru(Ad)(κ^{1}-OH_2)]PF_6 ($C_{31}H_{31}F_6N_4O_3PRu$) + 4H_2O: C, 45.09; H, 4.76; N, 6.79.

CHN found: C, 45.36; H, 4.74; N, 7.04.

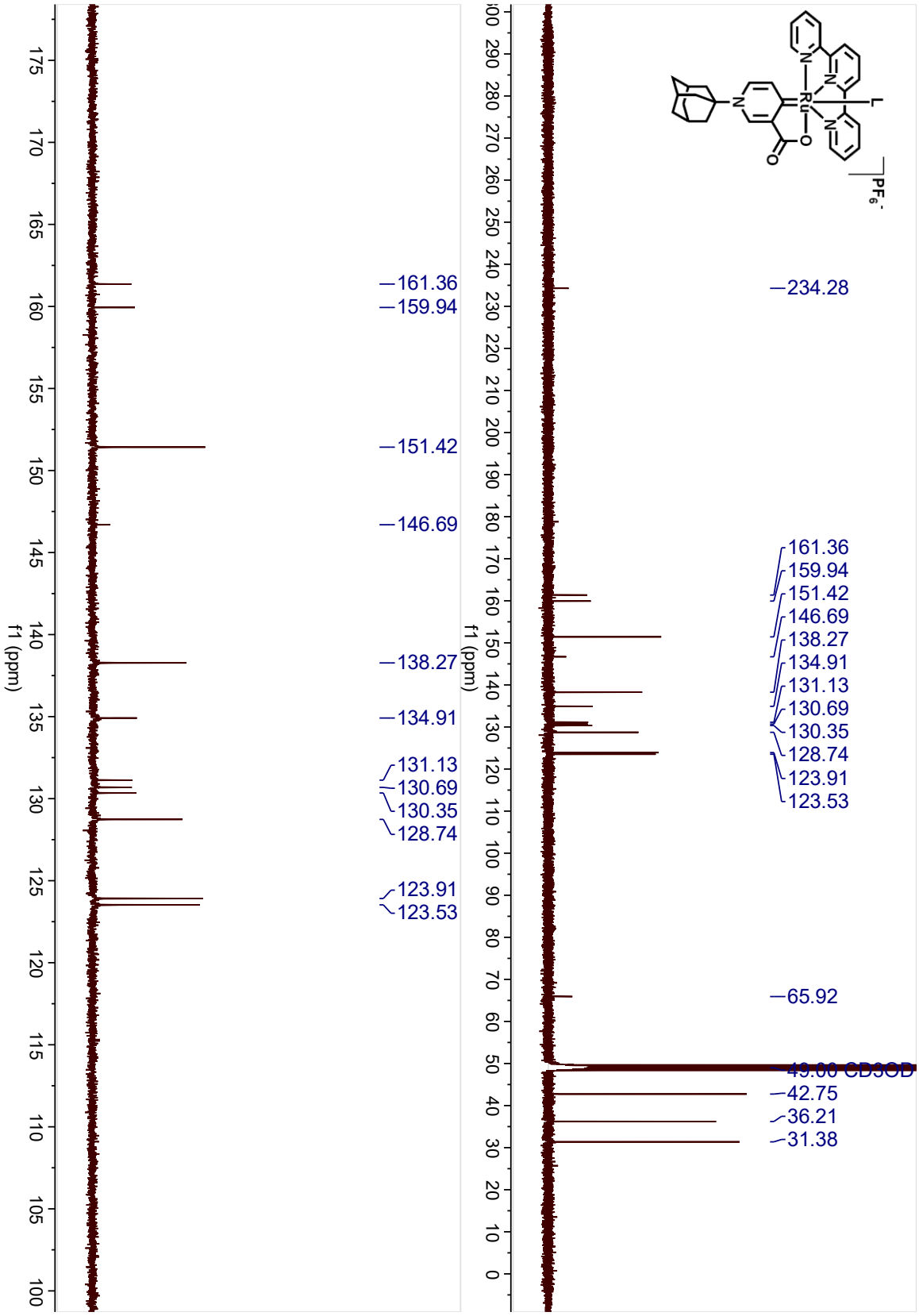
^{1}H NMR, CD_3CN


PF6-
CD3CN
f1 (ppm)
H (m) 8.31
G (td) 7.96
E (d) 8.36
B (d) 8.00
F (t) 7.89
C (ddd) 7.55
D (dd) 7.33
A (d) 6.21
J (d) 1.97
I (q) 1.67
1.99 3.93
1.03 1.98 1.02
1.93
0.99
1.00
5.93
6.43

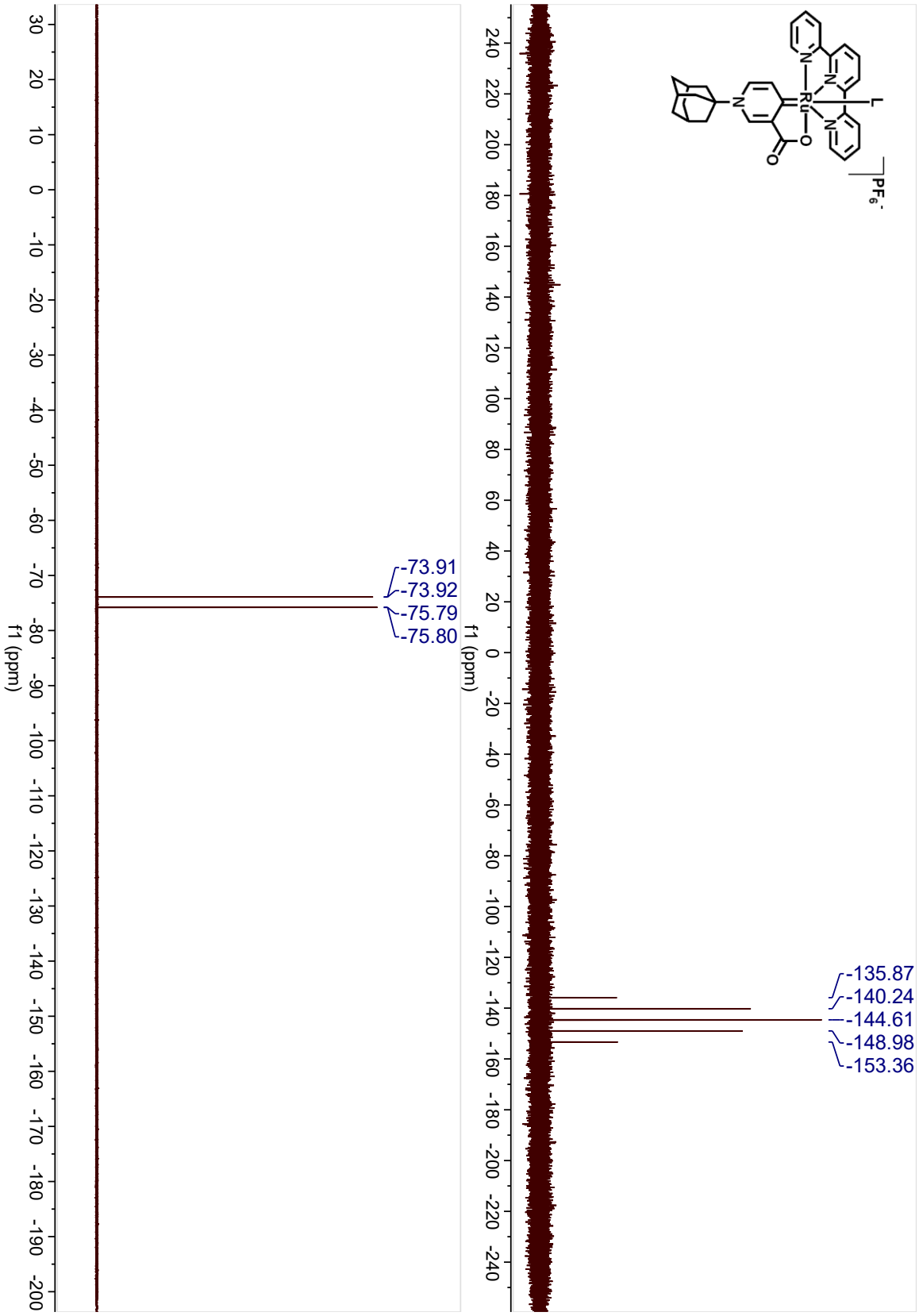
^{13}C NMR, CD_3CN



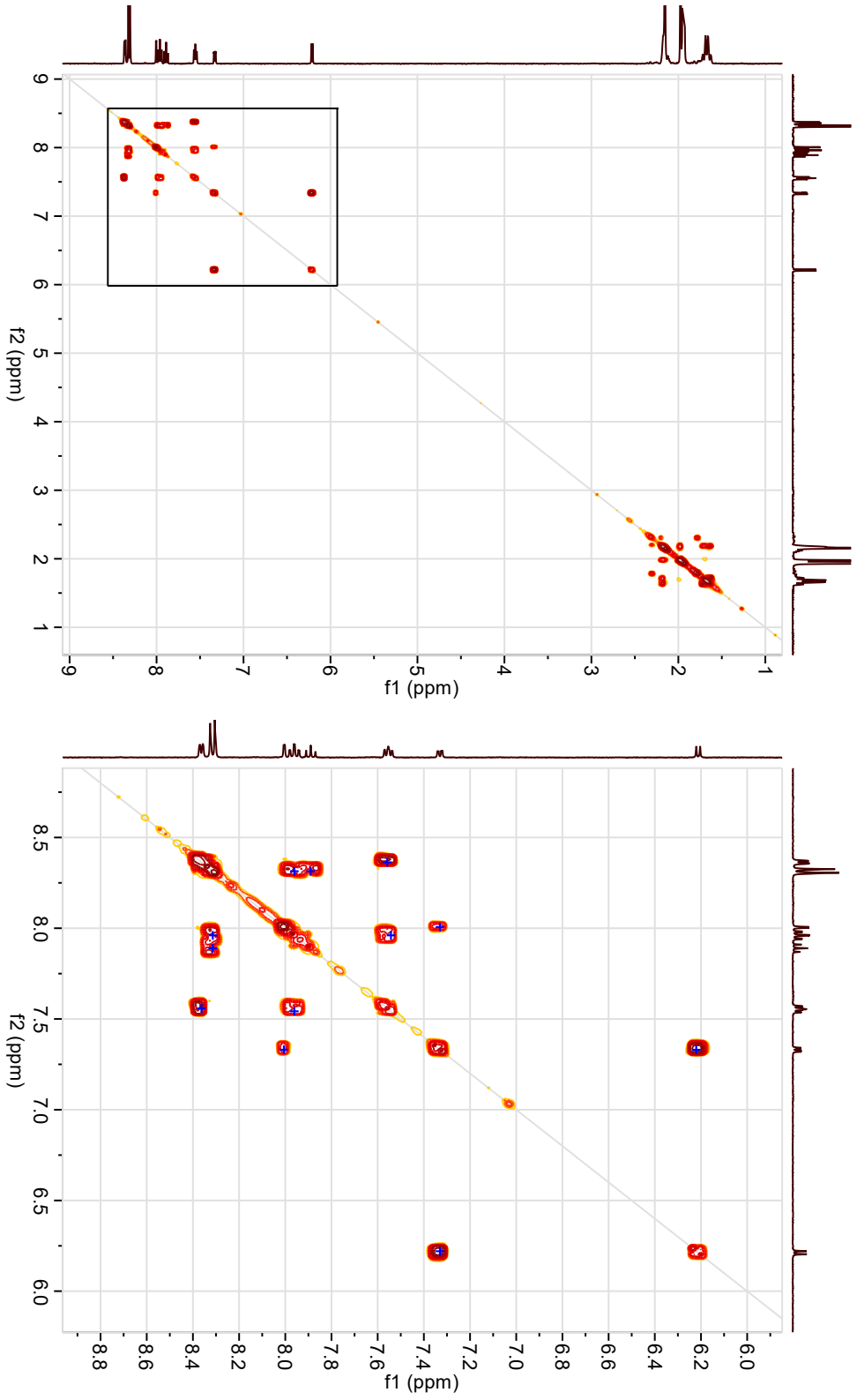
^{13}C NMR, CD_3OD



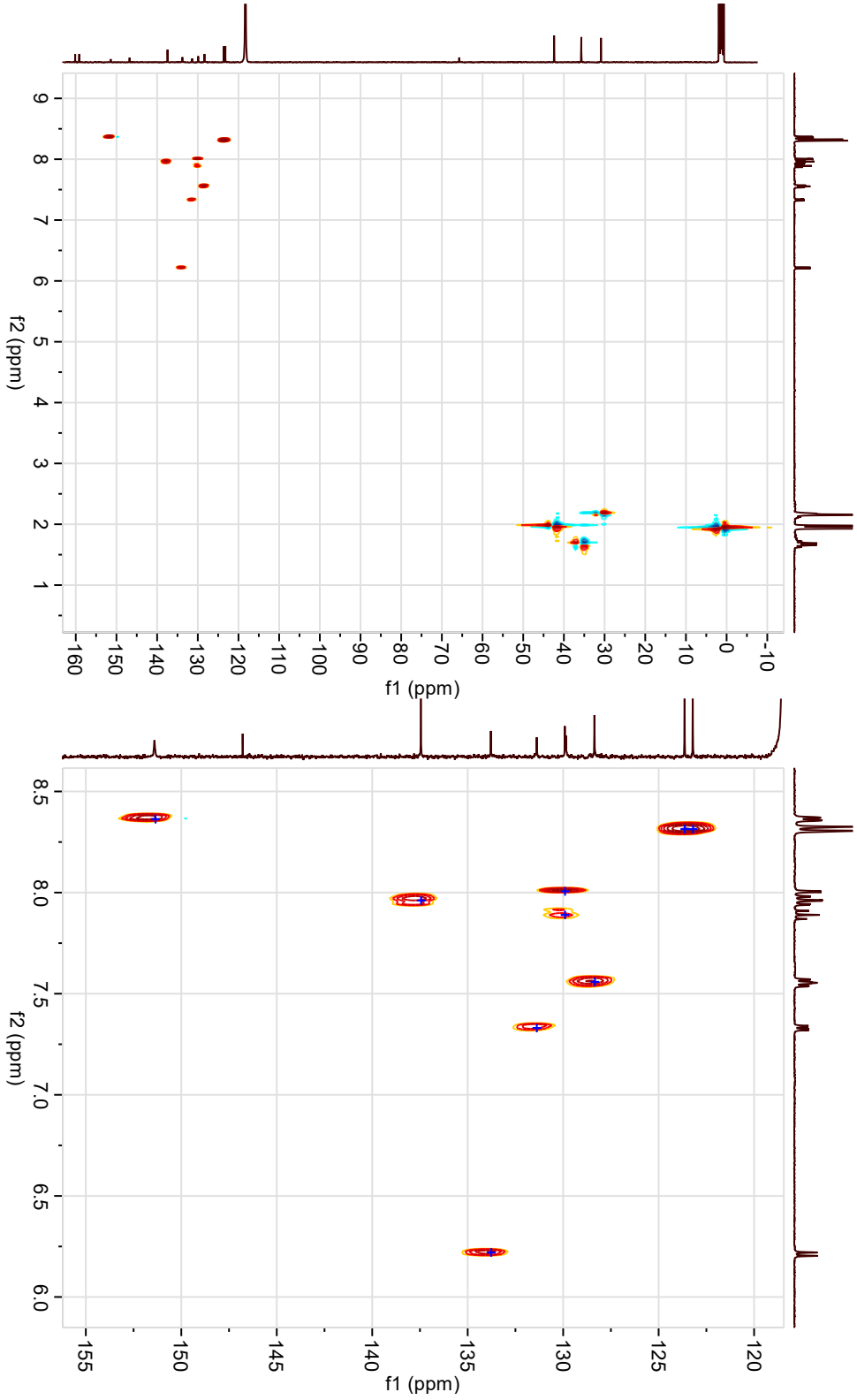
^{31}P & ^{19}F NMR, CD_3OD



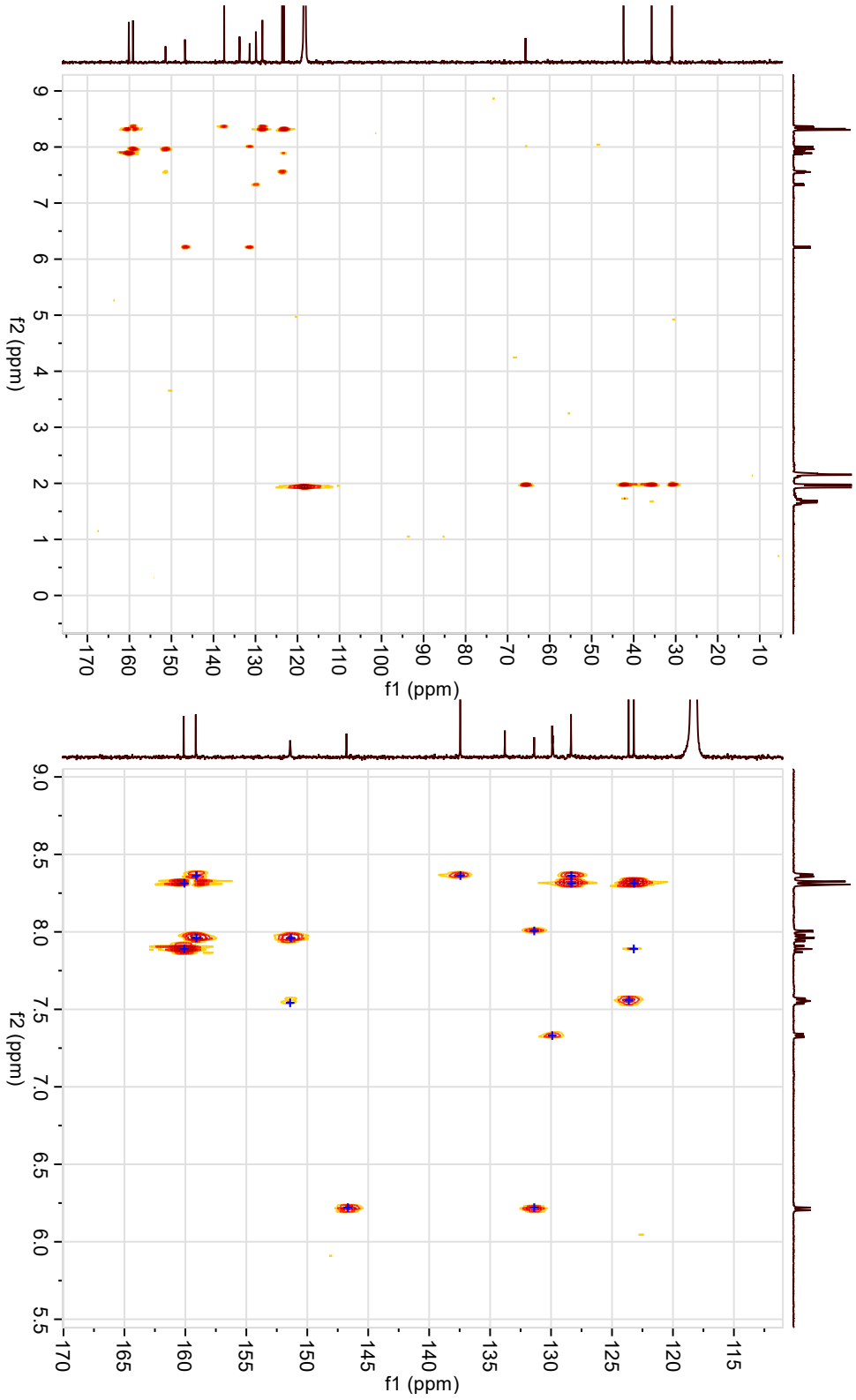
^{1}H-^{1}H COSY, CD_3CN



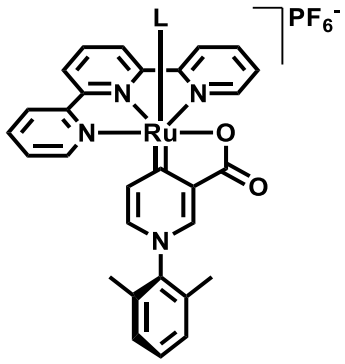
^{1}H-^{13}C HSQC, CD_3CN



^{1}H-^{13}C HMBC, CD_3CN



Ru(Ar)



Inside N_2 glovebox, a 20 mL vial was charged with **17** (107.3 mg, 0.4722 mmol), $[Cl_2Ru(tpy)]_2$ (191.3 mg), AgOAc (399.8 mg) and a magnetic stirrer added. The solids were suspended in methanol (about 3 mL) and the vial was sealed prior to heating and stirring at 70°C for 142 h (6 d). Under inert atmosphere, reaction mixture was filtered through a celite and a finely fritted funnel to remove insoluble AgCl salts. The crude product was rotoevaporated to dryness. Inside N2 glovebox, 50 mL deoxygenated deionized water and a magnetic stirrer was added. The flask was sealed and placed on an ultrasonic water bath (about 15 minutes), after which the contents became a thick brown purée. KPF_6 (401.0 mg) was added to the aqueous solution and stirring resumed for 19 h. A brownish red precipitate was collected over a fine fritted glass funnel. The mother liquor and 10 mL fresh deionized water was used to suspend and transfer material onto the frit, after which the solids on the frit was rinsed with water (3 x 3 mL). The solids were transferred to a vial, redissolved in CH_3CN, and passed through a kimwipe plug. Solvent was removed in vacuo to obtain red solids (164.0 mg, 47%).

^{1}H NMR (399.75 MHz, CD_3CN) δ 8.40 (dd, J = 5.5, 0.7 Hz, 2H), 8.37 – 8.30 (m, 4H), 8.00 (ddd, J = 8.2, 7.3, 1.5 Hz, 2H), 7.91 (t, J = 8.1 Hz, 1H), 7.63 (d, J = 1.6 Hz, 1H), 7.59 (ddd, J = 7.7, 5.5, 1.2 Hz, 2H), 7.30 (t, J = 7.7 Hz, 1H), 7.16 (d, J = 7.6 Hz, 2H), 6.92 (dd, J = 6.4, 1.7 Hz, 1H), 6.41 (d, J = 6.5 Hz, 1H), 1.73 (s, 6H).

^{13}C NMR (100.53 MHz, CD_3CN) δ 237.03, 175.74, 160.14, 159.10, 151.41, 147.48, 142.12, 137.71, 135.17, 134.79, 134.28, 133.27, 131.21, 130.55, 129.86, 128.44, 123.75, 123.28, 17.24.

^{31}P NMR (161.82 MHz, CD_3CN) δ -144.80 (hept, J = 706.3 Hz)

^{19}F NMR (376.11 MHz, CD_3CN) δ -73.10 (d, J = 706.5 Hz).

^{1}H-^{1}H COSY ((399.75, 399.75) MHz, CD_3CN) δ (8.40 7.59), (8.40 8.01), (8.34 7.59), (8.34 8.00), (8.33 7.91), (8.01 8.40), (8.00 7.59), (8.00 8.34), (7.91 8.33), (7.63 6.92), (7.59 8.34), (7.59 8.00), (7.59 8.40), (7.30 1.73), (7.30 7.15), (7.15 1.73), (7.15 7.30), (6.92 6.41), (6.92 7.63), (6.41 6.92), (1.73 7.15), (1.73 7.30).

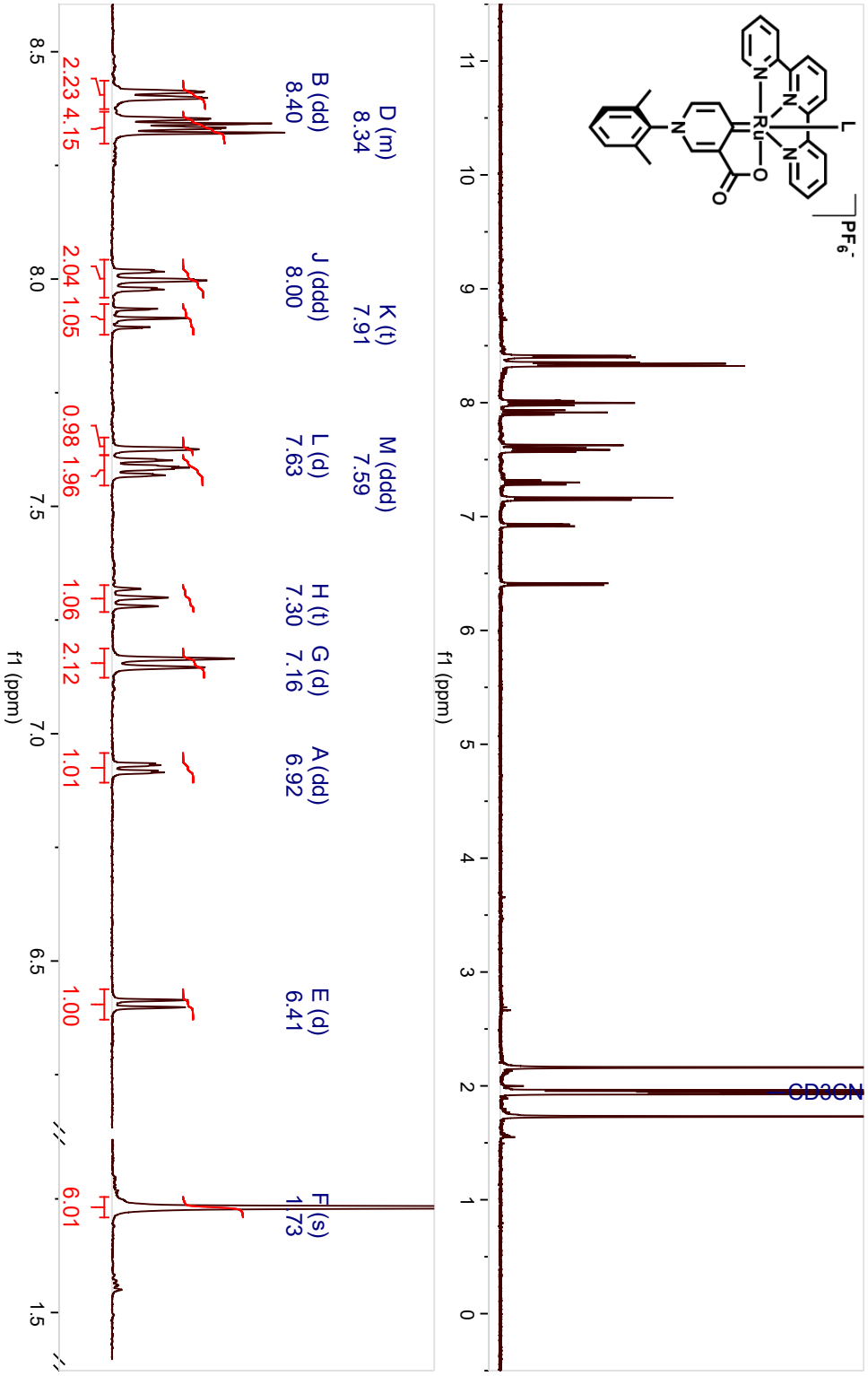
^{1}H-^{13}C HSQC ((399.75, 100.53) MHz, CD_3CN) δ (8.41 151.41), (8.34 123.75), (8.33 123.28), (7.99 137.71), (7.91 130.55), (7.63 133.27), (7.59 128.44), (7.30 131.21), (7.15 129.86), (6.93 135.17), (6.40 134.28), (1.73 17.24).

^{1}H-^{13}C HMBC ((399.75, 100.53) MHz, CD_3CN) δ (8.41 128.44), (8.41 137.71), (8.41 159.10), (8.34 128.44), (8.34 159.10), (8.33 123.28), (8.33 160.14), (7.99 151.41), (7.99 159.10), (7.91 123.28), (7.91 160.14), (7.63 135.17), (7.63 175.74), (7.59 151.38), (7.59 123.75), (7.30 134.79), (7.15 17.24), (7.15 129.86), (7.15 142.12), (6.93 133.27), (6.93 134.28), (6.40 135.17), (6.40 147.48), (1.73 129.86), (1.73 134.79), (1.73 142.12).

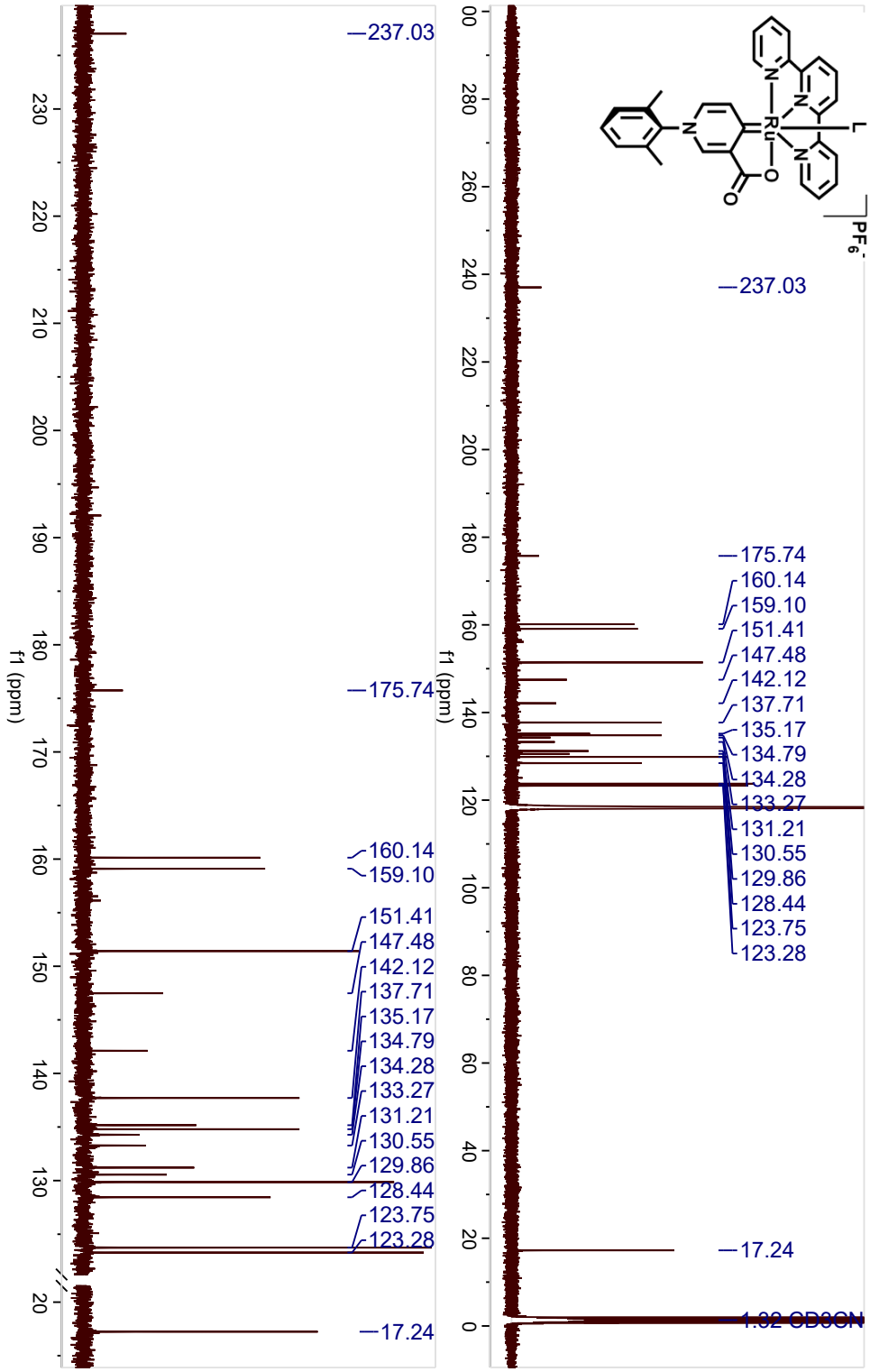
CHN calc'd for [**Ru(Ar)**(κ^{1}-CH_3CN)]PF_6 ($C_{33}H_{32}F_6N_5O_2PRu$) + 3H_2O: C, 47.71; H, 4.61; N, 8.43.

CHN found: C, 47.80; H, 3.24; N, 8.38.

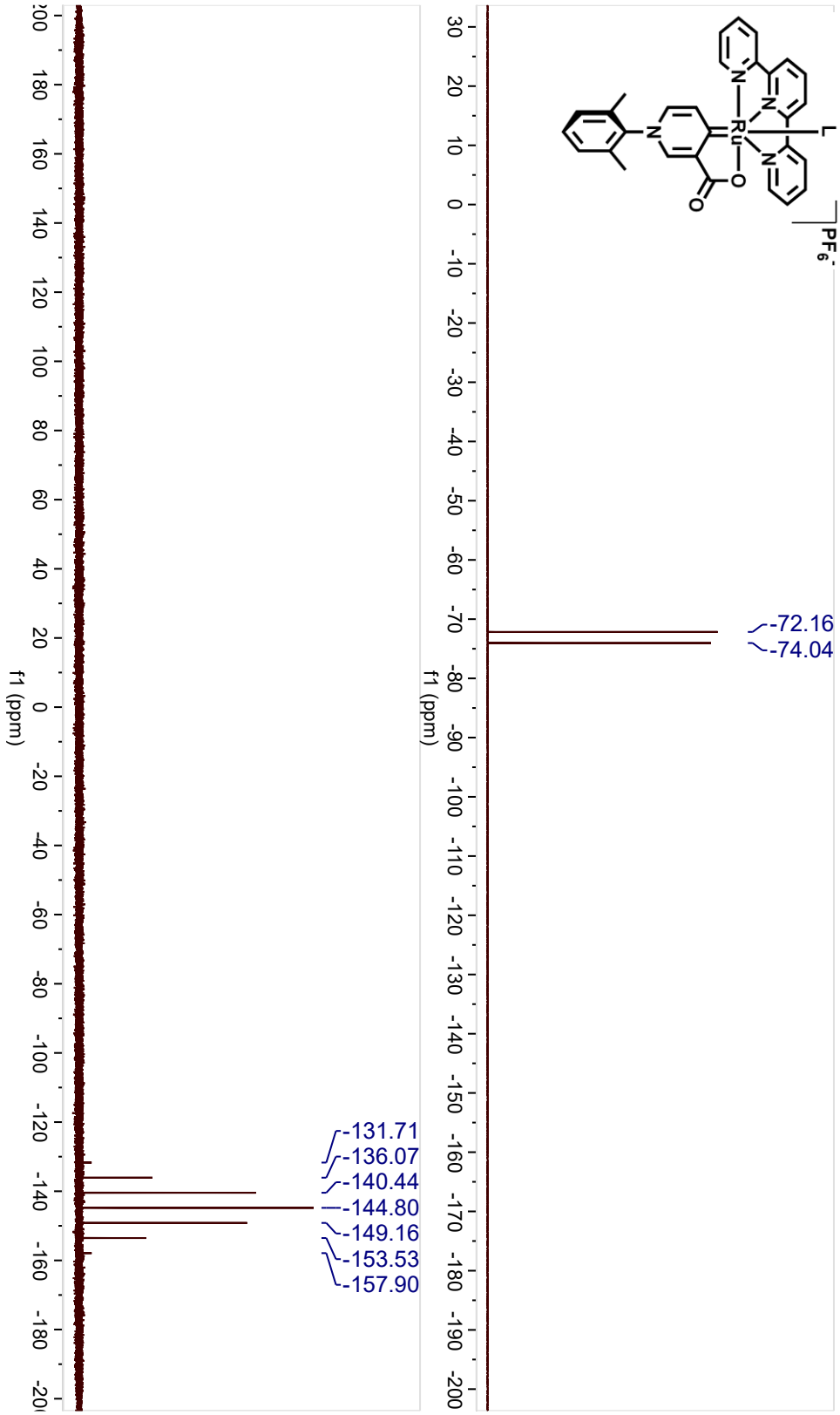
^{1}H NMR, CD_3CN


PF6-
CD3CN
f1 (ppm)
D (m) 8.34
K (t) 7.91
M (ddd) 7.59
B (dd) 8.40
J (ddd) 8.00
L (d) 7.63
H (t) 7.30
G (d) 7.16
A (dd) 6.92
E (d) 6.41
F (s) 1.73
2.23 4.15
2.04 1.05
0.98 1.96
1.06 2.12
1.01
1.00
6.01

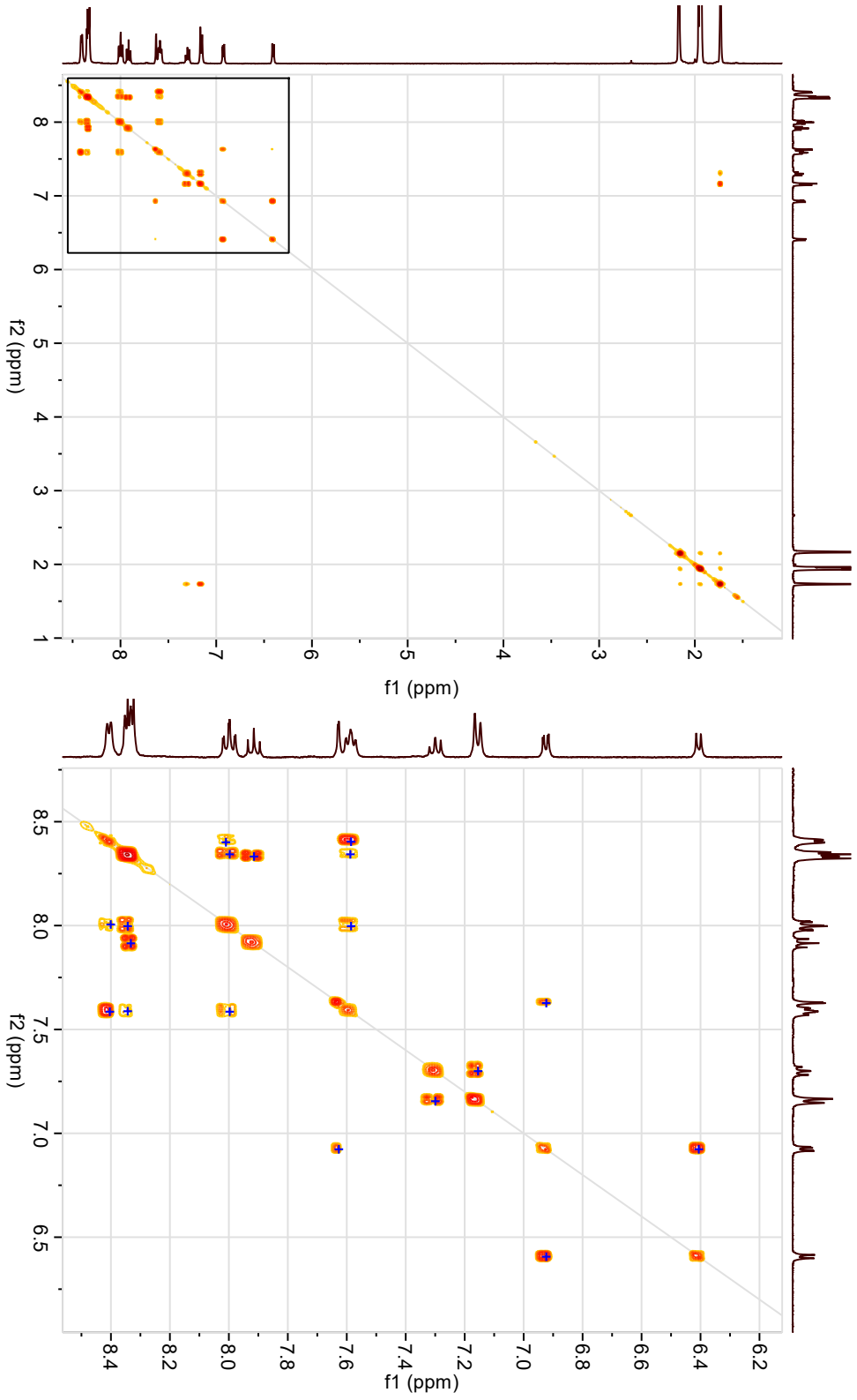
^{13}C NMR, CD_3CN



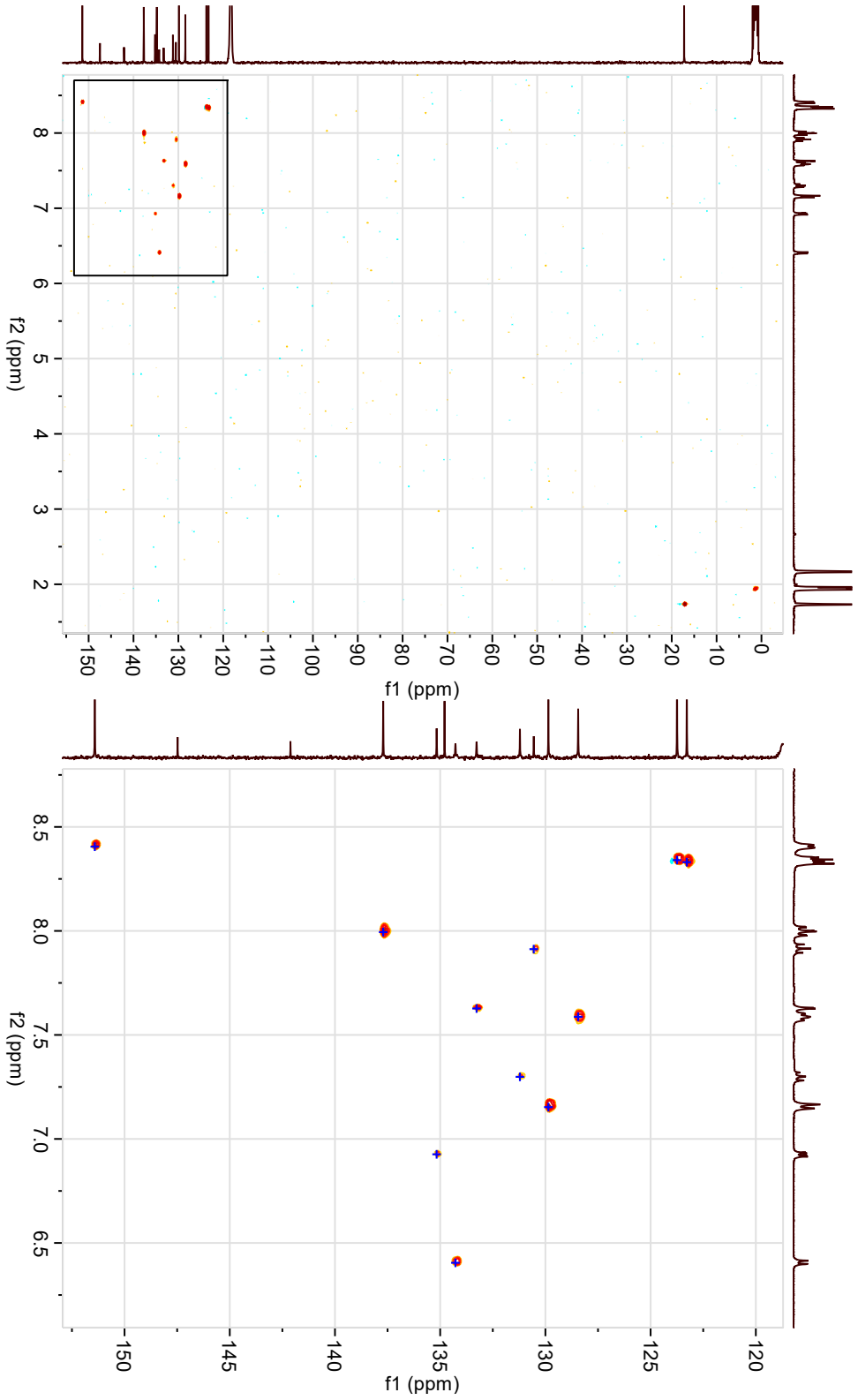
^{31}P NMR & ^{19}F NMR, CD_3CN



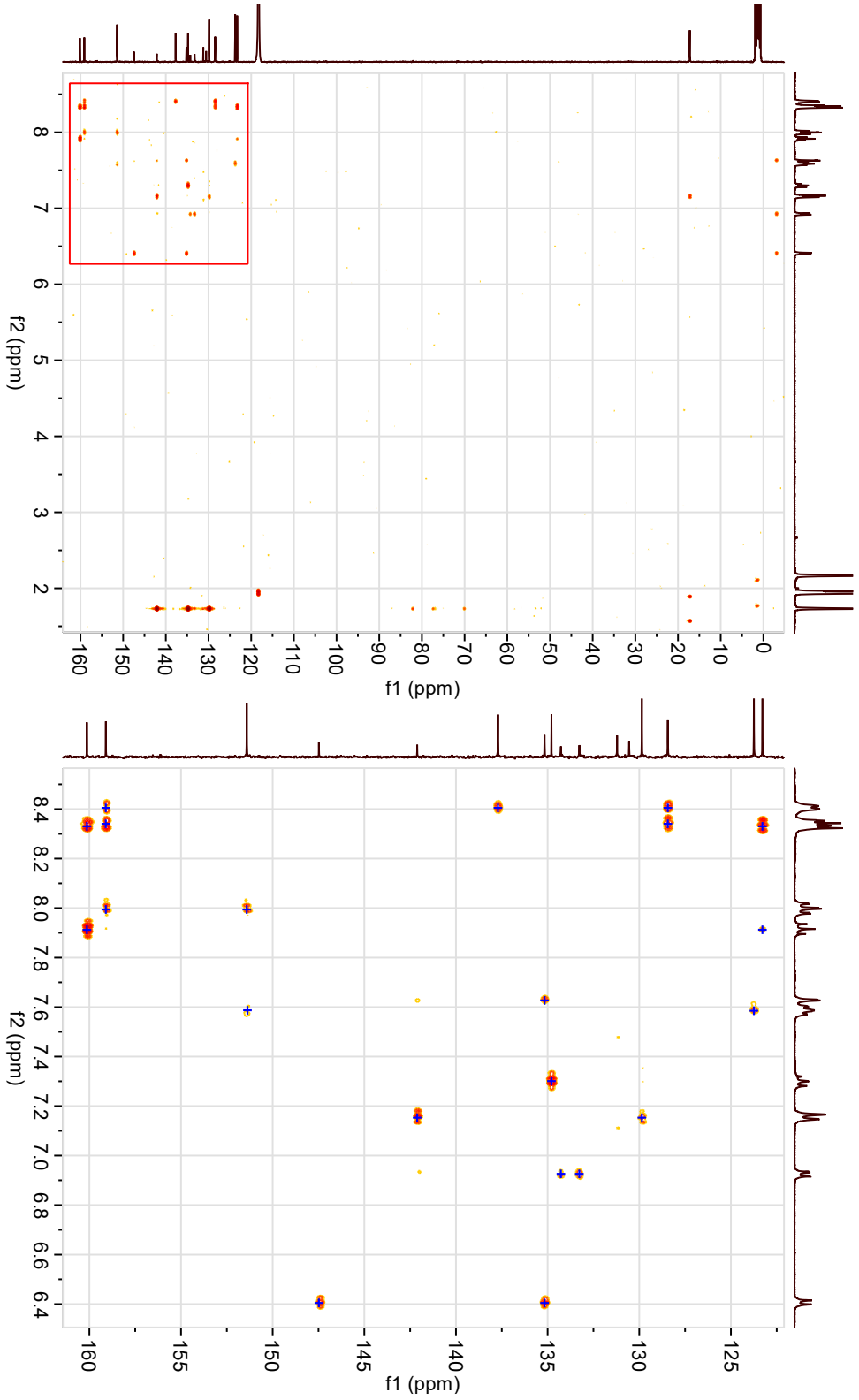
^{1}H-^{1}H COSY, CD_3CN



^{1}H-^{13}C HSQC, CD_3CN



^{1}H-^{13}C HMBC, CD_3CN



1.4.1.3. OCCO bipyridinium

The synthetic procedures for the compounds in **Figure 19** are presented in the following sections.

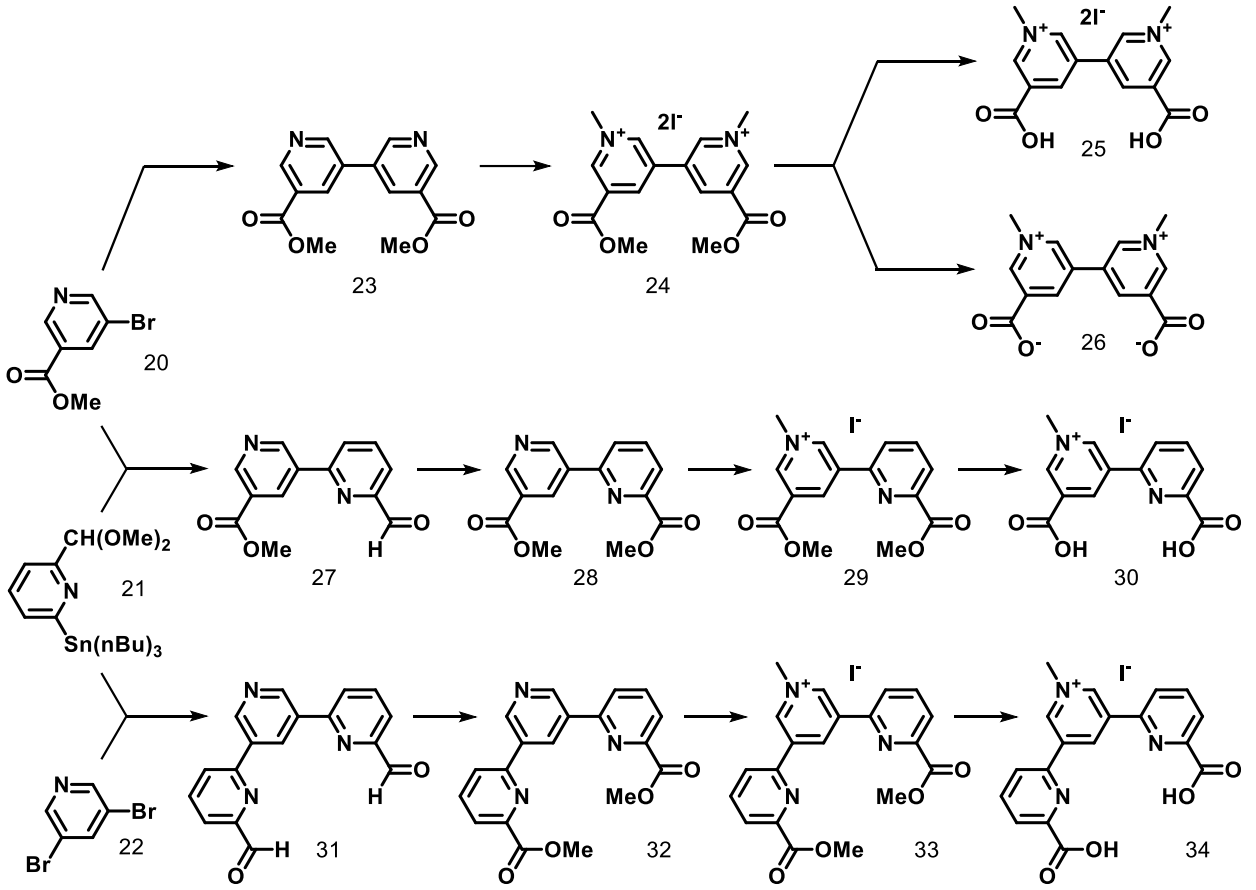
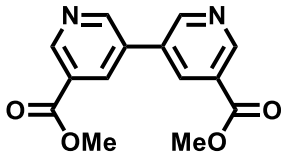


Figure 19. Synthetic scheme for polypyridyl analogues of **OC^{R}**

Dimethyl [3,3'-bipyridine]-5,5'-dicarboxylate



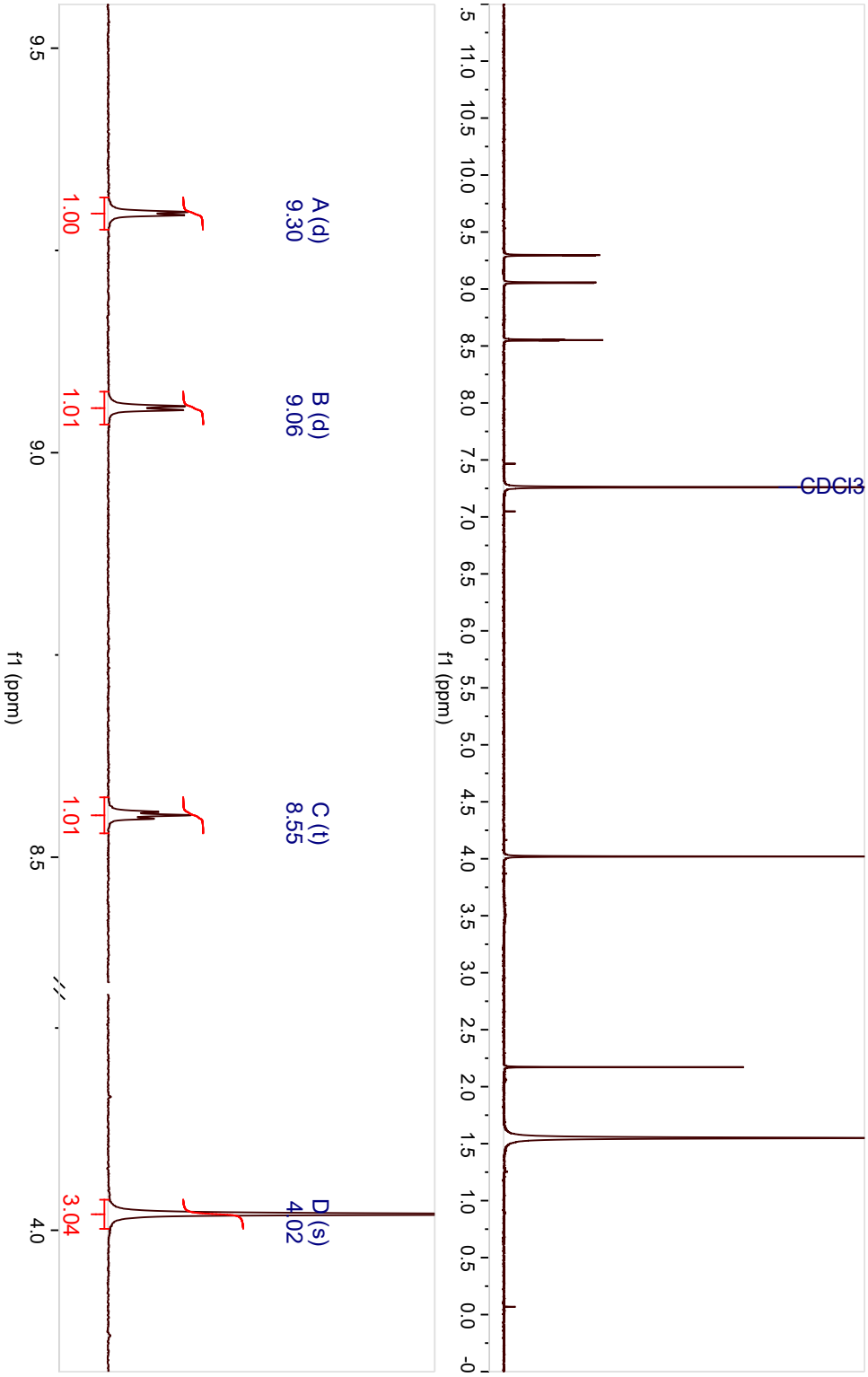
Reagents in this procedure were manipulated inside a nitrogen atmosphere drybox. The procedure was adapted from Oda et al.[35] A reaction vessel equipped with a Schlenk side-arm was charged with methyl 5-bromonicotinate (12.5800 g, 58.233 mmol), zinc dust (5.7610 g, 88.077 mmol), tetraethyl ammonium iodide (4.5112 g, 17.543 mmol), and $NiBr_2(PPh_3)_2$ (13.0062 g, 17.503 mmol). Dry deoxygenated tetrahydrofuran (100 mL) was added to the reaction vessel, and the resultant pale green suspension was heated at 60°C for 18 h under positive nitrogen pressure. Upon cooling, chloroform (100 mL) and aqueous ammonium hydroxide (200 mL) were added to the reaction mixture in portions, with vigorous stirring. Solids in the partitioned mixture were filtered out through a pad of Celite, after which the organic layer was extracted. The aqueous phase was extracted with additionally with chloroform (2 x 100 mL). All organic extracts were united and washed with aqueous ammonia (2 x 100 mL), deionized water (1 x 100 mL), and brine (2 x 100 mL). Removal of the organic solvent in vacuo gave a thick brown syrup that was redissolved to yield the product as a precipitate, which was collected by filtration and dried in vacuo (3.2329 g, 41%).

^{1}H NMR (499.94 MHz, $CDCl_3$) δ 9.30 (d, J = 2.0 Hz, 1H), 9.06 (d, J = 2.4 Hz, 1H), 8.55 (t, J = 2.1 Hz, 1H), 4.02 (s, 3H).

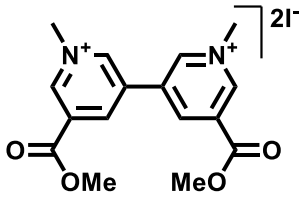
CHN calc'd for $C_{14}H_{12}N_2O_4$: C, 61.76; H, 4.44; N, 10.29.

CHN found: C, 61.69; H, 4.66; N, 10.55.

^{1}H NMR, $CDCl_3$



5,5'-bis(methoxycarbonyl)-1,1'-dimethyl-[3,3'-bipyridine]-1,1'-diium iodide



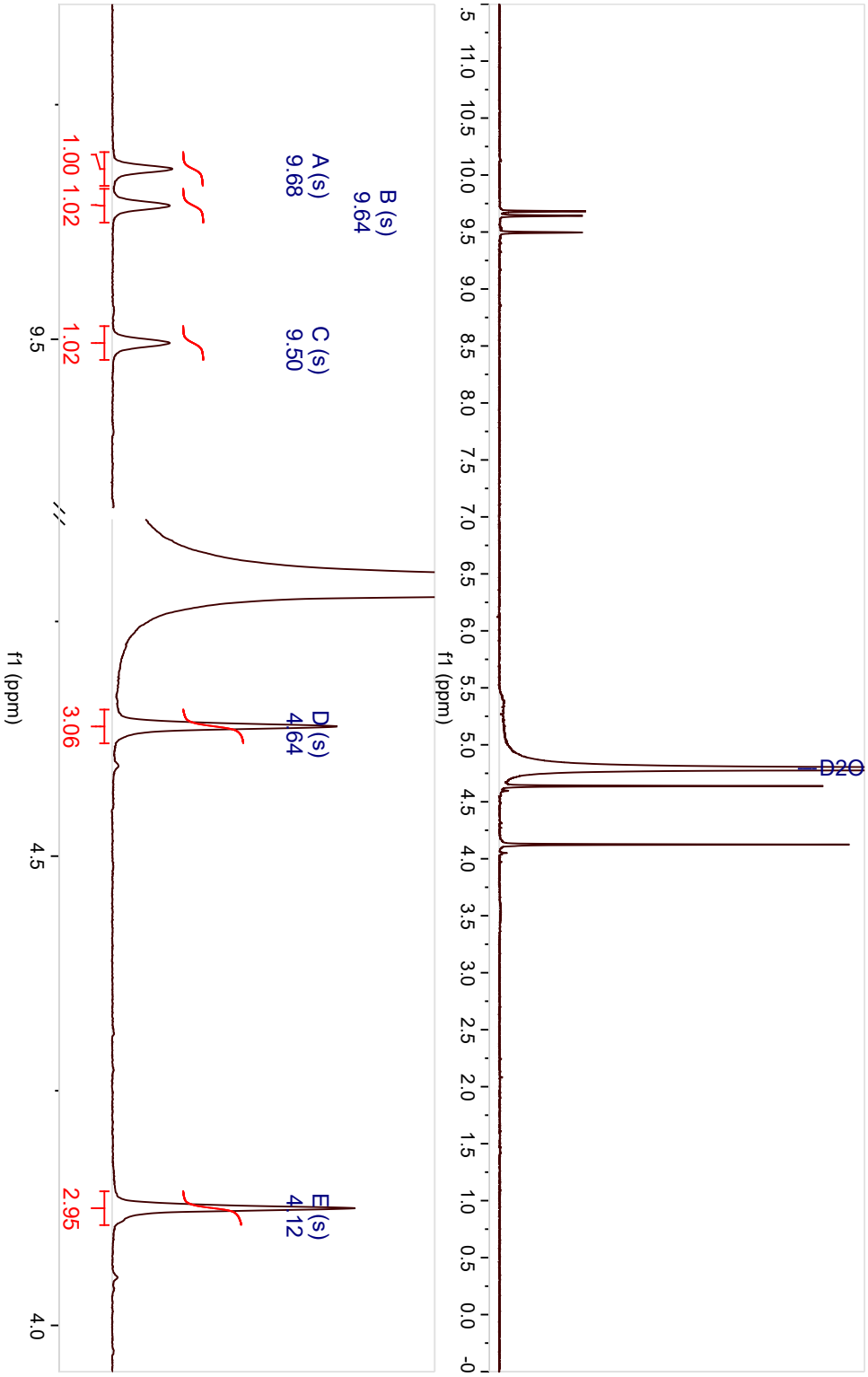
Dimethyl [3,3'-bipyridine]-5,5'-dicarboxylate (3.1882 g, 11.710 mmol) was suspended in an acetonitrile/chloroform solvent mixture (3:1, 8 mL) within a 20 mL scintillation vial. After the addition of methyl iodide (4.1533 g, 29.261 mmol), the vial was sealed and heated at 60°C for 92 h. The golden yellow crude material was filtered, rinsed with portions of acetone, and dried in vacuo to obtain the product as a hygrosopic yellow powder (6.1539 g, 99.9%).

^{1}H NMR (499.95 MHz, D_2O) δ 9.68 (s, 1H), 9.64 (s, 1H), 9.50 (s, 1H), 4.64 (s, 3H), 4.12 (s, 3H).

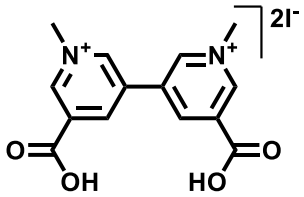
CHN calc'd for $C_{16}H_{18}I_2N_2O_4$: C, 34.56; H, 3.26; N, 5.04.

CHN found: C, 34.90; H, 3.35; N, 4.95.

^{1}H NMR, D_2O



5,5'-dicarboxy-1,1'-dimethyl-[3,3'-bipyridine]-1,1'-diium iodide



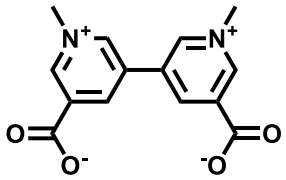
Diethyl [3,3'-bipyridine]-5,5'-dicarboxylate (1.3148 g, 2.2506 mmol) was dissolved in 20 mL deionized water inside a glass pressure reactor tube, after which hydrochloric acid (6 M, 0.361 mL) and a magnetic stirrer was added. The contents of the vessel were heated and stirred at 110 °C for 43 h. Acetone (about 20 mL) was added to the thick brown slurry, after which a black mud was filtered out using a fine frit. The residues were washed with 1:1 acetone:water (150 mL), concentrated down to about 20 mL, then redissolved in 1:1 acetone:water (300 mL) and refiltered. The crude material was dried *in vacuo* to obtain bright yellow solids (1.1884 g, 96.7% (monohydrate)).

CHN calc'd for $C_{14}H_{14}I_2N_2O_4$: C, 31.84; H, 2.67; N, 5.30.

CHN calc'd for $C_{14}H_{14}I_2N_2O_4 + 1H_2O$: C, 30.79; H, 2.95; N, 5.13

CHN found: C, 30.29; H, 3.09; N, 4.85

1,1'-dimethyl-[3,3'-bipyridine]-1,1'-diium-5,5'-dicarboxylate

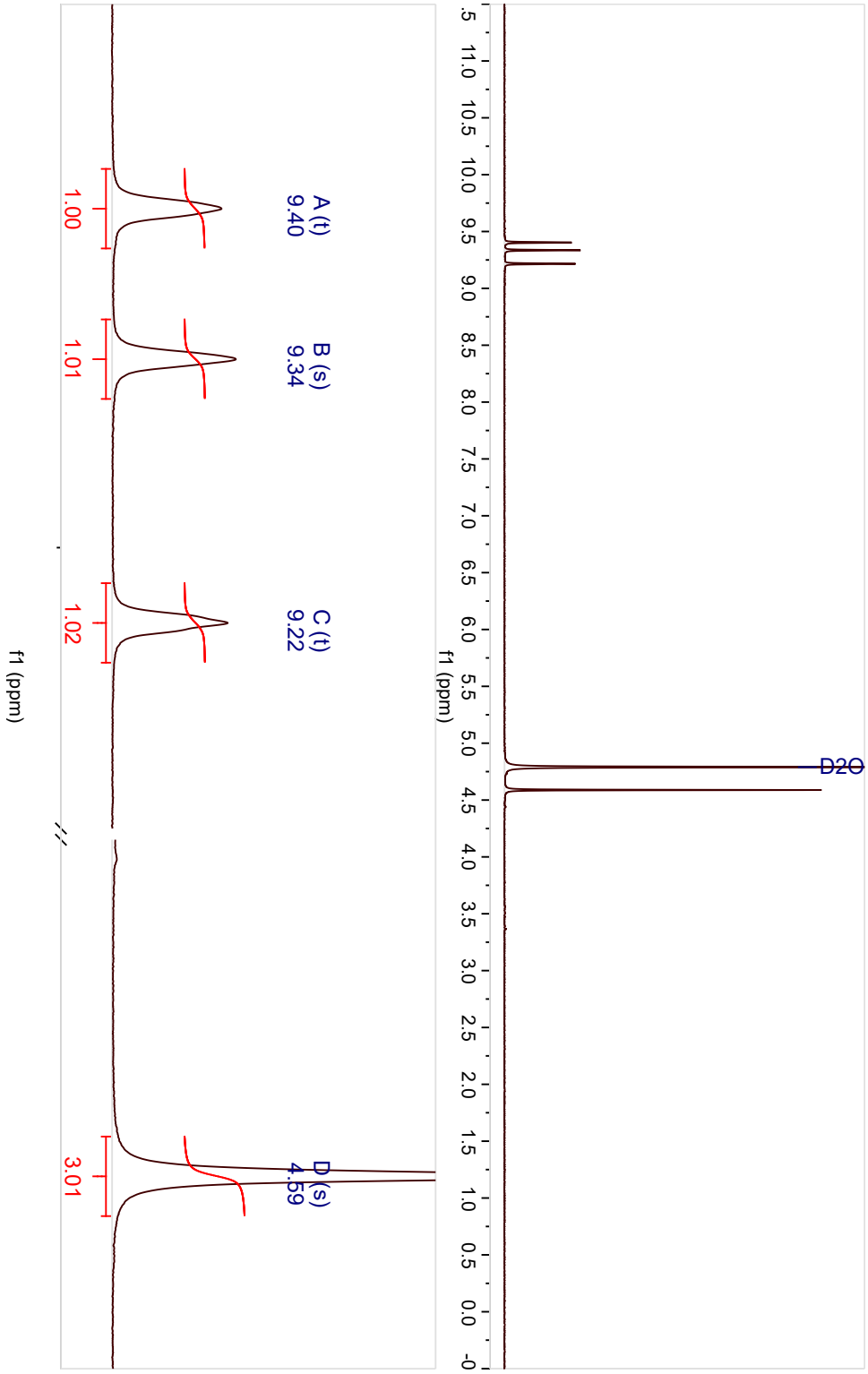


A yellow suspension of 5,5'-dicarboxy-1,1'-dimethyl-[3,3'-bipyridine]-1,1'-diium iodide (1.6097 g, 2.8944 mmol) in water (22 mL) turned orange when $LiOH{\cdot}H_2O$ (0.2491 g, 5.936 mmol) was added (total volume 32 mL). The mixture was stirred at room temperature for 19 h., after which water was removed on the rotary evaporator. The crude yellow solids were suspended in methanol (about 10 mL) and placed on ultrasonic water bath for 20 min., after which the off-white solids were filtered over a fine frit. The residues were rinsed with methanol (10 mL) and acetone (5 mL), and dried *in vacuo*. A small amount was dissolved in D_2O, where the ^7Li NMR spectra indicated a single peak and the pH of the sample was about 5. The solids were suspended in 2.5 mL water, sonicated, and combined with a solution of $LiOH{\cdot}H_2O$ (0.8058 g, 20 mL in water). The mixture was stirred at room temperature for 41 hours, then cooled on an ice bath. The precipitate was vacuum-filtered on a fine frit, after the frit was packed tightly with crushed ice. After the ice had melted, the solids were dried *in vacuo* to a snow-white powder (0.4121 g, 41.4 % (tetrahydrate)).

^1H NMR (499.95 MHz, D_2O) δ 9.40 (t, J = 1.5 Hz, 1H), 9.34 (s, 1H), 9.22 (t, J = 1.7 Hz, 1H), 4.59 (s, 3H).

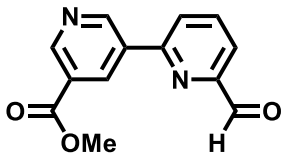
CHN calc'd for $C_{14}H_{12}N_2O_4$:	C, 61.76; H, 4.44; N, 10.29
CHN calc'd for $C_{14}H_{12}N_2O_4 + 4H_2O$:	C, 48.84; H, 5.86; N, 8.14.
CHN found:	C, 48.88; H, 5.81; N, 8.13.

^{1}H NMR, D_2O



1.4.1.4. ONCO bipyridinium

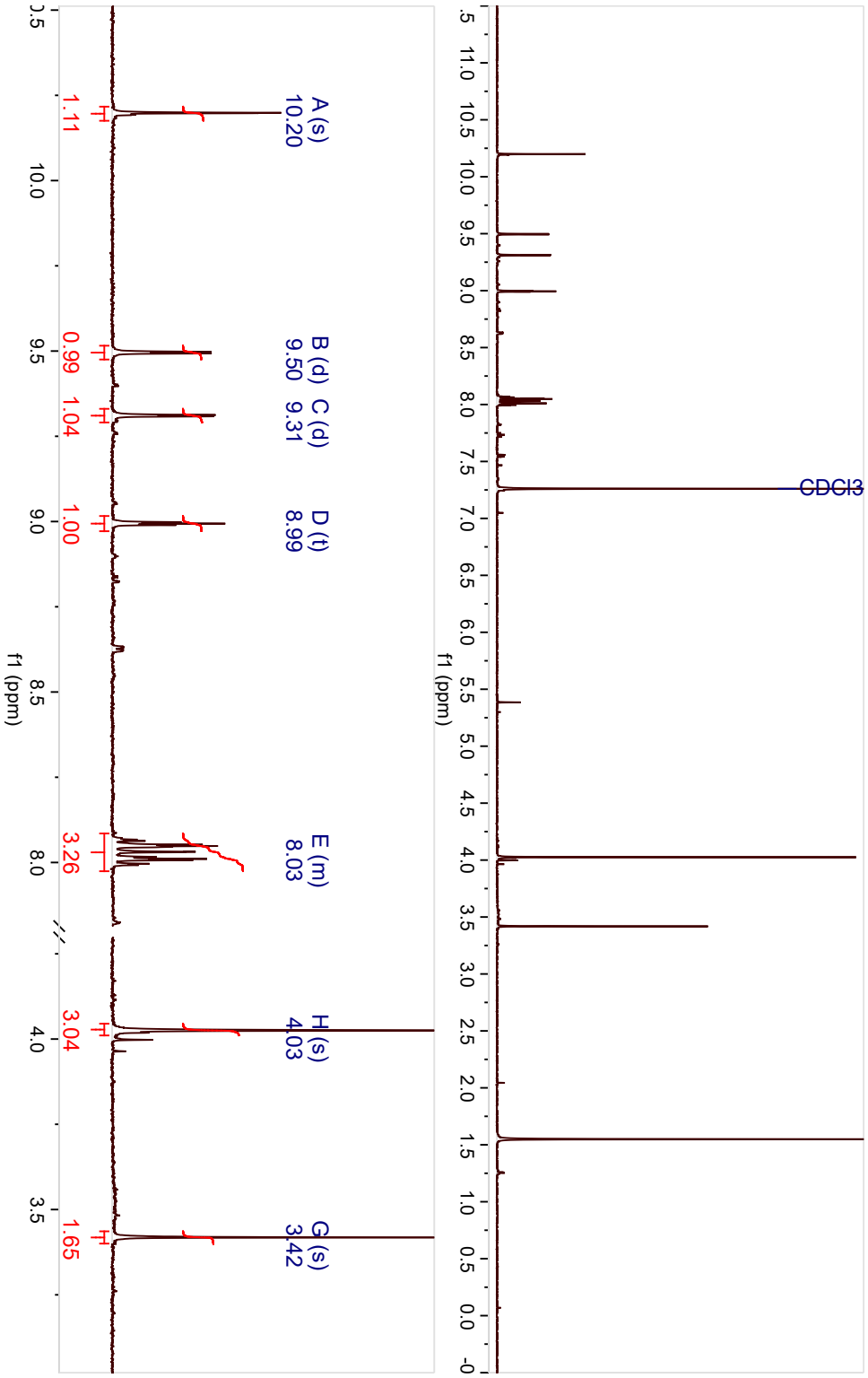
Methyl 6-formyl-[2,3'-bipyridine]-5'-carboxylate



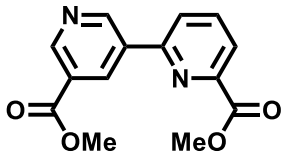
Reagents in this procedure were manipulated inside a nitrogen atmosphere drybox. A 20 mL scintillation vial was charged with 2-(dimethoxymethyl)-6-(tributylstannyl)pyridine (3.7100 g, 8.3893 mmol), methyl 5-bromonicotinate (1.2069 g, 5.5867 mmol), $Pd(PPh_3)_4$ (0.1230 g, 0.10644 mmol), and LiCl (0.4780 g, 11.275 mmol). The reagents were suspended in dry deoxygenated toluene (7 mL), after which the vial was sealed and heated at 100°C over 36 h. The contents of the vial were washed with portions of 6 M HCl (aq) (3 x 3 mL), and the washings filtered through a fritted funnel. The aqueous washings were collected and washed with dichloromethane (7 x 25 mL) during which the scarlet organic phases gradually turned pale yellow. The resulting aqueous phase was adjusted to neutral pH using $NaHCO_3$ (aq), and dichloromethane (ca. 50 mL) was added to partition the solution into two phases. The organic phase was extracted, washed with water (2 x 50 mL), brine (1 x 50 mL), then dried over anhydrous magnesium sulfate. Solvent was removed in vacuo to yield a brown solid (1.2075 g, 4.9849 mmol, 89%). Minor impurities were present in the product.

^{1}H NMR (499.94 MHz, $CDCl_3$) δ 10.20 (s, 1H), 9.50 (d, J = 2.2 Hz, 1H), 9.31 (d, J = 2.0 Hz, 1H), 8.99 (t, J = 2.1 Hz, 1H), 8.09 – 7.97 (m, 3H), 4.03 (s, 3H), 3.42 (s, 2H).

^{1}H NMR, $CDCl_3$


CDCl3
f1 (ppm)
A (s) 10.20
B (d) 9.50
C (d) 9.31
D (t) 8.99
E (m) 8.03
H (s) 4.03
G (s) 3.42
1.11
0.99
1.04
1.00
3.26
3.04
1.65

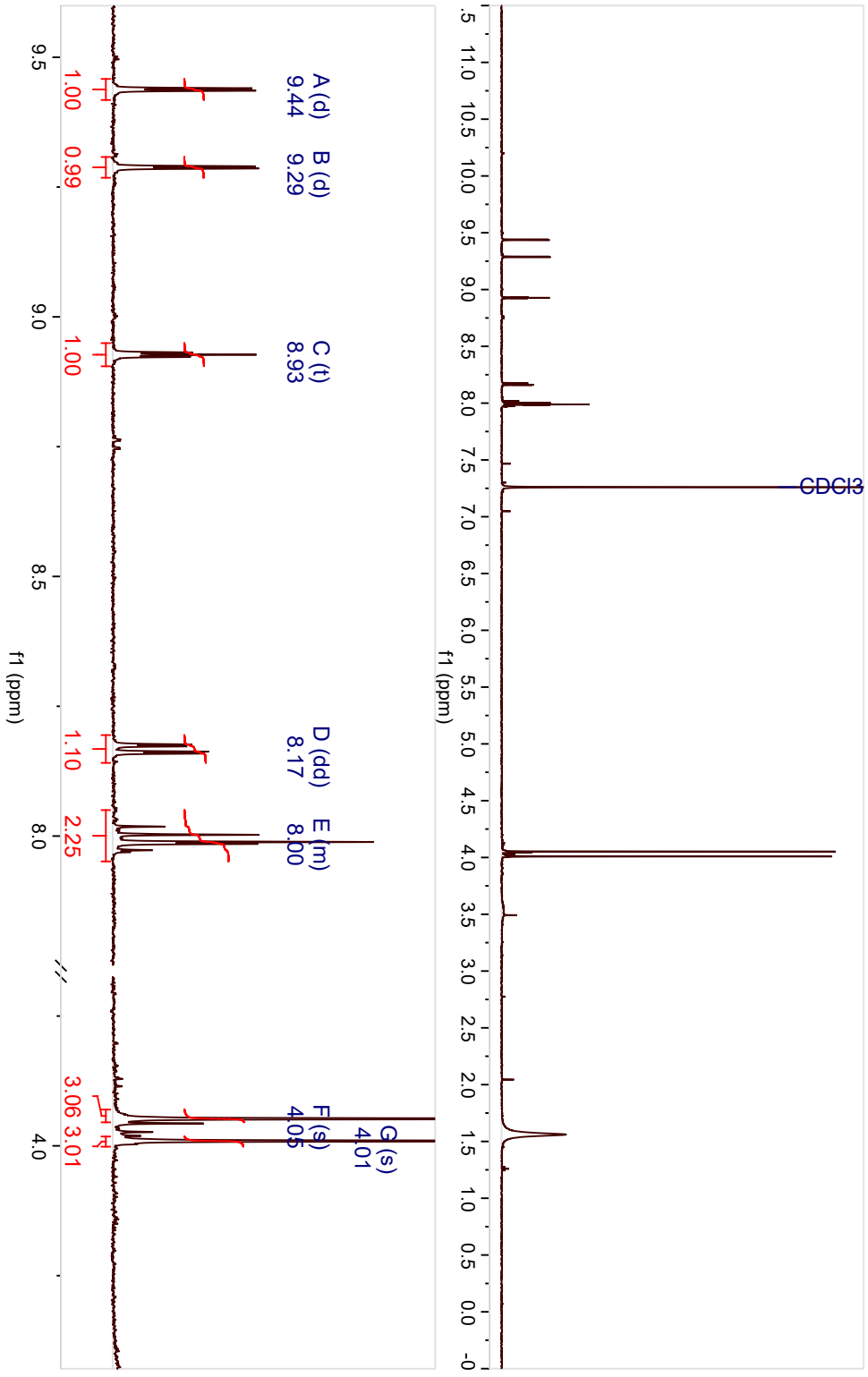
Dimethyl [2,3'-bipyridine]-5',6-dicarboxylate



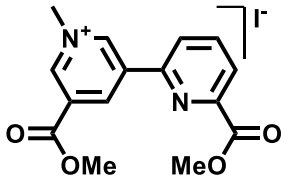
This procedure was adapted from Ghosh et al.[36] Aldehyde **21a** (1.3499 g, 5.5728 mmol), pyridine (0.425 mL, 5.28 mmol), and N-bromosuccinimide (1.9606 g, 11.015 mmol) were suspended in methanol (30 mL), and the mixture was heated and stirred at 40°C for 18 h under positive nitrogen pressure. The solution was concentrated by rotary evaporator to remove most of the methanol, and the residual aqueous portion was adjusted to pH 7 using saturated sodium bicarbonate (aq) to precipitate out the product. The precipitate was collected by filtration, washed well with portions of deionized water (ca. 150 mL total), and dried in a heat vacuum desiccator to obtain brown solids (1.1601 g, 4.3771 mmol, 79%).

^{1}H NMR (499.94 MHz, $CDCl_3$) δ 9.44 (d, *J* = 2.3 Hz, 1H), 9.29 (d, *J* = 2.0 Hz, 1H), 8.93 (t, *J* = 2.1 Hz, 1H), 8.17 (dd, *J* = 6.9, 1.8 Hz, 1H), 8.05 – 7.95 (m, 2H), 4.05 (s, 3H), 4.01 (s, 3H).

^{1}H NMR, $CDCl_3$


CDCl3
f1 (ppm)
A (d) 9.44
B (d) 9.29
C (t) 8.93
D (dd) 8.17
E (m) 8.00
F (s) 4.05
G (s) 4.01
1.00
0.99
1.00
1.10
2.25
3.06
3.01

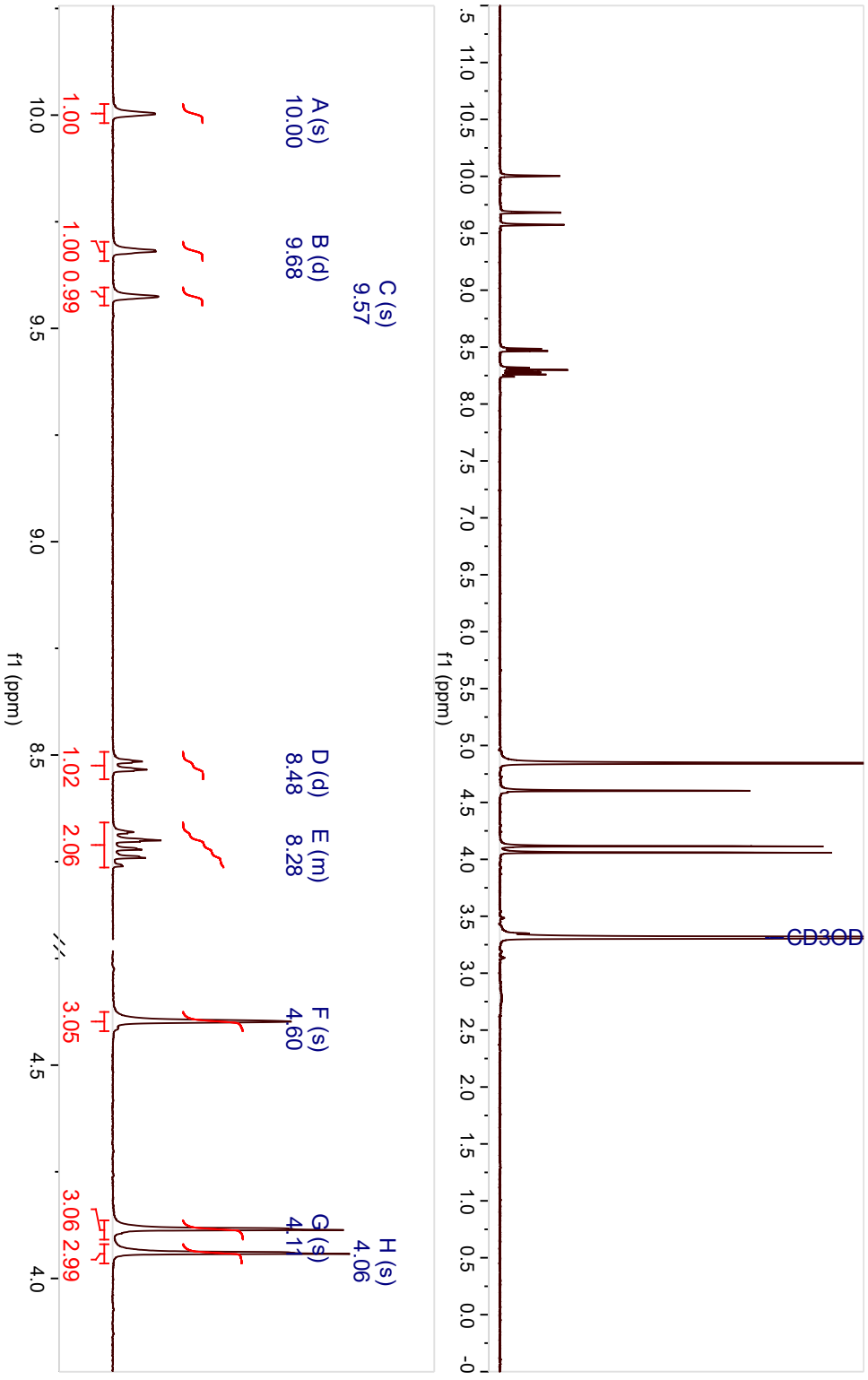
5',6-bis(methoxycarbonyl)-1'-methyl-[2,3'-bipyridin]-1'-ium iodide



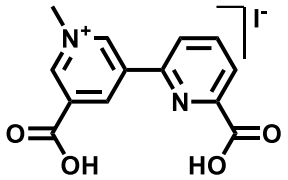
Diester **21b** (0.3596 g, 1.321 mmol) was suspended in chloroform (4 mL), and methyl iodide (0.11 mL, 1.8 mmol) was added. The reaction mixture was heated and stirred at 50°C for 23 h. An aliquot was taken for ^{1}H NMR spectroscopy, and heating was resumed at 60°C over 6 days. After solvent removal by rotary evaporator, the residue resuspended in acetone (10 mL). The crude solids were washed with small portions of acetone (5 x 2 mL) to obtain hygroscopic yellow solids (0.3143 g, 0.7587 mmol, 57%).

^{1}H NMR (399.75 MHz, CD_3OD) δ 10.00 (s, 1H), 9.68 (d, *J* = 1.1 Hz, 1H), 9.57 (s, 1H), 8.48 (d, *J* = 7.7 Hz, 1H), 8.34 – 8.24 (m, 2H), 4.60 (s, 3H), 4.11 (s, 3H), 4.06 (s, 3H).

^{1}H NMR, CD_3OD


CD3OD
f1 (ppm)
A (s) 10.00
B (d) 9.68
C (s) 9.57
D (d) 8.48
E (m) 8.28
F (s) 4.60
G (s) 4.11
H (s) 4.06
1.00
1.00
0.99
1.02
2.06
3.05
3.06
2.99

6-carboxy-1'-methyl-[2,3'-bipyridin]-1'-ium-5'-carboxylate



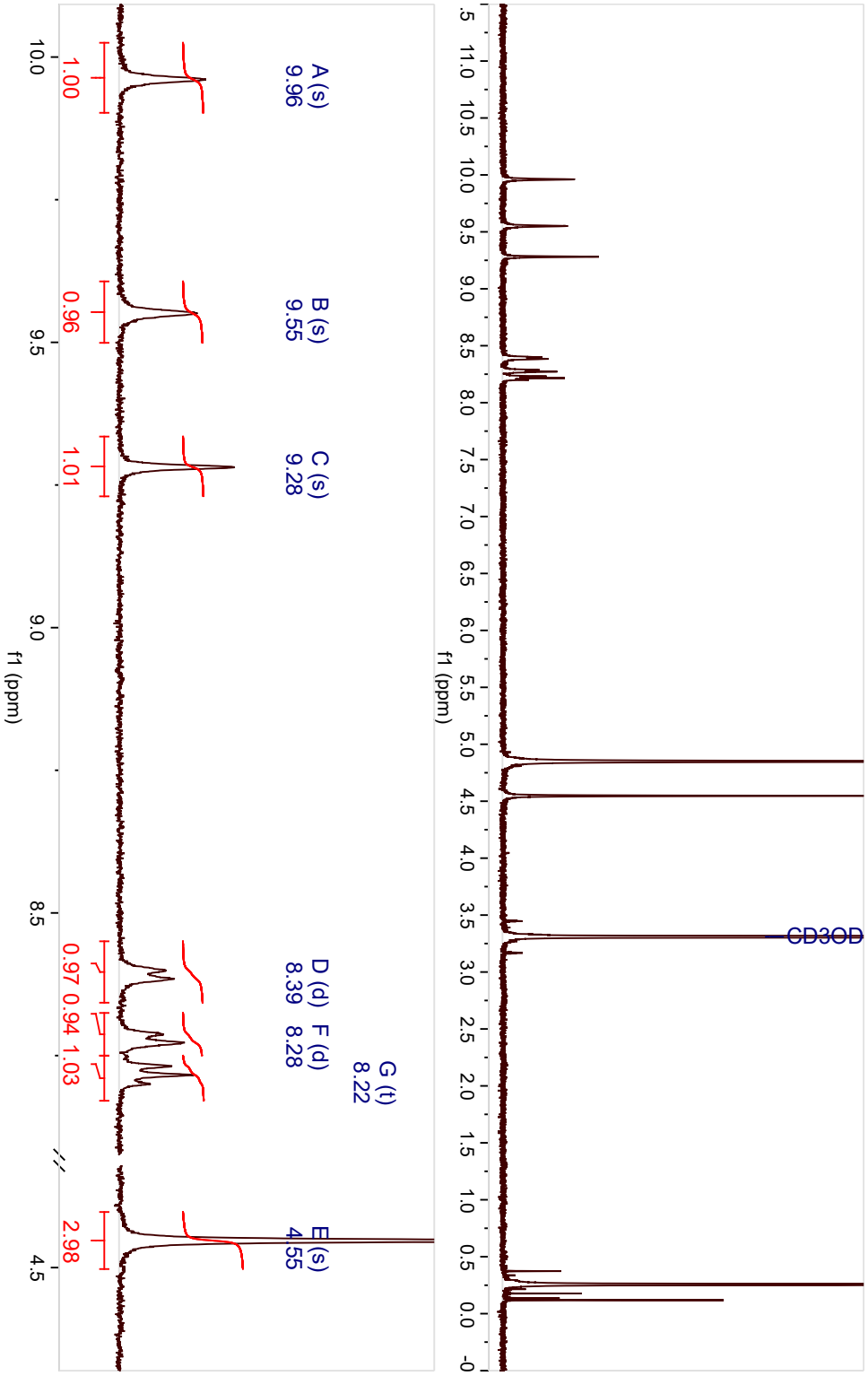
A 20 mL scintillation vial was charged with iodide salt **21c** (0.5123 g, 1.237 mmol) and 6 M HCl (aq) (4 mL). The contents of the vial was stirred and heated at 100°C for 20 h, resulting in the appearance of a black precipitate. Acetone was added to the aqueous solution to obtain a white precipitate, and the clear red supernate solution was decanted (3 x 2 mL). The residue was suspended in deionized water (2 mL) and an off-white solid could be filtered over a fine glass frit. The solids were dried in vacuo (0.2461 g, 0.9530 mmol, 77%). Aqueous solutions of **21d** tested neutral pH, and CHN indicated the zwitterionic species.

^{1}H NMR (499.95 MHz, CD_3OD) δ 9.96 (s, 1H), 9.55 (s, 1H), 9.28 (s, 1H), 8.39 (d, J = 7.4 Hz, 1H), 8.28 (d, J = 7.0 Hz, 1H), 8.22 (t, J = 7.8 Hz, 1H), 4.55 (s, 3H).

CHN calc'd for $C_{13}H_{10}N_2O_4 + 1H_2O$: C, 56.52; H, 4.38; N, 10.14.

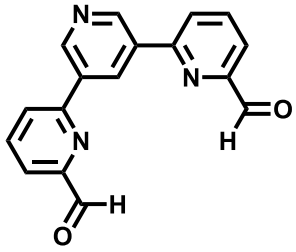
CHN found: C, 55.58; H, 4.39; N, 10.05.

^{1}H NMR, CD_3OD


CD3OD
f1 (ppm)
A (s) 9.96
B (s) 9.55
C (s) 9.28
D (d) 8.39
F (d) 8.28
G (t) 8.22
E (s) 4.55
1.00
0.96
1.01
0.97
0.94
1.03
2.98

1.4.1.5. ONCNO terpyridinium

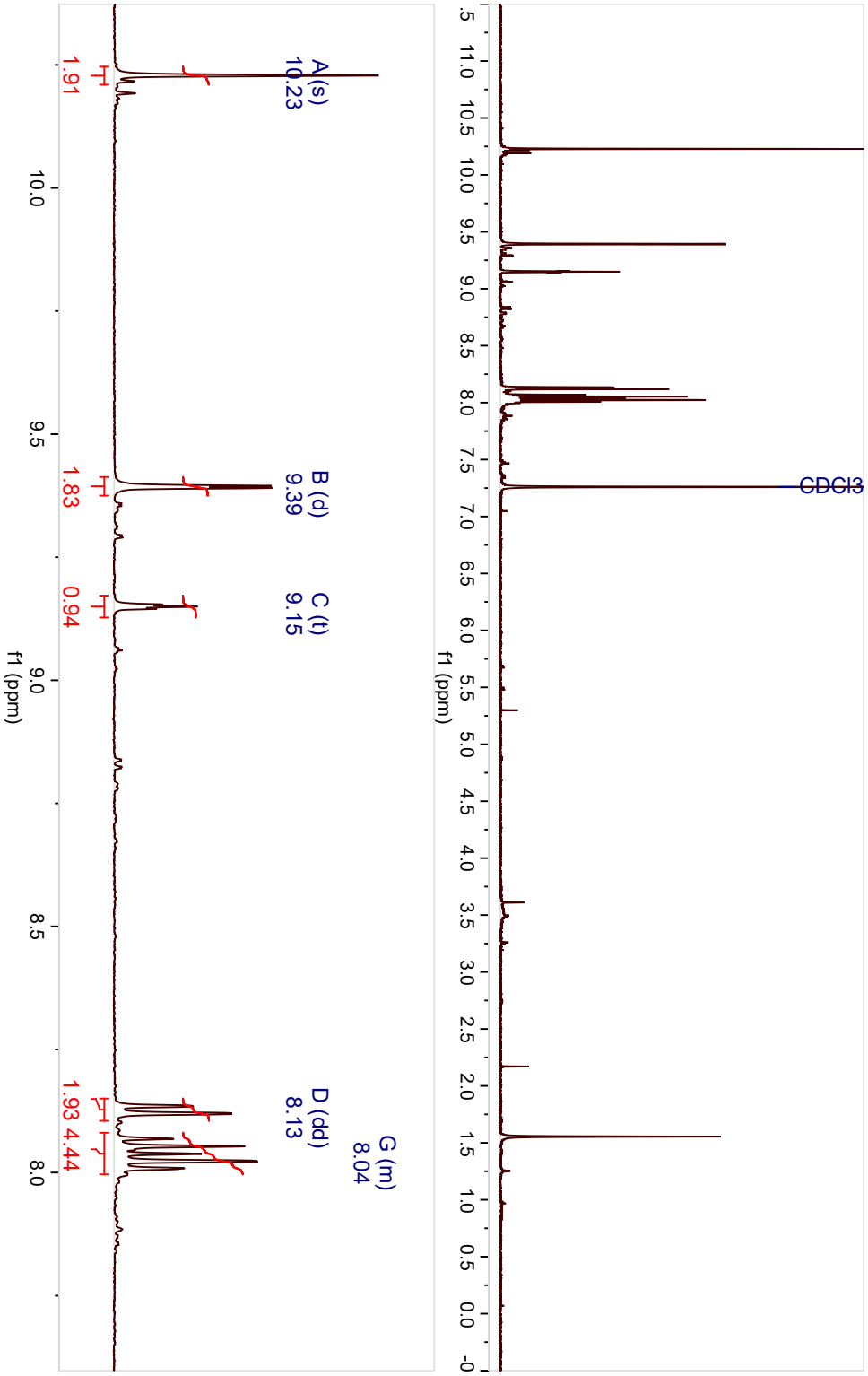
[2,3':5',2''-terpyridine]-6,6''-dicarbaldehyde



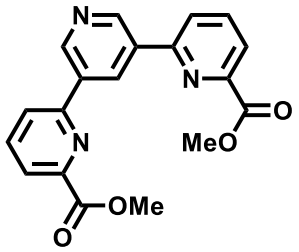
Reagents in this procedure were manipulated inside a nitrogen atmosphere drybox. A 20 mL scintillation vial was charged with 2-(dimethoxymethyl)-6-(tributylstannyl)pyridine (5.5323 g, 12.510 mmol), 3,5-dibromopyridine (1.0879 g, 4.5924 mmol), $Pd(PPh_3)_4$ (0.1575 g, 0.1363 mmol), and LiCl (0.7707 g, 18.18 mmol).was suspended in dry deoxygenated toluene (12 mL). The cloudy, orange-red solution was stirred at 100°C for 45 h. Upon cooling to room temperature, hydrochloric acid (6 M, 35 mL) was added, and the aqueous layer washed with dichloromethane(6 x 30 mL). The aqueous phase was adjusted to pH 7 by the addition of excess $NaHCO_3$ (aq), after which dichloromethane (200 mL) was added. The mixture was allowed to stir overnight, after which the organic layer was extracted. The aqueous layer was extracted additionally with dichloromethane (3 x 200 mL), after which the united organic layers were washed with deionized water (2 x 300 mL) and saturated aqueous sodium chloride (300 mL). Solvent was removed by rotary evaporation to yield the product (1.1035 g, 3.8172 mmol, 83%).

^{1}H NMR (499.94 MHz, $CDCl_3$) δ 10.23 (s, 2H), 9.39 (d, J = 2.2 Hz, 2H), 9.15 (t, J = 2.2 Hz, 1H), 8.13 (dd, J = 7.7, 1.4 Hz, 2H), 8.08 – 8.00 (m, 4H).

^{1}H NMR, $CDCl_3$


CDCl3
f1 (ppm)
A (s)
10.23
B (d)
9.39
C (t)
9.15
D (dd)
8.13
G (m)
8.04
1.91
1.83
0.94
1.93
4.44

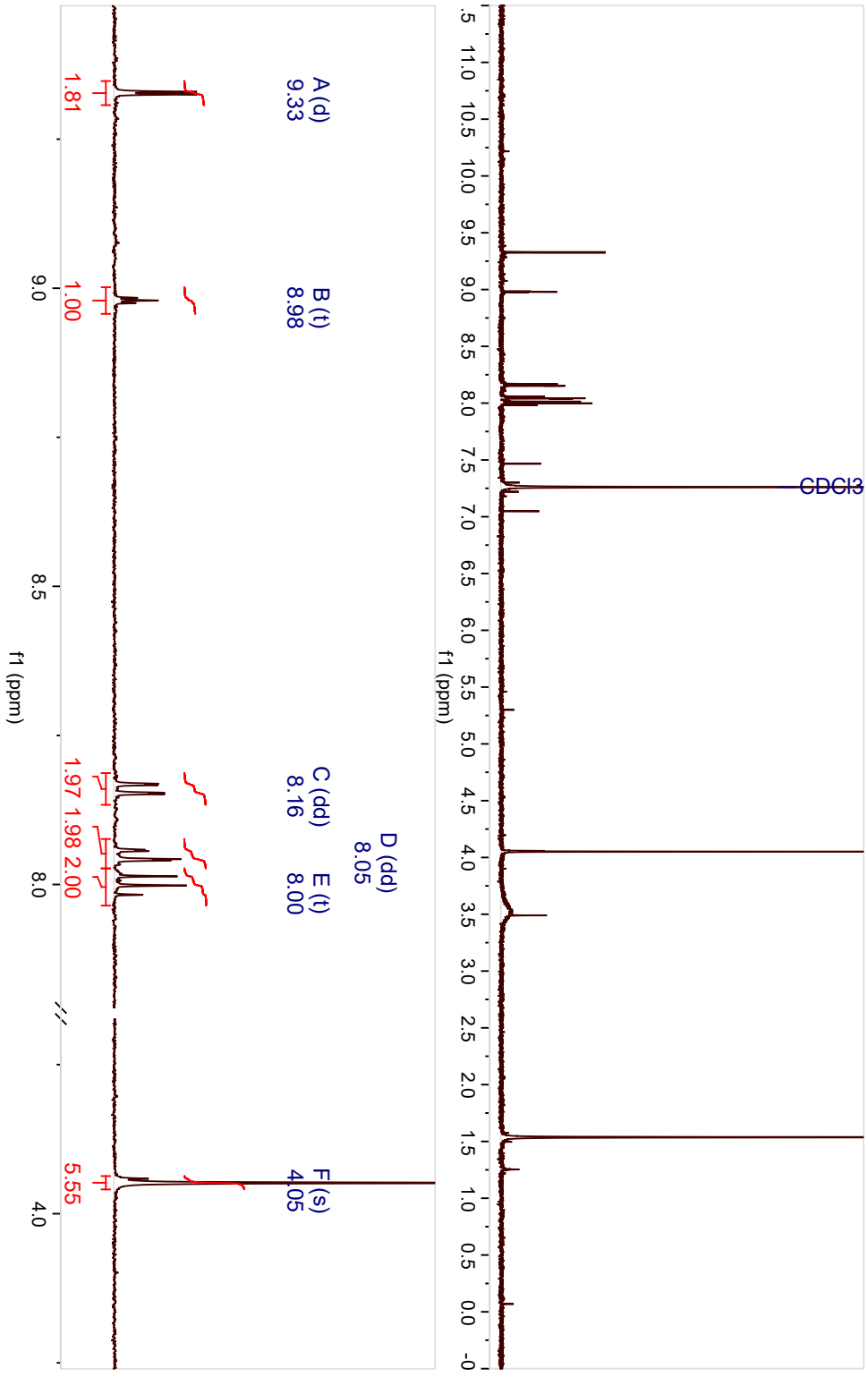
dimethyl [2,3':5',2''-terpyridine]-6,6''-dicarboxylate



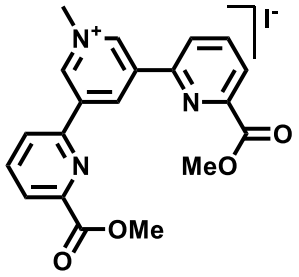
A methanol solution (15 mL) of [2,3':5',2''-terpyridine]-6,6''-dicarbaldehyde (1.1035 g, 3.8145 mmol), N-bromosuccinimide (2.7503 g, 15.451 mmol), and pyridine (0.3498 g, 4.422 mmol) was prepared. The reaction mixture was heated and stirred at 50°C for 23 h, after which it was allowed to cool to room temperature and the solvent removed by rotary evaporation. The brown-red crude residue was resuspended in deionized water (100 mL) and adjusted to pH 7 by the addition of saturated $NaHCO_3$ (aq). (20 mL). Dichloromethane (50 mL) was added to the aqueous solution, organic layer was extracted, and the aqueous layer extracted additionally with dichloromethane (2 x 60 mL). The united organic fractions were washed with deionized water (120 mL), brine (60 mL), and dried over anhydrous $MgSO_4$. Solvent was removed by rotary evaporation to an inhomogeneous brown powder, from which the product was obtained by recrystallation in $CHCl_3$ and hexanes (0.6615 g, 1.894 mmol, 50%).

^{1}H NMR (499.94 MHz, CD_3Cl) δ 9.33 (d, J = 2.2 Hz, 2H), 8.98 (t, J = 2.2 Hz, 1H), 8.16 (dd, J = 7.5, 1.2 Hz, 2H), 8.05 (dd, J = 7.9, 1.2 Hz, 2H), 8.00 (t, J = 7.7 Hz, 2H), 4.05 (s, 6H).

^{1}H NMR, CD_3Cl


CDCl3
f1 (ppm)
A (d) 9.33
B (t) 8.98
C (dd) 8.16
D (dd) 8.05
E (t) 8.00
F (s) 4.05
1.81
1.00
1.97
1.98
2.00
5.55

6,6''-bis(methoxycarbonyl)-1'-methyl-[2,3':5',2''-terpyridin]-1'-ium iodide



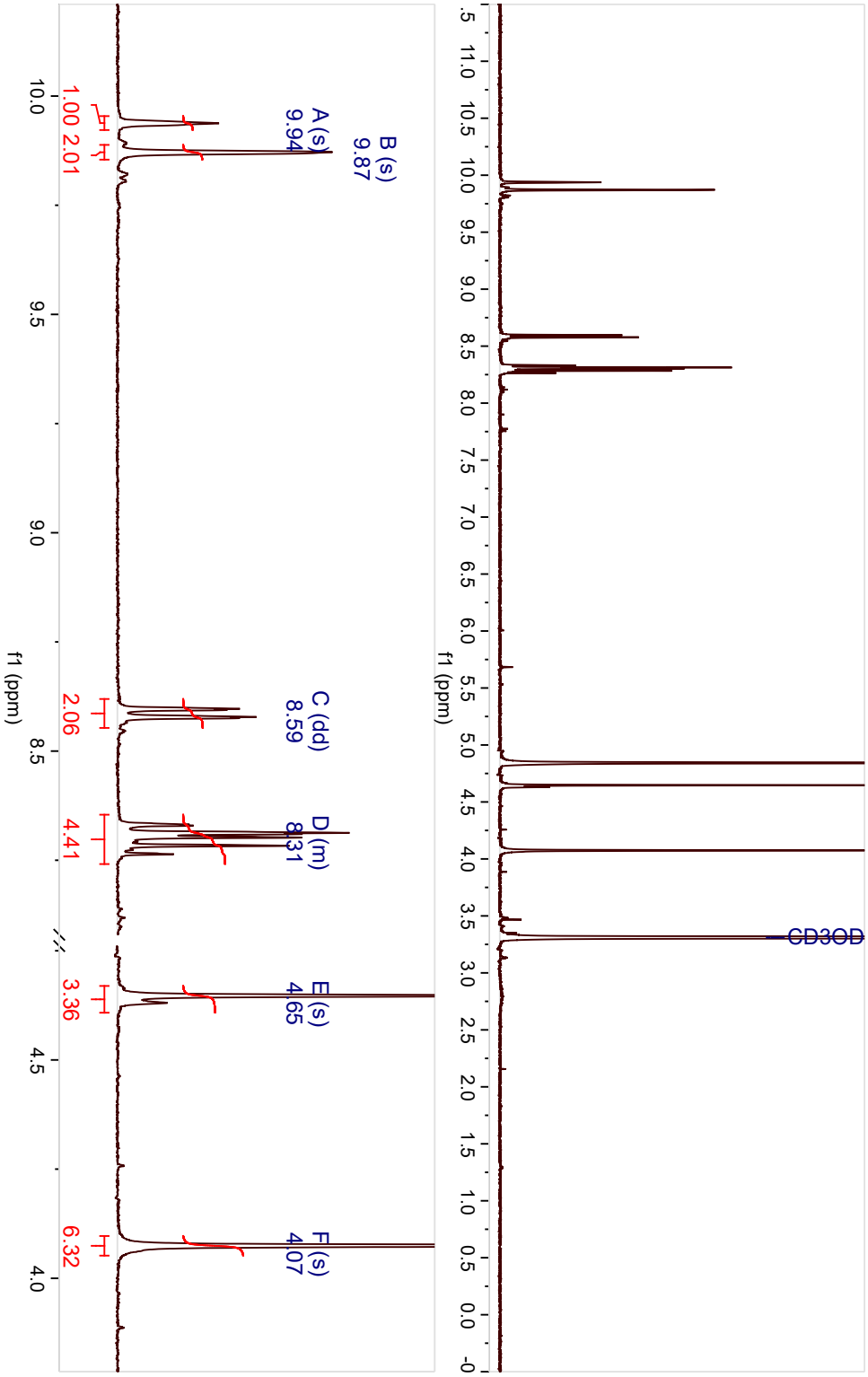
A chloroform (4 mL) suspension of dimethyl [2,3':5',2''-terpyridine]-6,6''-dicarboxylate (0.4045 g, 1.158 mmol) was combined with excess methyl iodide (0.11 mL, 1.5 equiv.) and heated at 61°C for 46 hours. After cooling, a yellowish solid was observed deposited in the dark brown solution. The solvent was removed by rotary evaporation, and the solids resuspended in acetone (4 mL). The crude product was filtered and washed with acetone (2 x 2 mL) and dried in vacuo to obtain light brown powder (0.4648 g, 0.9461 mmol, 82%).

^{1}H NMR (399.75 MHz, CD_3OD) δ 9.94 (s, 1H), 9.87 (s, 2H), 8.59 (dd, J = 7.5, 1.1 Hz, 2H), 8.35 – 8.24 (m, 4H), 4.65 (s, 3H), 4.07 (s, 6H).

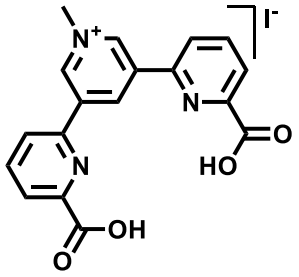
CHN calc'd for $C_{20}H_{18}IN_3O_4$: C, 48.90; H, 3.69; N, 8.55.

CHN found: C, 48.25; H, 4.16; N, 8.48.

^{1}H NMR, CD_3OD


CD3OD
f1 (ppm)
A (s) 9.94
B (s) 9.87
C (dd) 8.59
D (m) 8.31
E (s) 4.65
F (s) 4.07
1.00
2.01
2.06
4.41
3.36
6.32

6''-carboxy-1'-methyl-[2,3':5',2''-terpyridin]-1'-ium-6-carboxylate



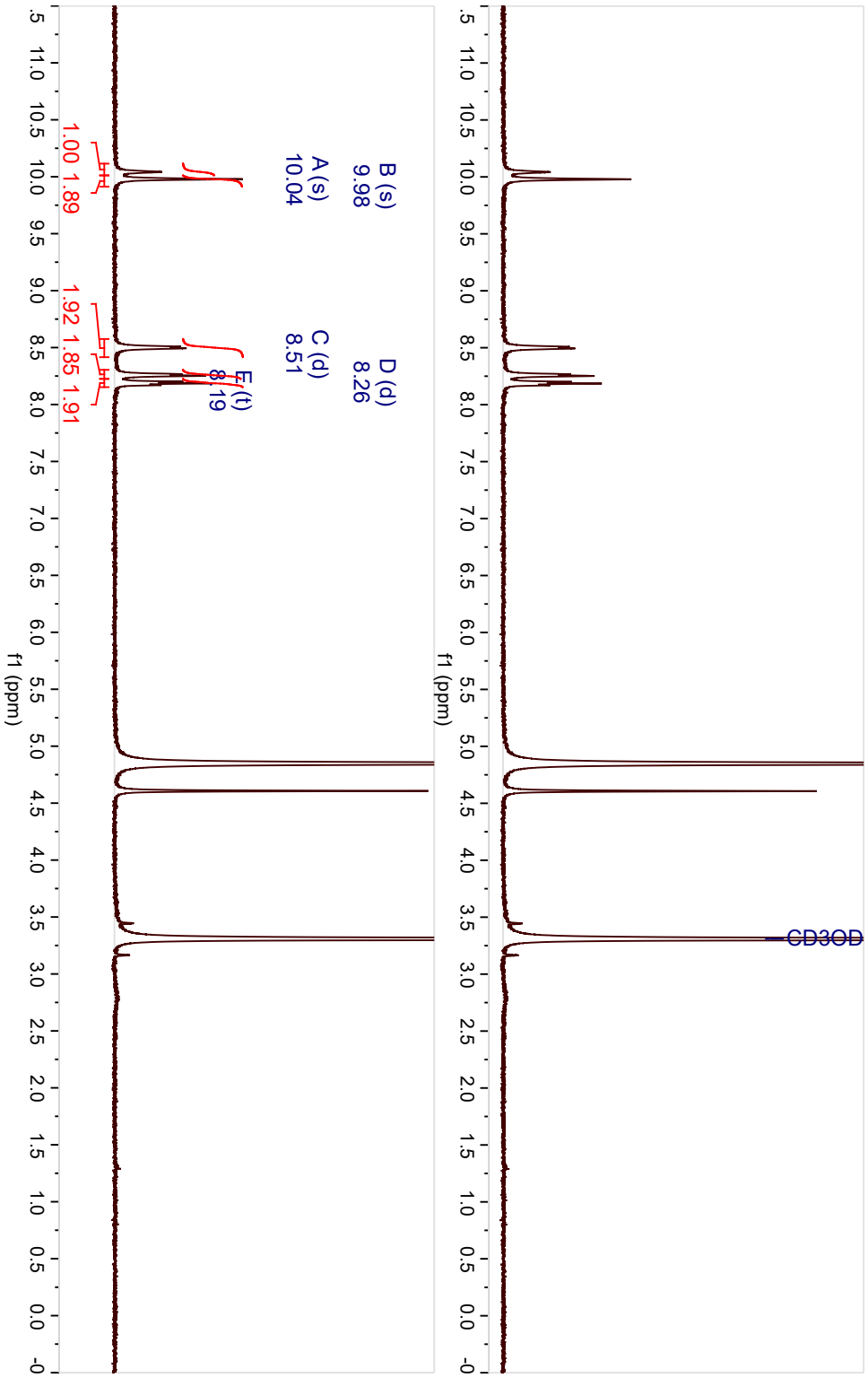
A reaction vessel was charged with 6,6''-bis(methoxycarbonyl)-1'-methyl-[2,3':5',2''-terpyridin]-1'-ium iodide (0.4583 g, 0.9327 mmol) and aqueous hydrochloric acid (6 M, 7 mL). The slurry was stirred and heated at 45°C for 35 h, after which the crude mixture was concentrated to yellow-red solids by rotary evaporation. The residue was resuspended in a mixture of equal portions water and methanol (20 mL), filtered, and washed with small portions of deionized water until the mother liquor became clear (Yield 0.1259 g, 0.2717 mmol, 29.1%)

^{1}H NMR (499.95 MHz, CD_3OD) δ 10.04 (s, 1H), 9.98 (s, 2H), 8.51 (d, J = 7.8 Hz, 2H), 8.26 (d, J = 7.7 Hz, 2H), 8.19 (t, J = 7.7 Hz, 2H).

CHN calc'd for $C_{18}H_{13}N_3O_4 + 6H_2O$: C, 48.76; H, 5.68; N, 9.48.

CHN found: C, 48.99; H, 4.48; N, 9.51.

^{1}H NMR, CD_3OD


CD3OD
f1 (ppm)
B (s)
9.98
A (s)
10.04
D (d)
8.26
C (d)
8.51
E (t)
8.19
1.00 1.89
1.92 1.85 1.91

1.4.2. Electronic Structure of Ru(OC^{R})

UV-visible spectroscopic observations were carried out in acetonitrile and aqueous solution to obtain insight into the electronic structure of **Ru(OC^{R})**. Stock solutions used for this purpose were stored in air, and additional spectroscopic observations were made over several days. This was done to identify spectral changes, which could serve as an indication of the complexes' stability in air.

Table 2. UV-visible spectroscopy of **Ru(OC^{R})** with comparison to related literature complexes. The solutions at pH = 1 and 7 were prepared from unbuffered Millipore water and 0.1 M HNO_3 (aq), respectively.

entry	Ru	conds.	λ_{max} (log(ε))
1	$[Ru^{II}(Me)]^+$	CH_3CN	276 (4.27), 312 (4.41), 390 (3.94), 483 (3.67), 528 (3.66)
2	$[Ru^{II}(Ad)]^+$	CH_3CN	276 (4.30), 311 (4.45), 393 (4.11), 488 (3.83), 530 (3.83)
3	$[Ru^{II}(Ar)]^+$	CH_3CN	276 (4.33), 310 (4.46), 400 (4.11), 481 (3.89), 522 (3.89)
4	$[Ru^{II}(Me)]^+$	pH = 7	276 (4.27), 313 (4.40), 385 (3.85), 528 (3.71)
5	$[Ru^{II}(Ad)]^+$	pH = 7	276 (4.26), 313 (4.42), 387 (4.00), 531 (3.84)
6	$[Ru^{II}(Ar)]^+$	pH = 7	275 (4.22), 312 (4.39), 395 (3.93), 524 (3.84)
7	$[Ru^{II}(Me)]^+$	pH = 1	276 (4.31), 313 (4.37), 383 (3.87), 524 (3.73)
8	$[Ru^{II}(Ad)]^+$	pH = 1	276 (4.30), 313 (4.39), 384 (3.96), 526 (3.80)
9	$[Ru^{II}(Ar)]^+$	pH = 1	275 (4.29), 312 (4.39), 393 (3.96), 519 (3.87)
11[22]	*cis*-$[Ru^{II}(tpy)(pic)(OH_2)]^+$	pH = 7	477 (3.80)
12[22]	*cis*-$[Ru^{II}(tpy)(pic)(Cl)]$	CH_3CN	519 (3.56), 389 (3.69)
13[22]	*cis*-$[[Ru^{III}(tpy)(pic)]_2O]^{2+}$	CH_3CN	698 (4.21)
14[24]	$Ru(bpy)_2$(4-rNHC(bpy))	CH_3CN	341 (4.11), 379 (3.98), 452 (4.13), 479 (sh),
15[24]	$Ru(bpy)_2$(3-rNHC(bpy))	CH_3CN	344 (3.93), 378 (sh), 431 (sh), 490 (3.70)
16[24]	$[Ru(bpy)_3]^{2+}$	CH_3CN	323 (sh), 356 (sh), 423 (sh), 451 (4.18)

In acetonitrile, UV-visible spectra of each **Ru(OC^{R})** complex exhibited intense absorptions at about 280, 300, and 400 nm, with a broad feature centered on 500 nm that were resolvable as two peaks. The **Ru(OC^{R})** peaks at 481-488 nm lies in between the 470 nm and 490 nm peaks reported for the 4-**NC** and 3-**NC** complexes, respectively (**Table** , entries 14 and 16). The former relationship is expected because both complexes bear a carbene at the *para* position of a 6-membered ring and the carboxylate of **OC^{R}** is a better donor than pyridine on 4-**NC**. Interestingly, the carbene at the less stable, *meta* position of 3-**NC** appear to exhibit a bathochromic shift (relative to 4-**NC**) of a magnitude like that seen between **OC^{R}** and 4-**NC**. Compared to the 451 nm shift of the **NN** compound **16**, the each carbene complex exhibit significant bathochromic shift due to destabilization of the metal t_{2g} orbital from the greater σ-character of the metal carbon bond.[24] This effect is also seen in aqueous

solutions at pH 7, where the **Ru(OC^{R})** at 524-531 nm. These wavelengths are bathochromic compared to the 477 nm peak of ON analogue **11** (**Figure 20**), consistent with the increase in donor ability of the carbene.

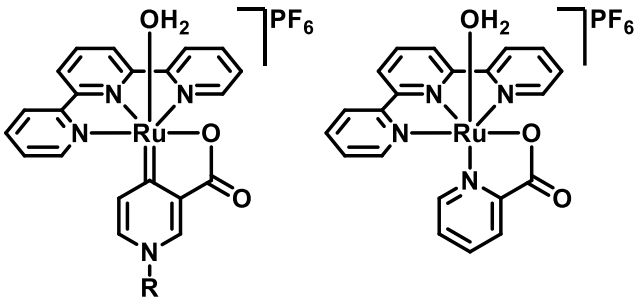


Figure 20. ON analogue[22] of **Ru(OC^{R})**

TDDFT has been commonly used to assist the interpretation of UV-visible spectra of Ru(tpy) complexes.[37–39] TDDFT calculations were performed using the M06[40] hybrid functional using geometries of **Ru(OC^{R})** optimized at the B3LYP/cc-pVDZ level (**Figure 21**, bottom). The simulated spectra of **Ru(OC^{R})** in acetonitrile were a good fit with the experimental, and excitation bands corresponding to all 5 peaks in the experimental spectra were present, although the present level of theory gave an overestimation of the energies.

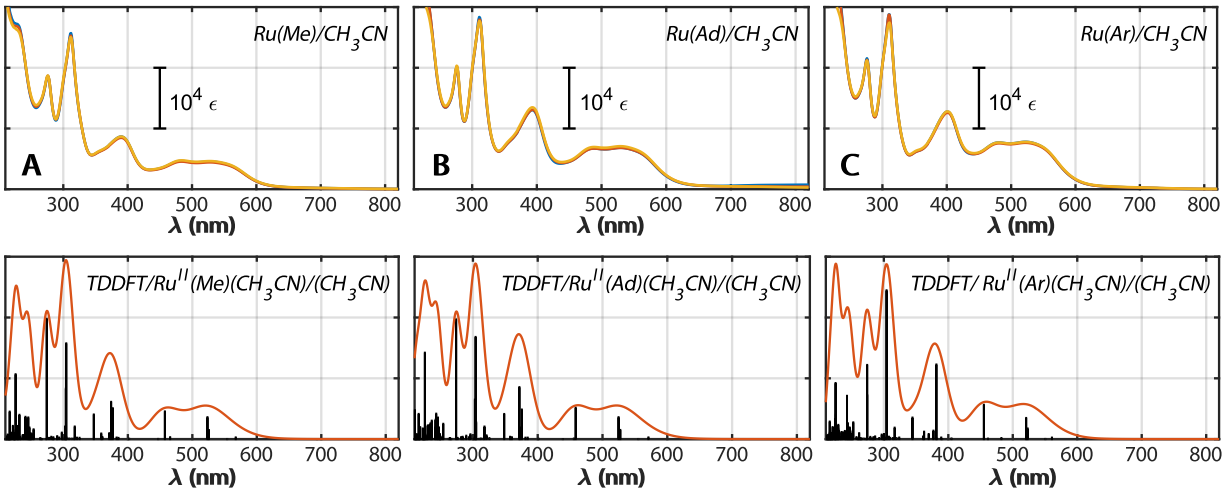


Figure 21. Top: UV-visible spectra of 1×10^{4} M **Ru(OC^{Me})**, **Ru(OC^{Ad})**, and **Ru(OC^{Ar})** (A, B, C, respectively) in acetonitrile at 0, 1, and 8 days. Bottom: simulated UV visible spectra

All three **Ru(OC^{R})** complexes appear air-stable in acetonitrile solution, as no spectral changes were seen for the complexes over the course of the 8 day observation period (**Figure 21**). After 18 days, a mass spectrum was

obtained for each sample to confirm this result. The mass spectra of the samples revealed relatively clean baselines and molecular ions consistent with [**Ru^{II}(OC^{R})**]$^{+}$ lacking the CH_3CN or H_2O ligand were observed at m/z 471.0363, 591.1336, and 561.0857, which correspond to the exact masses of **Ru(OC^{Me})**, **Ru(OC^{Ad})**, and **Ru(OC^{Ar})**, respectively (see 1.6.2.1 for spectra).

1.4.3. Formation of Ru(OC^{R}) Dimer at pH = 7

In aqueous solutions, **Ru(OC^{R})** appear to undergo pH-dependent changes over time. At pH 7, the UV-visible spectra of **Ru(OC^{R})** show the appearance of a broad new peak centered at about 830 nm, alongside a decrease in the intensity of peaks above 350 nm (**Figure 22**, top row). This transformation was likely due to oxidation of Ru^{II} to Ru^{III} in air. To confirm the oxidation hypothesis of **Ru(OC^{R})**, the 9-day old samples were treated with ascorbic acid (AA). Ascorbic acid is a chemical reductant that has been used to revert the oxidized forms of transition metal catalysts, in order to prove that the identity of the complex was not changed by the oxidation.[16,41] The addition of 1 equivalent of AA to **Ru(OC^{R})** samples resulted in the disappearance of the 830 nm peak and spectral profiles that closely resemble the initial spectra taken of **Ru(OC^{R})** (**Figure 22**, B, D, F). No further changes were seen upon the addition of excess AA to the samples. These results suggest that at neutral pH, **Ru(OC^{R})** undergoes reversible oxidation in the presence of air.

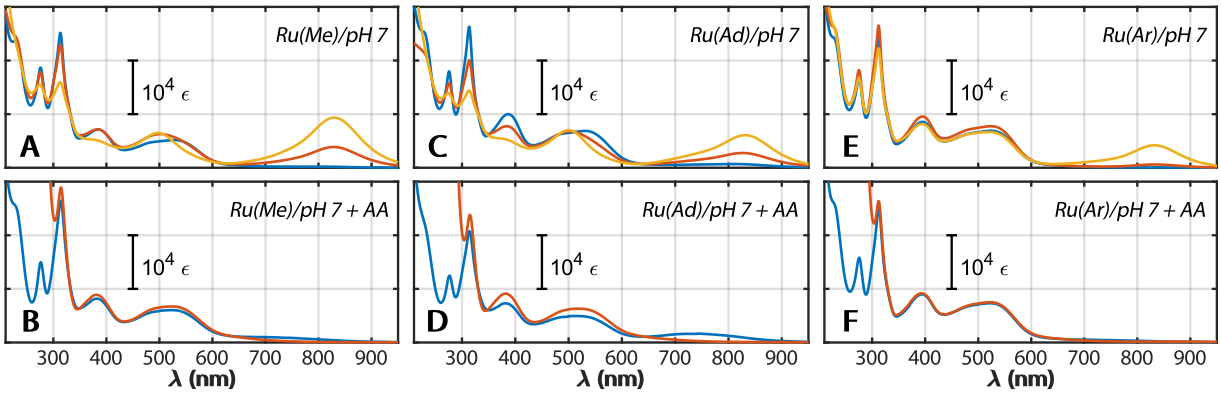


Figure 22. Top row: UV-visible spectra of 1 × 10^{4} M **Ru(OC^{Me})**, **Ru(OC^{Ad})**, and **Ru(OC^{Ar})** (A, C, E, respectively) in water taken at 0, 1, and 8 days. Bottom row: after adding 1 equivalent (blue) and excess (orange) ascorbic acid (aq).

We believe the identity of the oxidized species giving off the signal at 830 nm to be indicative of the formation of a [Ru^{III}-O-Ru^{III}]$^{2+}$ dimer, a behavior which is known to occur for the **ON** analogue reported by Llobet et al[22] (Figure 20, see also entry **13** in **Table**). Although the 830 nm peak of the tentative **Ru(OC^{R})** dimer occurs at

much longer wavelengths, such a bathochromic shift can be expected for a carbene relative to pyridine, as discussed previously.

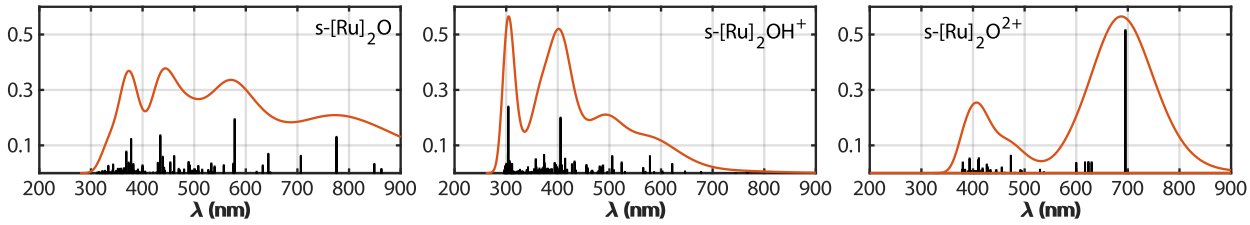


Figure 23. Predicted spectra for μ-oxo bridged **Ru(Ad)** dimers. The 's' prefix means the multiplicity was set to 1 for the TDDFT calculation.

Further support for a $[Ru^{III}\text{-}O\text{-}Ru^{III}]^{2+}$ dimer formation was obtained from TDDFT calculations of μ-oxo bridged **Ru(OC^{Ad})** dimers (**Figure 23**, at right). The predicted spectra of $[Ru^{III}\text{-}O\text{-}Ru^{III}]^{2+}$ showed a characteristic, intense excitation at about 700 nm, while the spectra of other candidates such as $[Ru^{II}\text{-}O\text{-}Ru^{II}]$ and $[Ru^{II}\text{-}[HO]\text{-}Ru^{II}]^{+}$ did not (see 1.6.3 for other examples). The higher energy of the predicted excitation can be expected since the computational methods used for our TDDFT calculations tend to give higher energy values for terpyridine ruthenium complexes.[42]

While all three complexes appeared to undergo dimerization, **Ru(OC^{Ar})** appeared to be most stable. To demonstrate this, **Ru(OC^{R})** solutions taken from the same stock as the previous experiments were treated with 1.1 equivalents of AA, and time-dependent spectral profiles were obtained (**Figure 24**). Each complex exhibited decreasing absorbance at about 385 nm (390 nm for **Ru(OC^{Ar})** in the first 0-4 hours. Over the course of 150 hours, the profiles of **Ru(OC^{Me})** and **Ru(OC^{Ad})** diverged from **Ru(OC^{Ar})**. The spectra of the methyl and adamantyl complexes exhibit significant change, while the spectra of **Ru(OC^{Ar})** remained relatively constant (**Figure 24**).

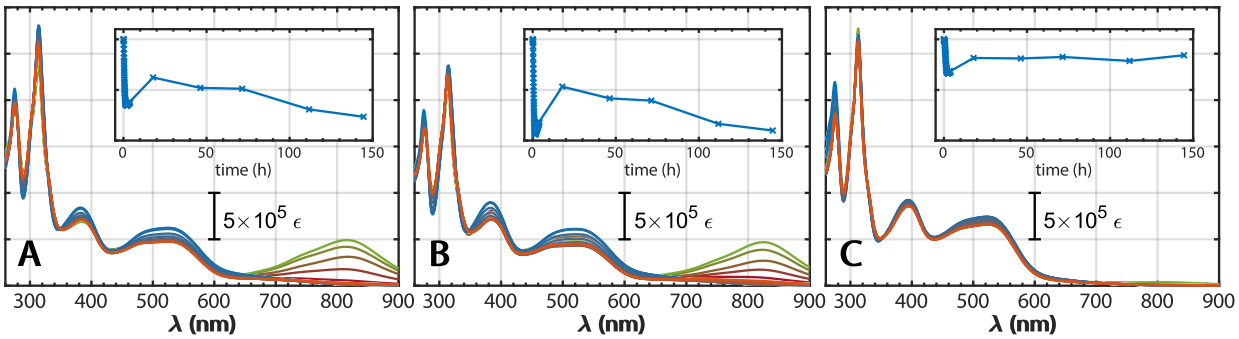


Figure 24. Time-dependent UV-visible spectra 5×10^5 M **Ru(OC^{Me})**, **Ru(OC^{Ad})**, and **Ru(OC^{Ar})** (A, B, C, respectively) after addition of 1.1 equivalents of freshly prepared ascorbic acid. Inset: spectral changes at 385 nm (390 nm for **Ru(OC^{Ar})**) observed over 150 hours in absorbance units.

High accuracy mass spectroscopy was used in attempt to identify the species corresponding to the 830 nm feature. Ruthenium complexes can be easily distinguished from background peaks due to a characteristic isotopic distribution with prominent peaks clusters at m/z values of 98 - 101 and 104 appearing at 40-60% relative abundance compared to the main ^{102}Ru peak. After 18 days of storage in air, aliquots from a pH = 7 aqueous solution of **Ru(OC^{R})** were injected into a QTOF mass spectrometer (**Figure 25**, top row). Then, a second aliquot was taken, treated with AA, and also injected (**Figure 25**, bottom row).

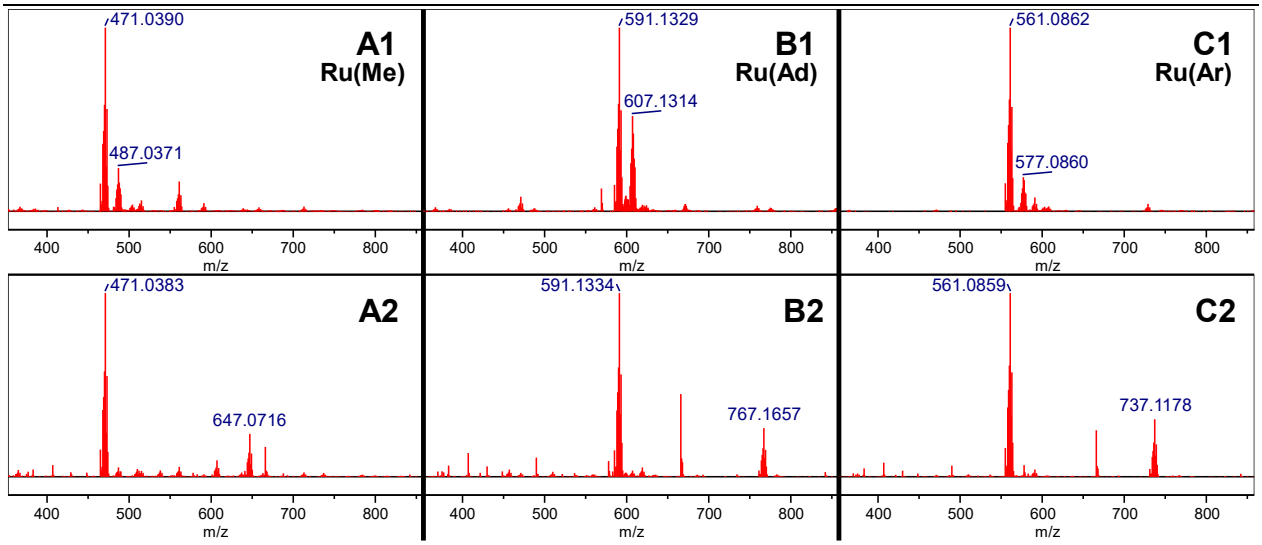


Figure 25. Mass spectra of 1×10^{-4} M **Ru(OC^{R})** samples prepared in unbuffered water (top), and after adding excess (solid) ascorbic acid (bottom).

The mass spectra of the samples not treated with AA revealed peaks consistent with the molecular ion (M^+) of **Ru(OC^{R})** and $[M + O]^+$ (**Figure 25,** top row). On the other hand, aliquots with AA showed only M^+ and a $[M + AA]^+$ peak (**Figure 25**, bottom row). Interestingly, peaks were not seen at the m/z values expected for a dimeric

species, which would appear as a $[M_2 + O]^{2+}$ peak for a $[Ru^{III}\text{-}O\text{-}Ru^{III}]^{2+}$ species (see 1.6.2 for expanded spectra). These observations were consistent across all three **Ru(OC^R)** complexes.

The lack of an observed $[M_2 + O]^{2+}$ cation can be explained if a $[Ru^{III}\text{-}O\text{-}Ru^{III}]^{2+}$ dimer was to undergo disproportionation upon ionization inside the mass spectrometer (**Figure 26**). Breaking the μ-oxo bridge on a $[Ru^{III}\text{-}O\text{-}Ru^{III}]^{2+}$ to yield $[Ru^{IV}\text{-}O]^{+}$ and $[Ru^{II}]^{+}$ species corresponding to the M^{+} and $[M + O]^{+}$ cations that were in fact observed in the mass spectra of **Ru(OC^R)** aliquots not treated with AA (**Figure 26**, A). On the other hand, if $[Ru^{III}\text{-}O\text{-}Ru^{III}]^{2+}$ is chemically reduced by AA to $[Ru^{II}]^{+}$ prior to entering the mass spectrometer, only a M^{+} peak would be seen.

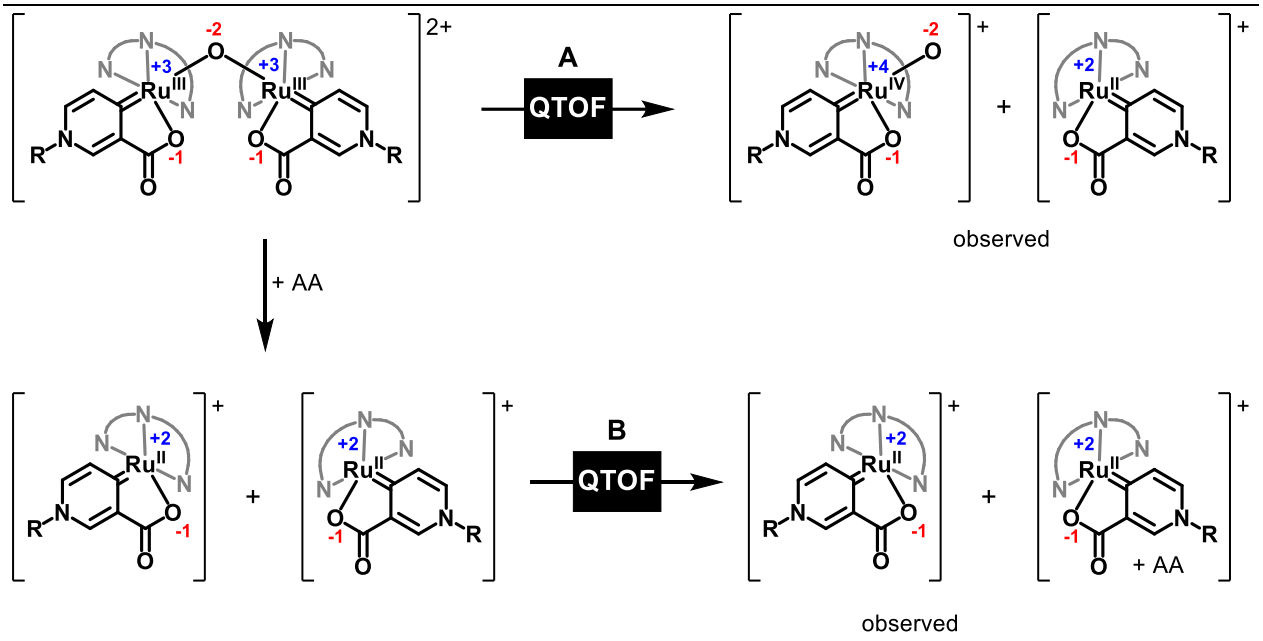


Figure 26. Possible scenaria for disproportionation of $[Ru^{III}\text{-}O\text{-}Ru^{III}]^{2+}$. **A**: dimer enters "black box" of QTOF-MS instrument and ionizes into the observed peaks for $[Ru^{II}]^{+}$ and $[Ru^{IV} + O]^{+}$. **B**. chemical reduction of sample generates monomeric $[Ru^{II}]^{+}$ prior to measurement.

1.4.4. Redox chemistry of Ru(OC^R) at pH = 1

A popular and relatively easy method for screening coordination complexes for water oxidation activity by using a sacrificial oxidant such as ceric ammonium nitrate (CAN) to provide the oxidation potentials needed for water oxidation[43]. This is a reaction that is typically carried out at acidic pH values due to the instability of CAN at high pH.[44] We wished to characterize the stability of **Ru(OC^R)** under acidic conditions, in this case, in aqueous HNO_3 (aq), since a catalyst is no good if it is unstable under chemical conditions used for catalysis.

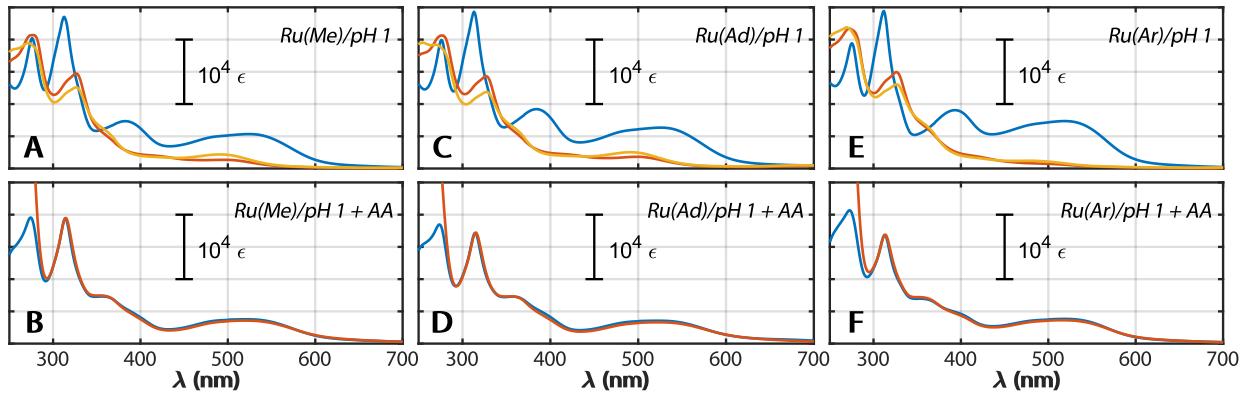


Figure 27. Top row: UV-visible spectra of **Ru(OC^{Me})**, **Ru(OC^{Ad})**, and **Ru(OC^{Ar})** (A, C, E, respectively) in 0.1 M HNO_3 (aq) taken at 0, 1, and 8 days. Concentration of complexes. Bottom row: after adding 1 equivalent (blue) and excess (orange) ascorbic acid (aq).

In 0.1 M HNO_3, samples of **Ru(OC^{R})** at pH = 1 turned colorless over time, and the UV-vis spectra of the likewise show a bleaching of major MLCTs (**Figure 27**, top row). An attempt was made to chemically reverse this using ascorbic acid (AA) as a reductant, however, the addition of ascorbic acid to 10 days-old samples resulted in only a partial return of the original spectral features of **Ru^{II}(OC^{R})** (**Figure 27**, bottom row).

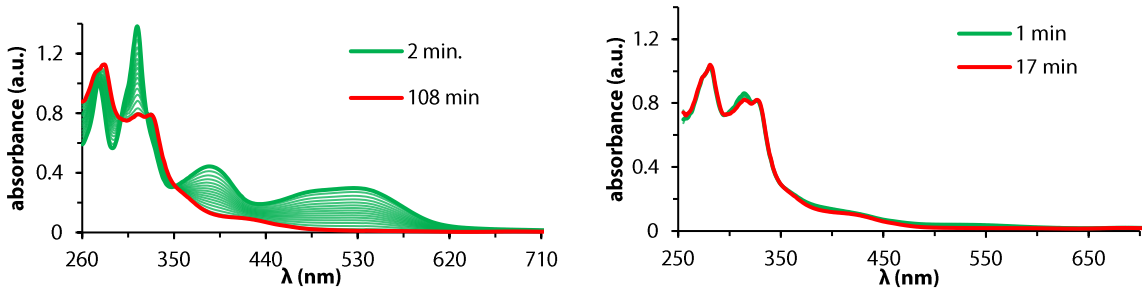


Figure 28. UV-visible spectra of **Ru(OC^{Ad})**. At left: 1×10^{-4} M, 0.1 M HNO_3(aq). Δt = 4min; at right: 2.5×10^{-5} M, 0.1 M HNO_3(aq), 1eq CAN. Δt=6 min.

Freshly prepared samples of **Ru(OC^{Ad})** were treated with 1 equivalent of CAN to oxidize Ru^{II} to Ru^{III}. This resulted in UV-visible changes almost identical to that which occurs for samples simply exposed to aerial oxygen, albeit over a much shorter timeframe (**Figure 28**). To test whether the observed MLCT bleaching was occurring as a result of pH or the nitrate ion, time-dependent spectral profiles were acquired for freshly prepared samples of **Ru(OC^{Ar})** in aqueous solutions of either HNO_3 or KNO_3. Bleaching occurred in the presence of HNO_3 (aq), but not M KNO_3 or control samples (**Figure 29**). Moreover, the bleaching occurred faster in 0.1 than 0.05 M HNO_3 (aq) samples, suggesting a pH dependence.

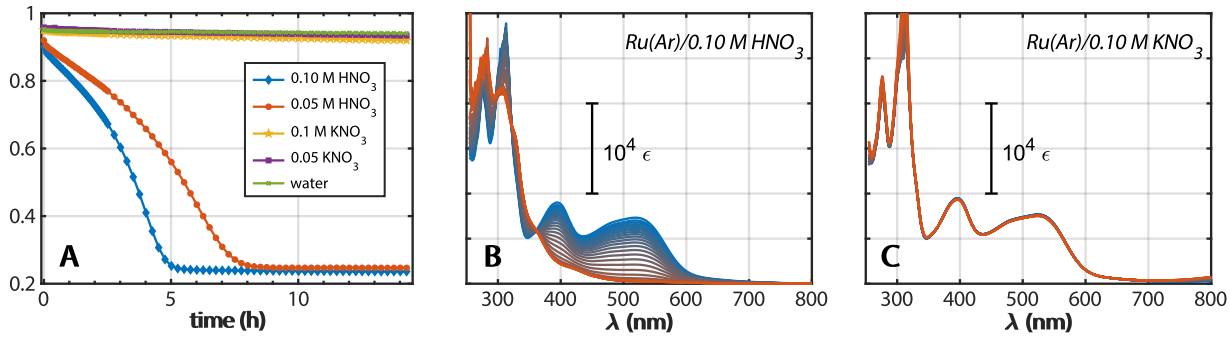


Figure 29. Spectral changes observed for 1×10^{-4} M **Ru(OC^{Ar})** in the presence of HNO_3 and KNO_3. (A) plot of absorbance changes at 395 nm. Spectral changes observed over 5 h for (B) 0.1 M HNO_3 (aq) and (C) 0.1 M KNO_3 (aq).

These results suggest that under acidic conditions, **Ru(OC^{R})** undergoes oxidation from Ru^{II} to Ru^{III}, an interpretation supported by the simulated spectra for **Ru^{II}(OC^{R})** and **Ru^{III}(OC^{R})** obtained through TDDFT calculations (**Figure 30**). However, this does not explain why AA seems unable to reverse this oxidation, especially since electrochemical data indicates that the $Ru^{II/III}$ redox couple is *more* reversible at low pH (see 1.4.5).

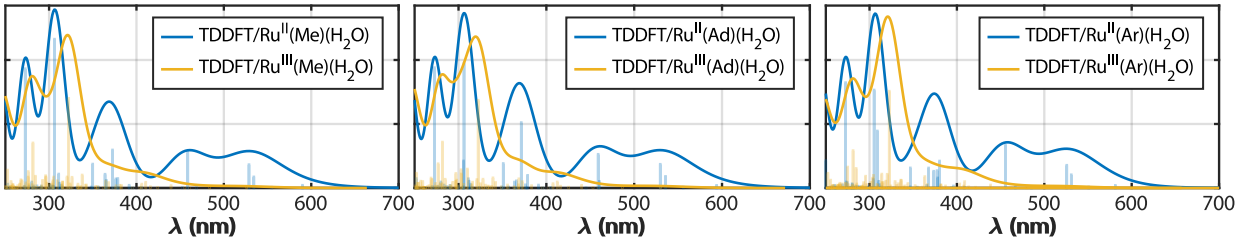


Figure 30. TDDFT simulated spectra of **Ru^{II}(OC^{R})(H$_2$O)** and **Ru^{II}(OC^{R})(H$_2$O)** in water.

QTOF-MS was used to characterize samples of **Ru(OC^{R})** treated and untreated with AA (**Figure 31**, top; see also 1.6.2.3 for expanded spectra) after 18 days of storage in air. The spectra of untreated samples were complex (see 1.6.2.7), and the presence of species with m/z values lower than the M^+ and M^{2+} ions appeared to indicate fragment loss from the 4-pyridylidene ligand. This was notably prominent in the case of **Ru(OC^{Ad})** where the loss of adamantyl group is evidenced by prominent peaks at the m/z values for $[Ad - 1]^+$ and $[Ru(Ad) - (Ad - 1)]^+$, an observation explained by the stability of the adamantyl cation[45,46]. No evidence was seen for the loss of an aryl cation from **Ru(OC^{Ar})** since it would likely occur via a high-energy pathway.

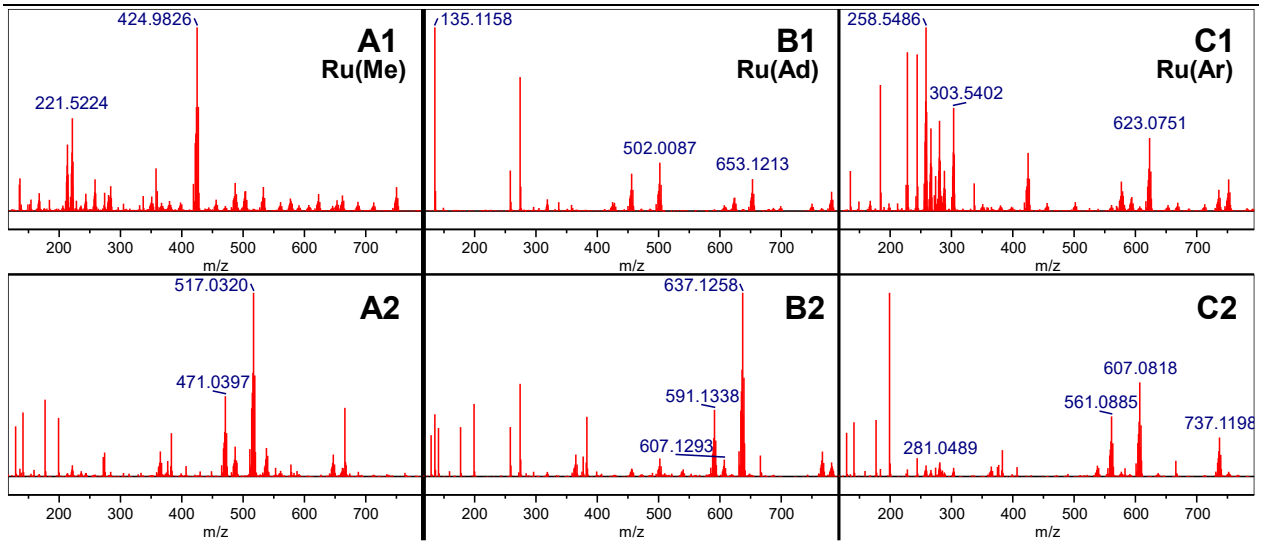


Figure 31. Mass spectra of 1×10^{-4} M **Ru(R)** samples prepared in 0.1 M HNO_3 (aq) (top), and after adding excess (solid) ascorbic acid (bottom). Note the absence of masses lower than M^+ or M^{2+} in samples treated with AA; the M^+ and $M^+ + NO_2$ peak is seen.

Surprisingly, spectra of samples treated with AA cleaned up to give M^+ and $[M + NO_2]^+$ peaks (**Figure 31**, top). Notably, peaks from the untreated samples suggestive of possible decarboxylation of the **OC^R** ligand were absent after AA addition. Moreover, while neither M^+ nor M^{2+} cations were seen in the untreated samples, the samples treated with AA showed relatively abundant M^+ and higher mass peaks. This suggests that the treated samples, which originated from the same stock as the untreated samples, consisted largely of intact **Ru(OC^R)** complex. These results suggest that the **OC^R** ligand was not decomposing in solution, but upon ionization within the QTOF mass spectrometer.

Further time-dependent QTOF-MS studies were performed for solutions of **Ru(OC^R)** after the addition of 20 equivalents of ceric ammonium nitrate (CAN) to determine the stability of the complex in the presence of excess oxidant. After these data were acquired, other QTOF-MS experiments conducted by Drs. Grotjahn and Elliott indicated the data may have been affected from contamination generated from injecting relatively large amounts of ruthenium-containing catalysts and CAN from previous runs on the instrument. The spectral data is available in sections 1.6.2.4, 1.6.2.5, and 1.6.2.6 for **Ru(OC^{Me})**, **Ru(OC^{Ad})**, and **Ru(OC^{Ar})**, which showed similar peaks to that seen as discussed above. Further efforts in this area were halted due to the COVID-19 pandemic.

1.4.5. Electrochemistry of Ru(OC^{Ad})

The background-subtracted cyclic voltammagrams of **Ru(OC^{Ad})** at various pH are shown in **Figure 32**. At all pHs, the cathodic sweep revealed a $Ru^{II/III}$ peak and a poorly resolved feature that appeared in the shoulder of the catalytic current at higher potentials. The $Ru^{II/III}$ couple at pH 1 indicated a reversible process and the peak separation (ΔE_p) for the $Ru^{II/III}$ couple was 64 mV, close to the 57 mV Nernestian ideal for a $1e^-$ process.[47]

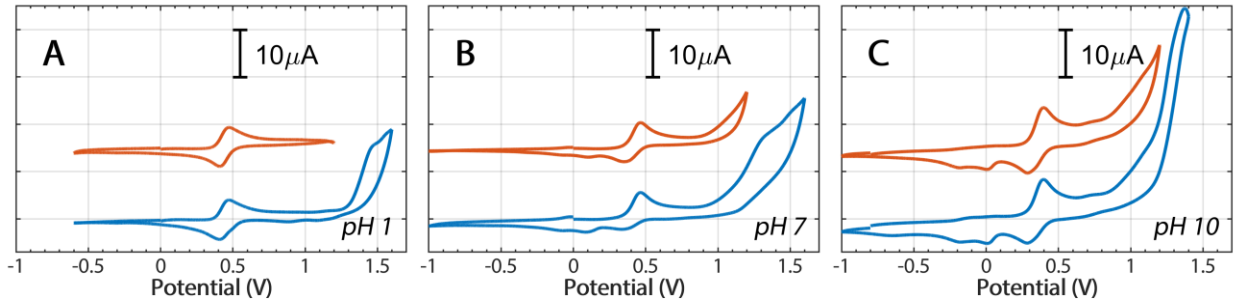


Figure 32. CVs of **Ru(OC^{Ad})**. A: in 0.1 M HNO_3; B: in 0.1 M PO_4^{3-} (pH 7) buffer; C: in 0.1 M CO_3^{2-} buffer

The $Ru^{II/III}$ couple of **Ru(OC^{Ad})** was less reversible at pH 7 and pH 10, appearing to break up into at least two additional peaks on the anodic sweep. The peak separation for the largest peak (presumably Ru^{III} -> Ru^{II}) was 131 and 112 mV, respectively, at pH 7 and 10 (**Table 2**).

Table 2. Electrochemical parameters (Ag/AgCl). Average values from 4, 8, and 6 runs for pH 1, 7, and 10, respectively.

Ru(Ad)	E_p1	E_p2	E_h1	E_h2	$E_{1/2}$	ΔE_p
pH 1	0.473	0.409	0.415	0.469	0.441	0.064
pH 7	0.466	0.335	0.405	0.439	0.401	0.131
pH 10	0.397	0.285	0.333	0.378	0.341	0.112

To verify that the electroactive species is freely diffusing, CVs were acquired at scan rates of 5 to 0.1 V/s (**Figure 33**, **A**/**B**). The plots of i_p vs. the square root of the scanrate (**A1/B1**) and concentration (**A2/B2)** showed a linear relationship, which is consistent with a freely diffusing electroactive species.[48]

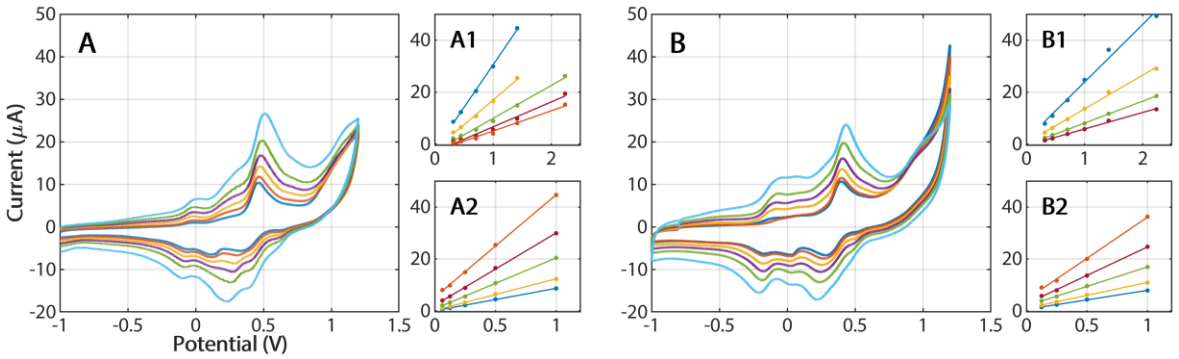


Figure 33. CV of **Ru(Ad)** at scan rates varying from 5 to 0.1 V / s. The uppermost aqua traces **A** and **B** are at 5 V / s and lowest is at 0.1 V / s. **A** is pH 7, **B** is at pH 10. **A1** and **B1** are plots of i_p vs square root of the scan rate, showing linearity indicative of diffusion-limited transfer. **A2** and **B2** show the changes in i_p for the II/III couple as a function of analyte concentration in mM. For details see section 6.2.2.

A Pourbaix (potential vs pH) diagram was constructed from electrochemical measurements of Ru(Ad) from pH 1 to pH 11.5 (**Figure 34**). The II/III couple appears at the same potential between pH 1 and 9, indicating that oxidation occurs without proton loss. However above pH 9, the potential decreases with a slope of -62.5 mV per pH unit, consistent with oxidation by PCET. The significance of the magnitude of the slope is that it is very close to the ideal of 59 mV per pH unit for a loss of x electrons as well as x protons, which is taken as evidence for PCET, and can only mean the presence of a water molecule on **Ru(OC^{Ad})** as the source of the proton. The pK_a of the Ru^{III}-OH_2 species is thus 9, which is much higher than the pKa 3.7 for the pyridine-2-carboxylato analogue reported by Llobet et al.[22] (**Figure 20**). The decreased acidity of the Ru^{III}-OH_2 species may be attributed to the effects of the rNHC ligand trans to the aquo.

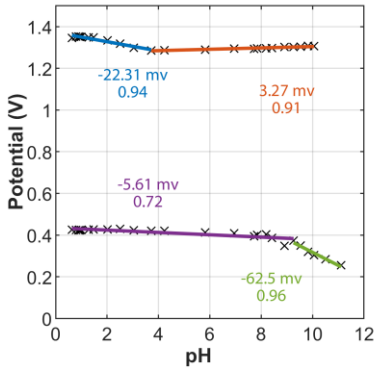


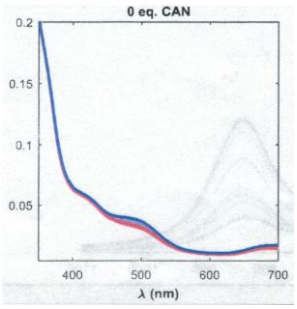
Figure 34. potential vs pH diagram

Electrochemical experiments involving **Ru(OC^{Me})** and **Ru(OC^{Ar})** could not be completed due to the COVID-19 pandemic.

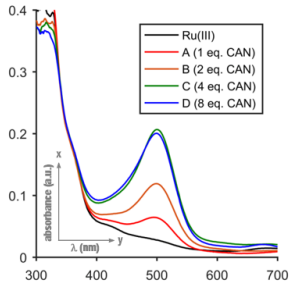
1.4.6. UV-vis redox titrations of Ru(OC^{Ad})

Stoichiometric titrations of ruthenium-based WOCs with a one electron oxidant such as CAN serves as a useful tool for probing the identity of intermediates formed during water oxidation[9,38,39]. A solution of air-oxidized **Ru(OC^{Ad})** was treated with 1, 2, 4, and 8 equivalents of CAN to observe the spectral profiles of high-valent species formed in the process (**Table**).

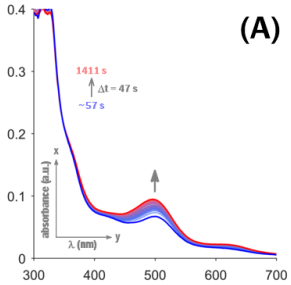
Table 3. Spectra of **Ru(OC^{Ad})** after titration of Ru^{III} with equivalents of CAN in 0.1 M HNO_3 (aq)



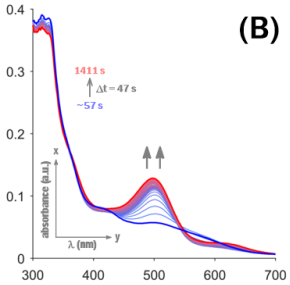
0 equiv.



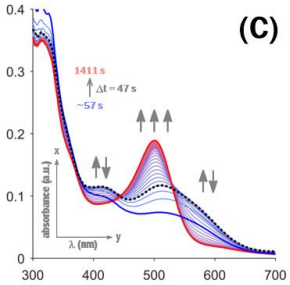
A-E after 24 h.



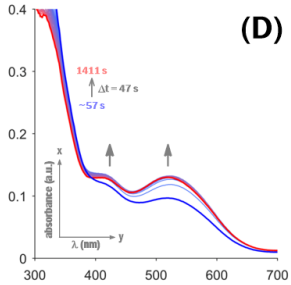
1 equiv.



2 equiv.



4 equiv.



8 equiv.

Titration of **Ru^{III}(OC^{Ad})** (air-oxidized sample denoted by 0 equiv.) with one or two equivalents of CAN results in the appearance of a new peak centered at 500 nm (A, B). At 4 equivalents, two broad features appear at 410 and 510 nm; after about 120 seconds, the peaks disappear and only the 500 nm peak is seen (C). When 8 equivalents of CAN are added, the 410 and 510 nm peaks remain for the duration of the observation period (D). After 24 h, only the 500 nm peak remains, and the absorbance values of the 500 nm peak for the 4 and 8 equiv samples were the same. These observations suggest that **Ru^{III}(OC^{Ad})(H_2O)** undergoes to an unstable species (410 and 510 nm) that decomposes to a longer-lived species (500 nm).

1.4.7. Evaluation of Ru(OC^{R}) for Water Oxidation Catalysis

The activity of a prospective WOC can be measured by injecting solutions of catalyst into sealed reaction cell containing an aqueous solution containing a sacrificial oxidant such as ceric ammonium nitrate.[13,15] The pressure generated within the vessel can be measured, and the amount of O_2 produced by the catalyst can be calculated from the ideal gas law, PV = nRT (although production of other gases such as CO_2 from ligand oxidation requires caution in interpreting the results[49,50]).

Samples of **Ru(OC^{Ad})** and **Ru(OC^{Ar})** were injected . Pressure increases were recorded immediately upon injection. The resolution of the data at early time points poor since the sampling rate of the pressure transducer setup was configured for slower catalysts. Moreover, pressure drops were seen due to the removal of the needle after injection into the reactor cell. We can reasonably conclude based on the shapes of the pressure curves that **Ru(OC^{Ad})** and **Ru(OC^{Ar})** undergo an initial period of rapid O_2 production before plateauing after about 40-100 turnovers. At these turnover numbers, the pressure increase due to injection of the catalyst solution was relatively low (<5 TON), as confirmed by the injection of a blank sample of the same volume as the initial catalyst injection at the end of each run. Due to the COVID-19 pandemic, additional runs could not be performed.

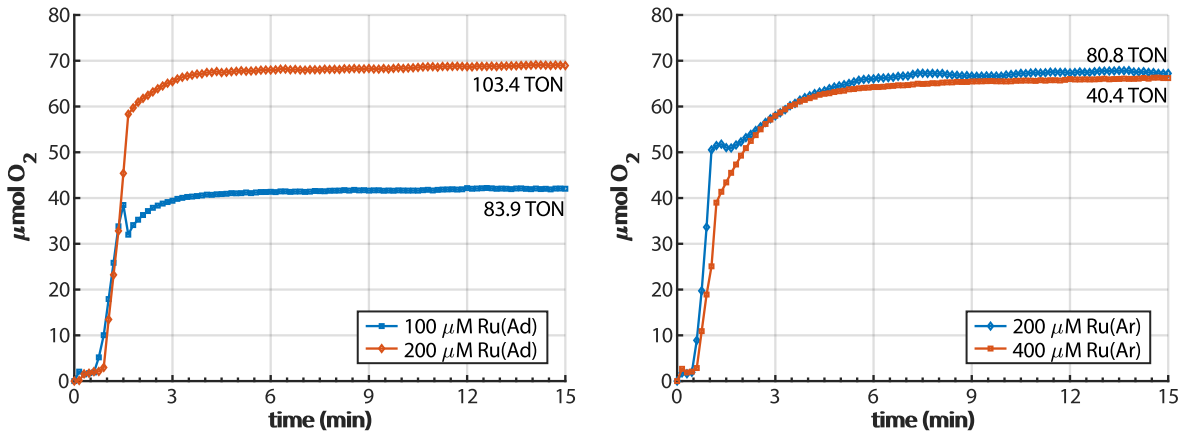


Figure 35. O_2 production using ceric ammonium nitrate (CAN) as a sacrificial oxidant.

1.5. Conclusion/Future work

We have shown that the reaction of $[Cl_2Ru^{II}(tpy)]_2$ with N-alkyl- or N-arylated 3-carboxypyridninium salts produce *para* substituted 4-pyridylidene complexes of ruthenium. Moreover, we have shown that the Zincke reaction can be applied towards deactivated 3-carboxypyridines to install bulky substituents on the quaternary nitrogen atom of the pyridinium ligand precursor. The flexibility of the Zincke reaction allows facile derivatization of the functionality on the quaternary nitrogen, which could enable fine-tuning of the electronic or geometric properties of 4-pyridylidene complexes through modification of their ligand architecture. Thus, we believe our methodology is a step towards expanding the presently underdeveloped areas in pyridylidene chemistry.[25]

The **Ru(OC^{R})** complexes in this work are, to our knowledge, the first 4-pyridylidene complexes of ruthenium to have been shown to be competent water oxidation catalysts. The available evidence suggests that while **Ru(OC^{R})** appears to promote fast WOX, catalytic activity ceases after 40-100 turnovers. Using combined UV-visible and mass spectroscopic methods, we were able to gain insight into the pH-dependent changes to **Ru(OC^{R})** in solution. We have identified possible ligand decomposition pathways via mass spectrometry, although decomposition is not seen if the samples are chemically reduced prior to injection into the spectrometer. The QTOF-MS results suggest that the **OC^{R}** ligand is stable to time and pH, but unfortunately, we are unable to conclude from the spectra for **Ru(OC^{R})** samples treated with excess oxidant as to what changes are occurring at oxidation states higher than Ru^{III}.

The scientific work in this project encountered significant disruptions consequent of the COVID-19 pandemic in 2020. Much future work is needed to characterize the electrochemical properties of **Ru(OC^{Ar})** and **Ru(OC^{Me})**, and to determine optimal reaction conditions for obtaining pressure transducer data during the time in which **Ru(OC^{R})** is actively oxidizing water.

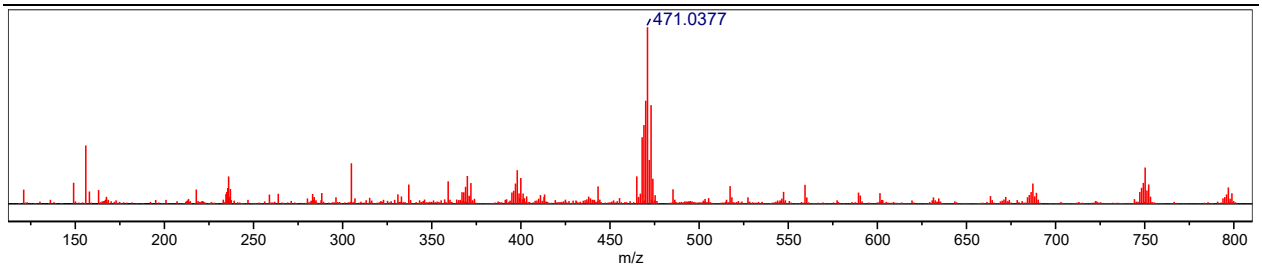
1.6. Appendix 1

1.6.1. Methods

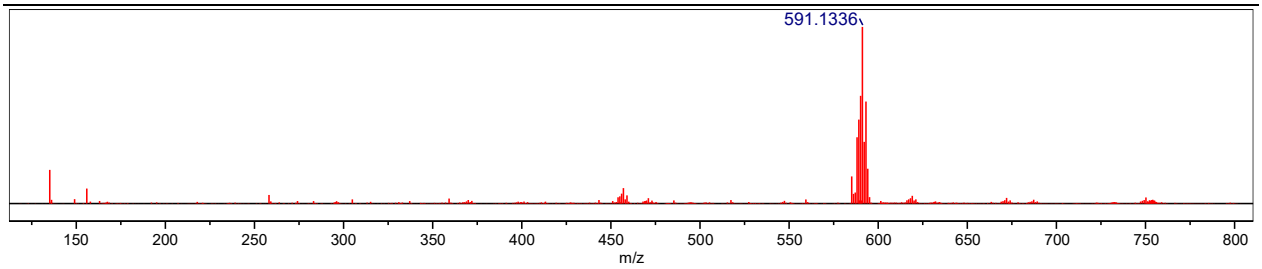
Reagents were purchased from Sigma-Aldrich, ACROS, or Combi-Blocks and used without further purification. NMR solvents purchased from Cambridge Isotopes were used as-is. NMR spectra was obtained from Varian 400 MHz, Bruker 400 MHz, and Varian 500 MHz spectrometers. UV-visible spectroscopy data was obtained using Shimadzu UV-2600 and JASCO V-730 spectrometers. All UV-visible spectroscopic data was acquired at room temperature using single-use PTFE or quartz cuvettes. Electrochemical data was obtained using a CH Instruments 600 or 700 series potentiostat. A glassy carbon working electrode, a Pt wire counter electrode, and Ag/AgCl reference was used for electrochemical experiments, which were performed at room temperature. All electrochemical solutions were deoxygenated with nitrogen or argon gas prior to data collection. DFT calculations were carried out using the Gaussian 09 and Gaussian 16 suite of computational chemistry software on an Intel Linux cluster. The B3LYP method was used with Grimme's D2 empirical dispersion[51] correction and a basis set consisting of Dunning's[52] cc-PVDZ (main group atoms) and Peterson's[53] aug-cc-PVDZ (Ru).

1.6.2. Mass spectra

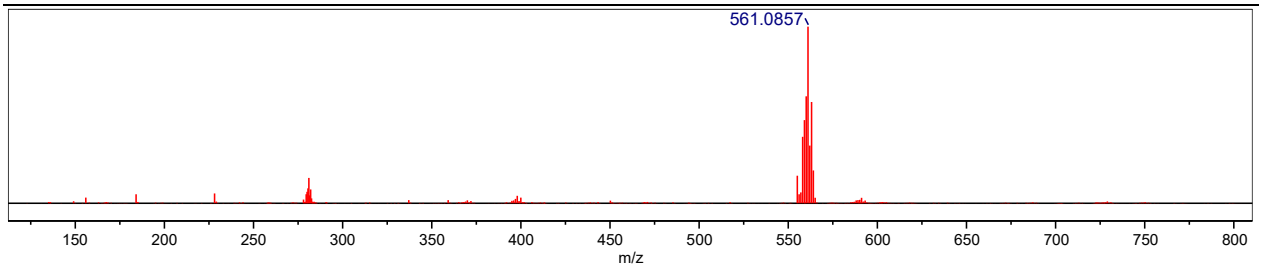
1.6.2.1. Ru(R) in CH_3CN



Ru(Me) in CH_3CN, 18 days after dissolution.

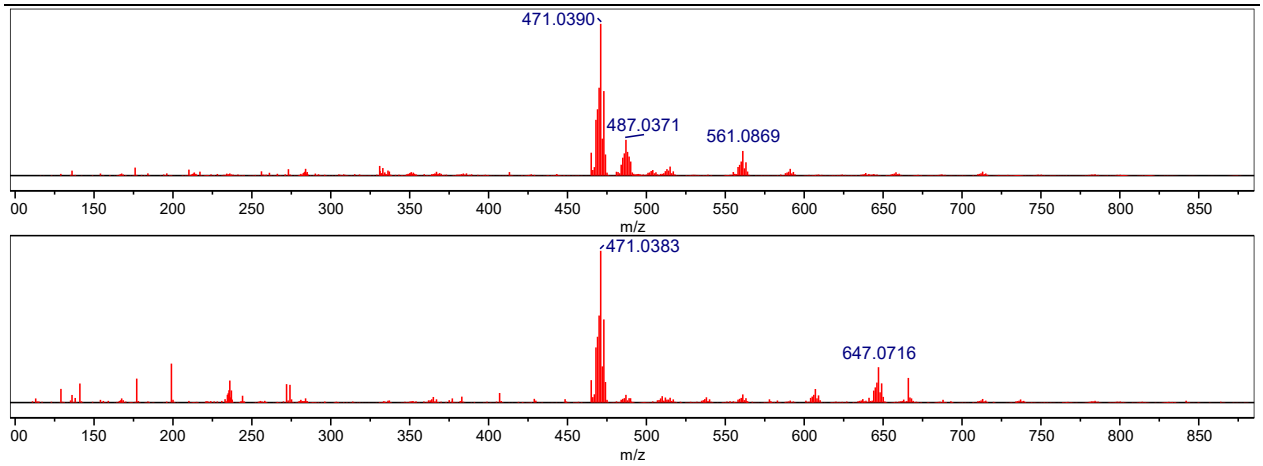


Ru(Ad) in CH_3CN, 18 days after dissolution.

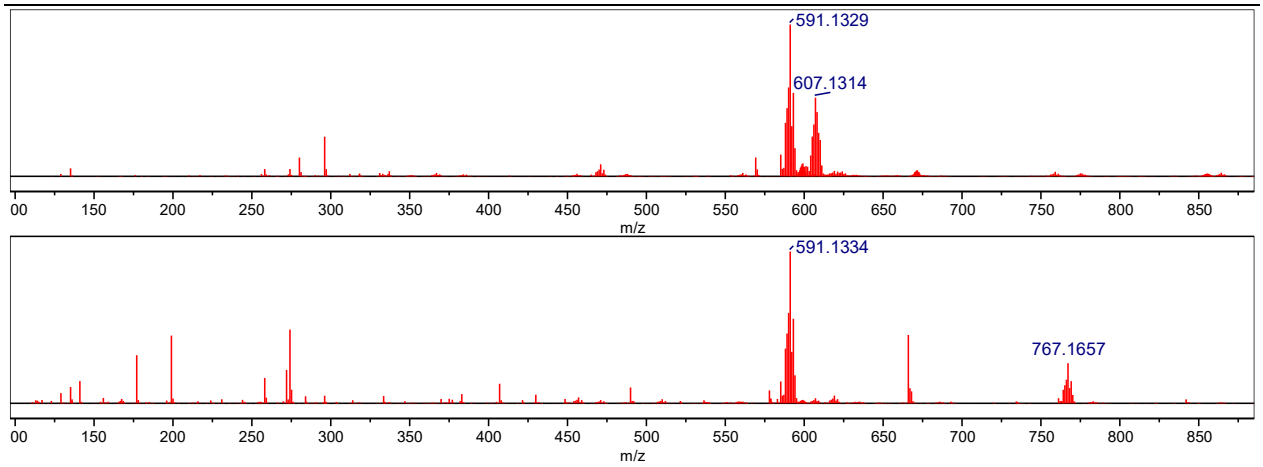


Ru(Ar) in CH_3CN, 18 days after dissolution.

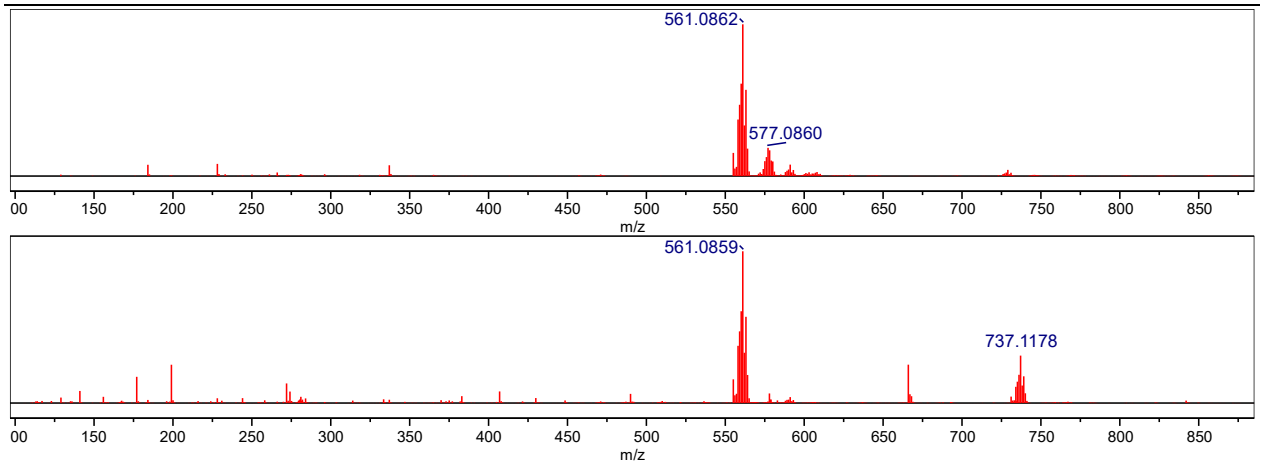
1.6.2.2. pH 7 / +AA (18 days); H_2O (unbuffered)



Top: 18-day old sample of **Ru(Me)** in deionized water; bottom: after treatment with an excess of ascorbic acid.

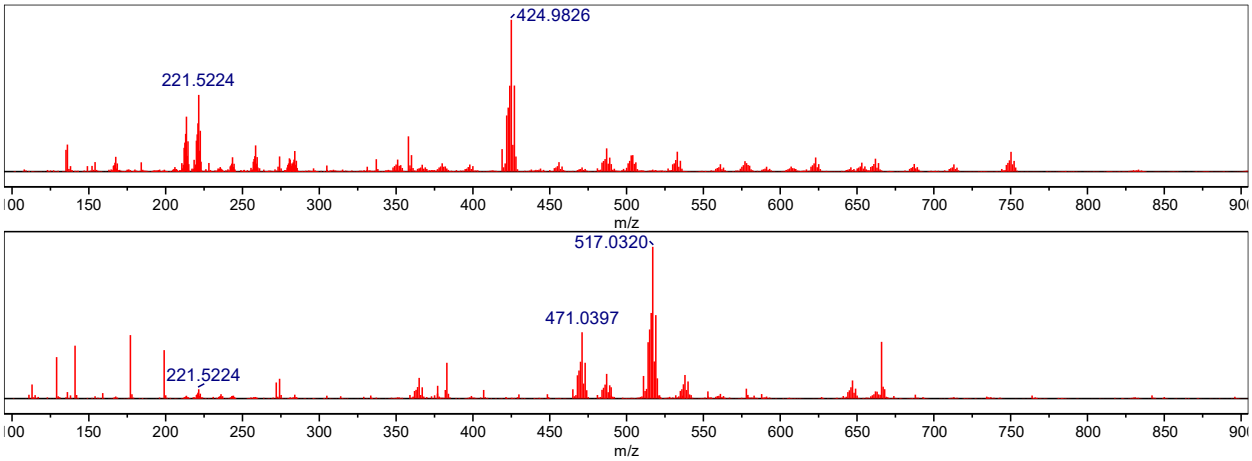


Top: 18-day old sample of **Ru(Ad)** in deionized water; bottom: after treatment with an excess of ascorbic acid.

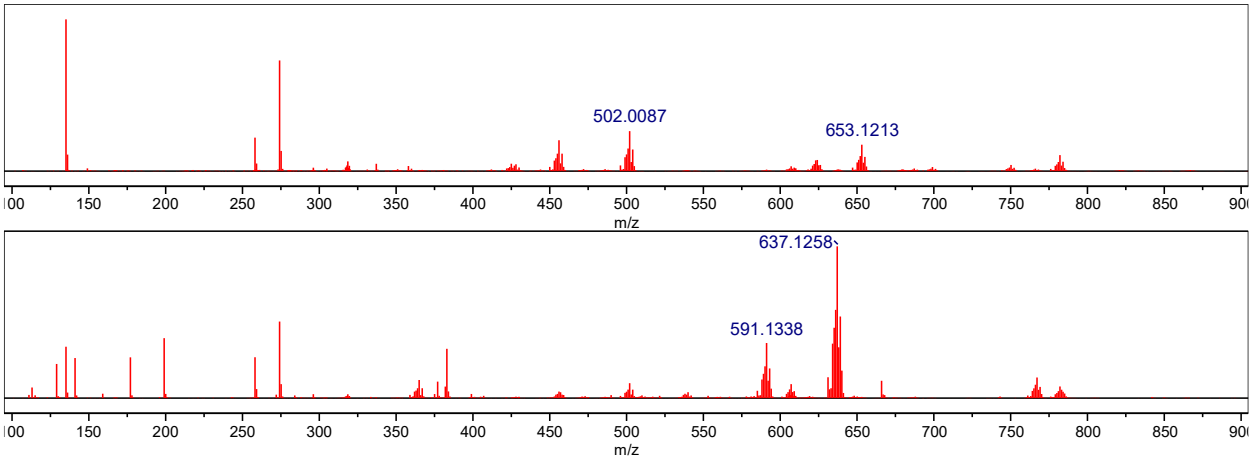


Top: 18-day old sample of **Ru(Ar)** in deionized water; bottom: after treatment with an excess of ascorbic acid.

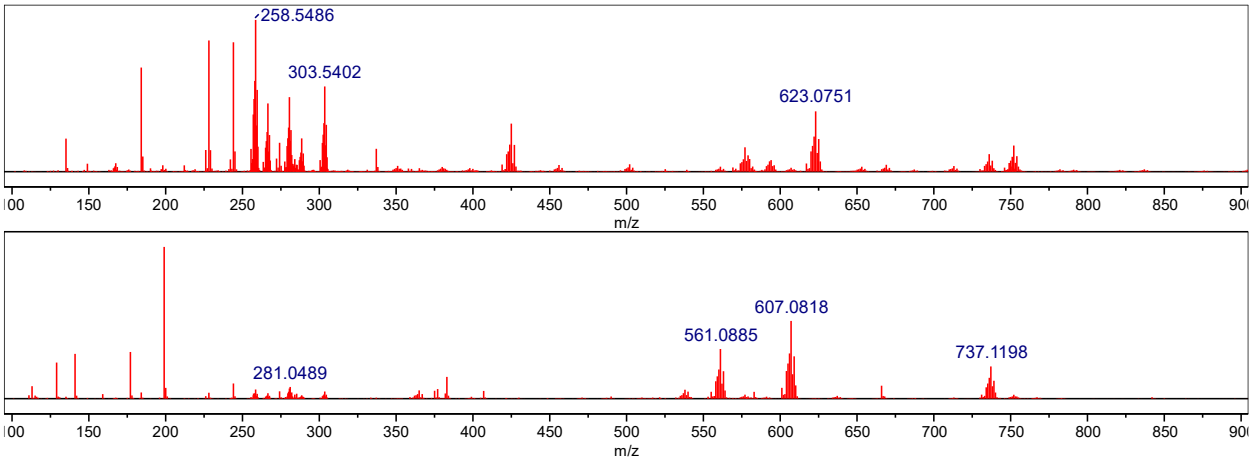
1.6.2.3. pH 1 / +AA (18 days); 0.1 M HNO_3 (aq)



Top: 18-day old sample of **Ru(Me)** in 0.1 M HNO_3 (aq); bottom: after treatment with an excess of ascorbic acid.



Top: 18-day old sample of **Ru(Ad)** in 0.1 M HNO_3 (aq); bottom: after treatment with an excess of ascorbic acid.

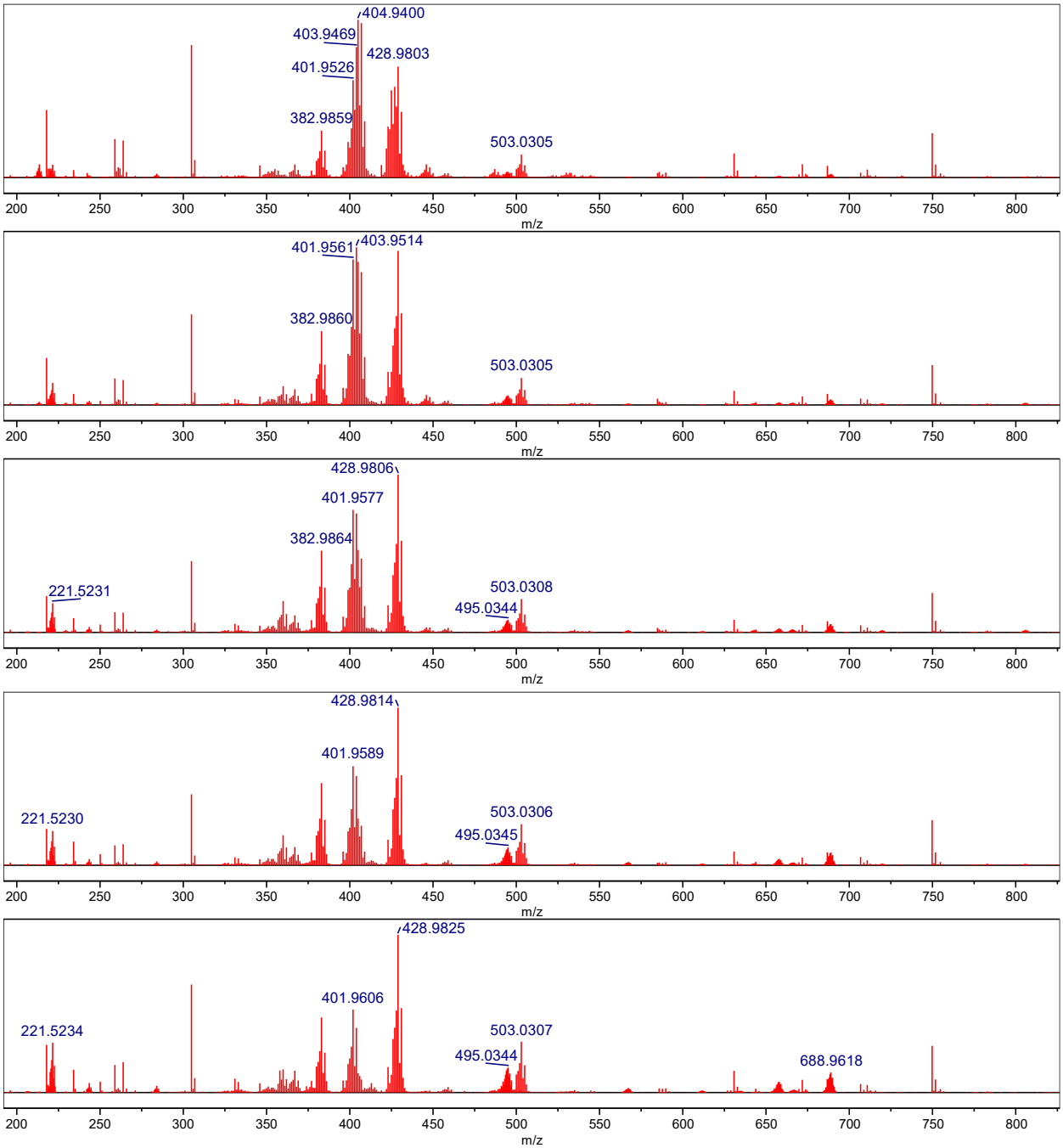


Top: 18-day old sample of **Ru(Ar)** in 0.1 M HNO_3 (aq); bottom: after treatment with an excess of ascorbic acid.

1.6.2.4. Ru(Me), 0.1 M HNO_3 + 20 (?) equiv. CAN

times; 1134, 1139, 1150, 1205, 1235 (descending)

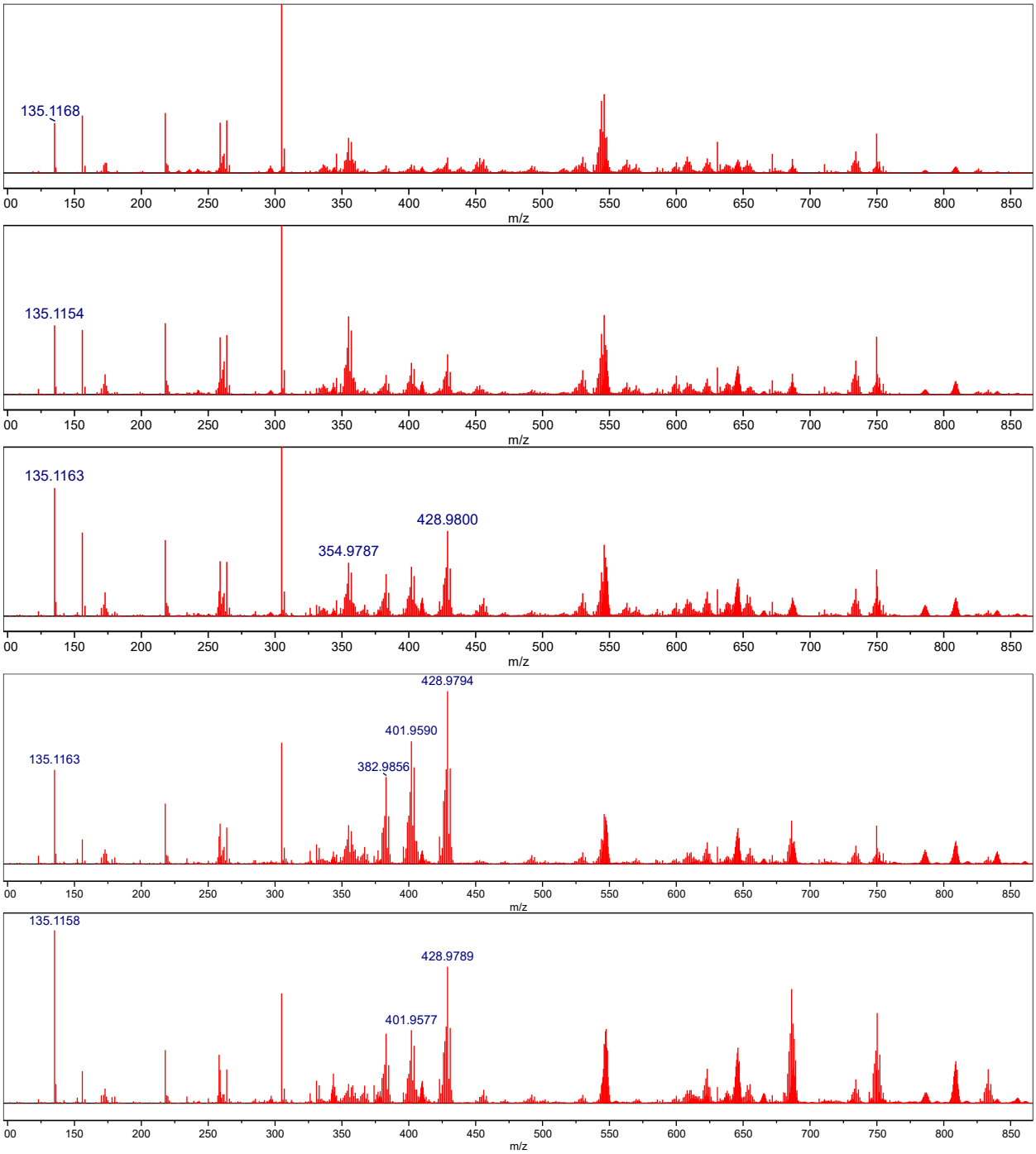
Ru(Me) – $C_{22}H_{17}N_4O_2Ru$; $M^+ = 471.0395$; $M^{2+} = 235.5198$



1.6.2.5. Ru(Ad), 0.1 M HNO_3 + 20 (?) equiv. CAN

times; 1007, 1012, 1016, 1021, 1039

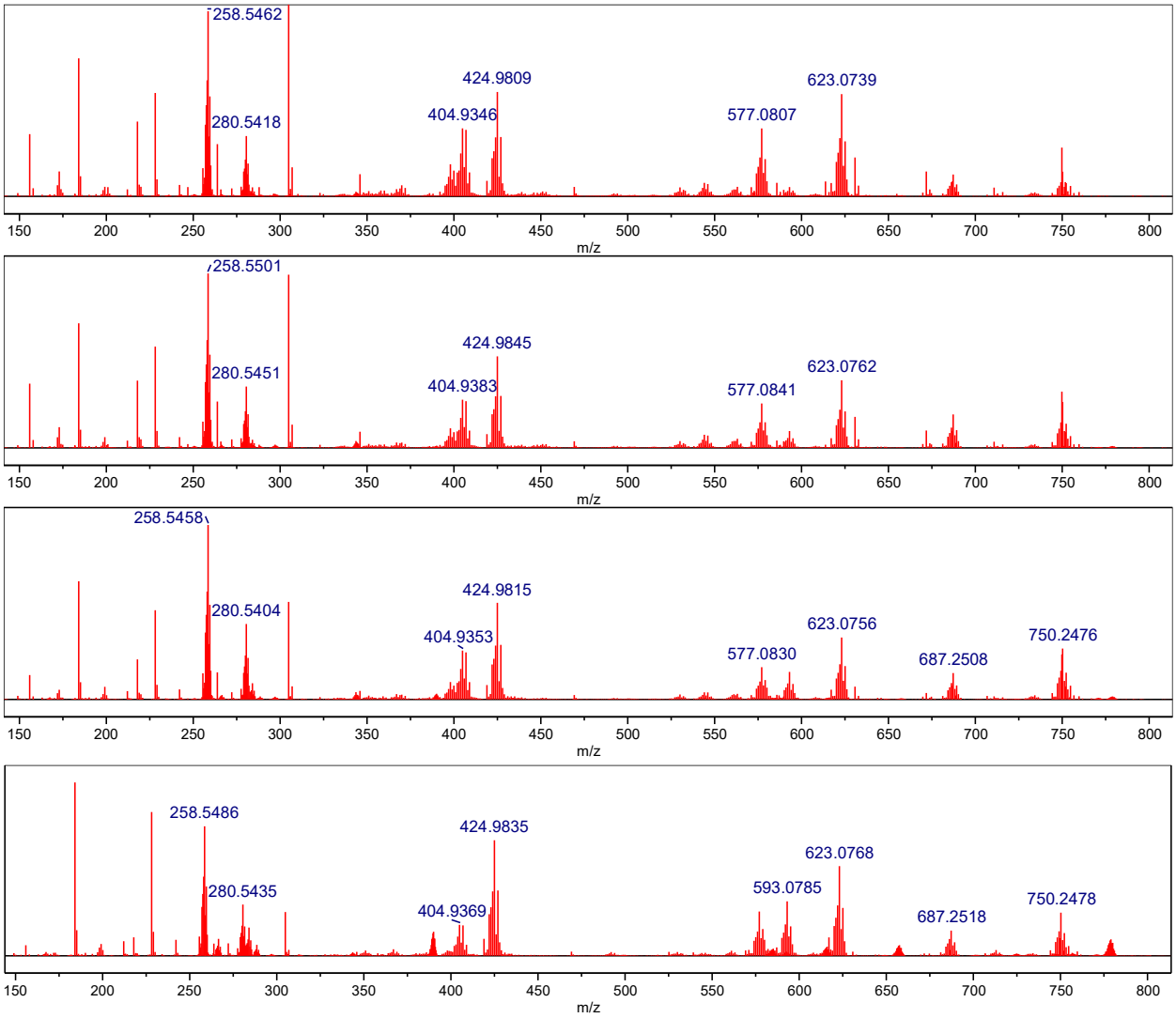
Ru(Ad) – $C_{31}H_{29}N_4O_2Ru$; $M^+ = 591.1334$; $M^{2+} = 295.5667$



1.6.2.6. Ru(Ar), 0.1 M HNO_3 + 20 equiv. (?) CAN

times; 1511, 1522, 1530, 1623 (descending)

Ru(Ar) – $C_{29}H_{23}N_4O_2Ru$; $M^+ = 561.0865$; $M^{2+} = 280.5433$



1.6.2.7. Table of peaks at pH 1 / +AA (18 days)

Ru(Me) – $C_{22}H_{17}N_4O_2Ru$; $M^+ = 471.0395$; $M^{2+} = 235.5198$

Ru(Me), 0.1 M HNO_3 (aq), 18 days			
Observed		Calculated	
M	z	Proposed	M/z
213.5248	2+	$[Ru(Me)]^{2+} - CO_2$	213.5249
221.5224	2+	$[Ru(Me)]^{2+} - CO$	221.5223
424.9826	1+	unid	n/a

After AA			
Observed		Calculated	
M	z	Proposed	M/Z
471.0397	1+	$[Ru(Me)]^+$	471.0395
517.0320	1+	$[Ru(Me)]^+ + NO_2$	517.0324

Ru(Ad) – $C_{31}H_{29}N_4O_2Ru$; $M^+ = 591.1334$; $M^{2+} = 295.5667$

Ru(Ad), 0.1 M HNO_3 (aq), 18 days			
Observed		Calculated	
M	z	Proposed	M/z
456.0156	1+	$[Ru(Ad)]^+ - (Ad\text{-}1)$	456.0160
502.0087	1+	$[Ru(Ad)]^+ - (Ad\text{-}1) + NO_2$	502.0089
653.1213	1+	$[Ru(Ad)]^+ + NO_3$	653.1212
782.0902	1+	unid	n/a

After AA			
Observed		Calculated	
M	z	Proposed	M/z
591.1338	1+	$[Ru(Ad)]^+$	591.1334
637.1258	1+	$[Ru(Ad)]^+ + NO_2$	637.1263

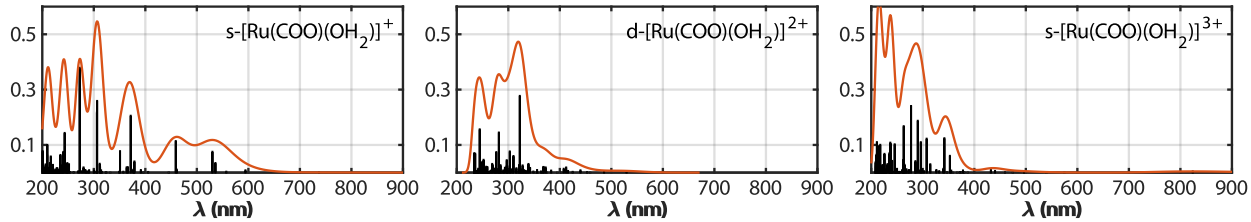
Ru(Ar) – $C_{29}H_{23}N_4O_2Ru$; $M^+ = 561.0865$; $M^{2+} = 280.5433$

Ru(Ar), 0.1 M HNO_3 (aq), 18 days			
Observed		Calculated	
M	z	Proposed	M/z
258.5486	2+	$[Ru(Me)]^{2+} + NO_2$	258.5162
266.5460	2+	$[Ru(Ar)]^{2+}$ - CO	266.5458
280.5438	2+	$[Ru(Ar)]^{2+}$	280.5433
303.5397	2+	$[Ru(Ar)]^{2+} + NO_2$	303.5397
424.9821	1+	unid	n/a
577.0821	1+	$[Ru(Ar)]^+ + O$	577.0814
623.0751	1+	$[Ru(Ar)]^+ + NO_3$	623.0743

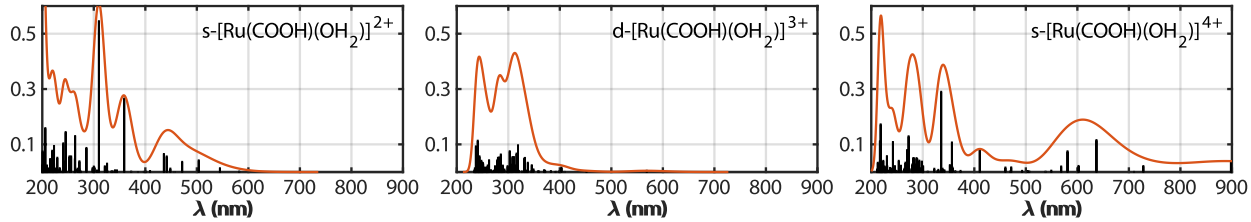
After AA			
Observed		Calculated	
M	z	Proposed	M/z
561.0885	1+	$[Ru(Ar)]^+$	561.0865
607.0818	1+	$[Ru(Ar)]^+ + NO_2$	607.0794
737.1198	1+	$[Ru(Ar)]^+ +$ AA	737.1185

1.6.3. TDDFT

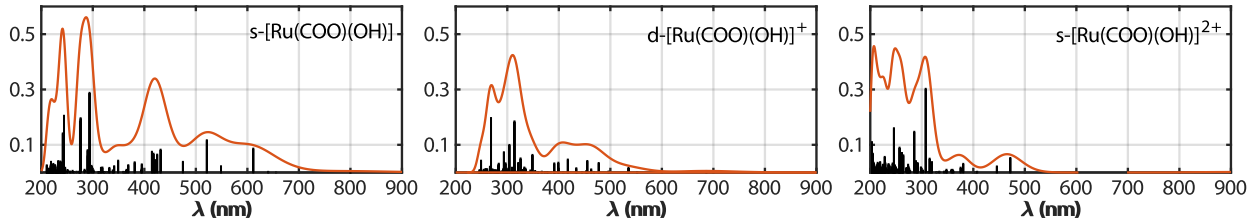
1.6.3.1. TDDFT UV-vis spectra of Ru(Ad)



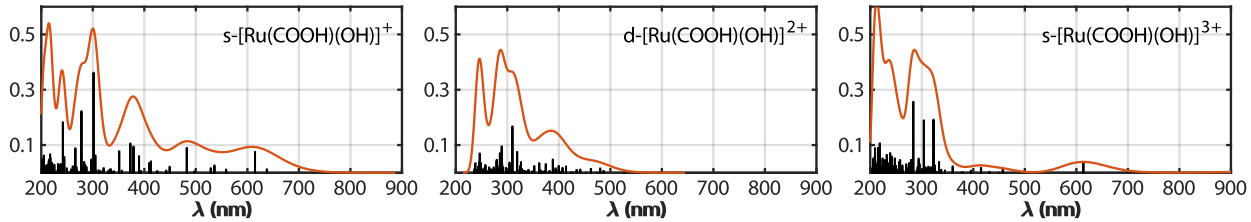
Ru(II), doublet Ru(III), and Ru(IV) aquo complexes.



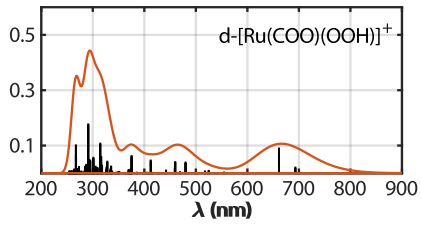
Ru(II), doublet Ru(III), and Ru(IV) aquo complexes, protonated carboxylate.

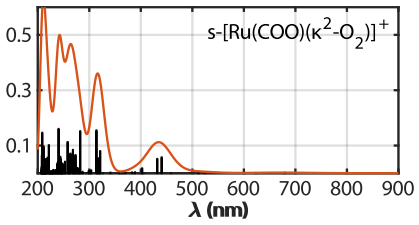


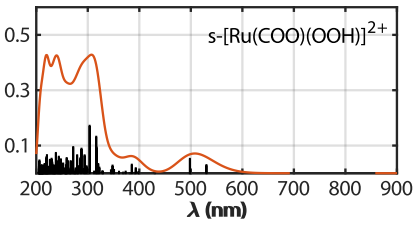
Ru(II), doublet Ru(III), and Ru(IV) hydroxo complexes



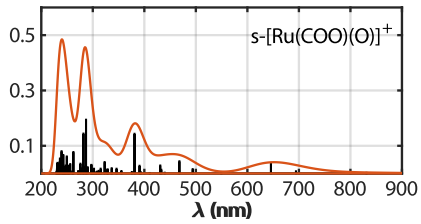
Ru(II), doublet Ru(III), and Ru(IV) hydroxo complexes, protonated carboxylate

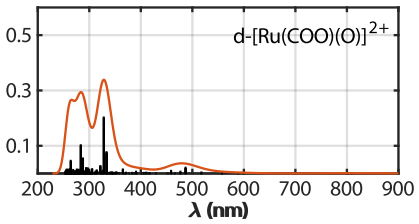


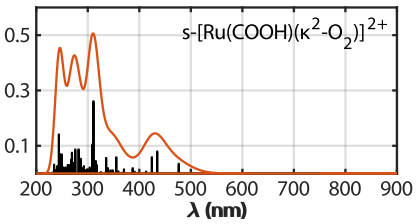




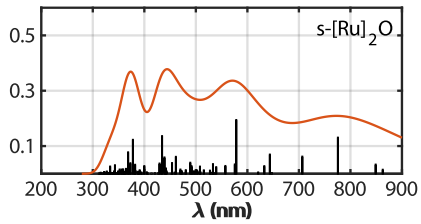
Ru OOH and Ru O_2 complexes

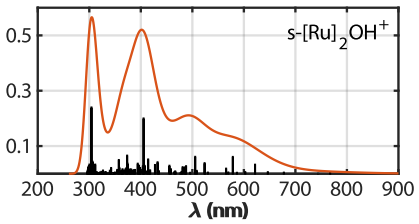


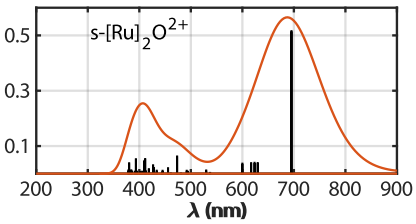




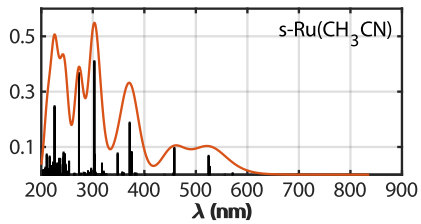
Assorted Ru O_x complexes





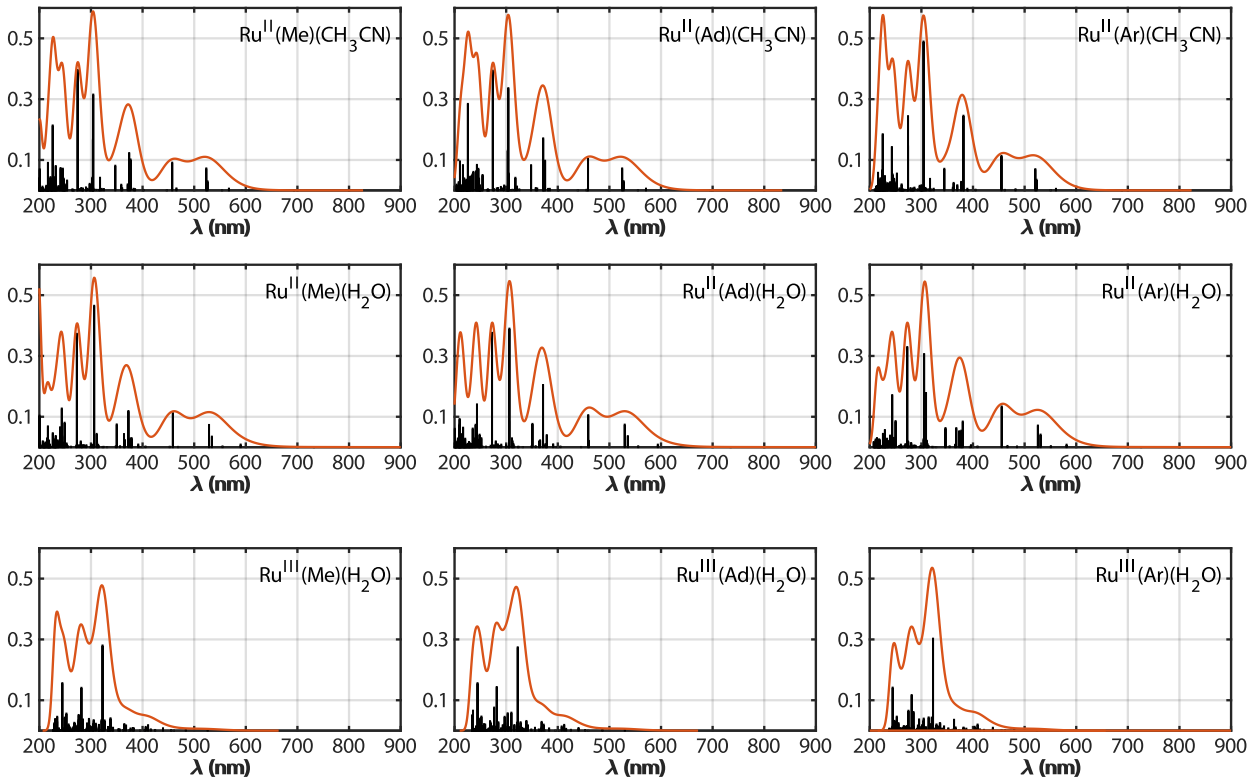


Ru dimers



Ru(CH_3CN)

1.6.3.2. TDDFT of Ru(R) complexes



1.6.4. Tables of data

1.6.4.1. $Ru^{II/III}$ couple

1.0 mM Ru(Ad) in 0.1 M HNO_3(aq); pH 1

entry	Max E	Ep V	Eh V	ip A	Ah C
bgs10	1.0V	0.473	0.415	3.95E-06	2.42E-06
		0.409	0.468	-3.79E-06	-2.51E-06
bgs12	1.2 V	0.474	0.414	4.48E-06	2.95E-06
		0.409	0.469	-4.05E-06	-2.74E-06
bgs14	1.4 V	0.473	0.414	4.32E-06	2.73E-06
		0.409	0.47	-4.07E-06	-2.81E-06
bgs16	1.6 V	0.473	0.415	4.22E-06	2.65E-06
		0.409	0.489	-4.01E-06	-3.36E-06

1.0 mM Ru(Ad) in 0.1 M PO_4^{3-}(aq); pH 7

entry	Max E	Ep V	Eh V	ip A	Ah C
10a	1.0 V	0.463	0.404	5.20E-06	3.47E-06
		0.357	0.443	-3.90E-06	-3.53E-06
10b	1.0 V	0.465	0.403	5.30E-06	3.74E-06
		0.349	0.442	-3.98E-06	-3.85E-06
12a	1.2 V	0.463	0.403	5.28E-06	3.57E-06
		0.349	0.442	-3.38E-06	-3.26E-06
12b	1.2 V	0.465	0.405	4.91E-06	3.33E-06
		0.344	0.441	-3.41E-06	-3.43E-06
14a	1.4 V	0.464	0.404	5.04E-06	3.45E-06
		0.344	0.44	-2.63E-06	-2.61E-06
14b	1.4 V	0.467	0.406	4.74E-06	3.25E-06
		0.333	0.439	-2.62E-06	-2.85E-06
16a	1.6 V	0.465	0.403	5.04E-06	3.54E-06
		0.334	0.438	-2.15E-06	-2.27E-06
16b	1.6 V	0.467	0.405	4.92E-06	3.40E-06
		0.329	0.437	-2.13E-06	-2.33E-06

1.6.4.2. Scanrate/concentration dependence

Ru(Ad) in 0.1 M PO_4^{3-} (aq); pH 7; max E = 1.0 V

1.0 V	**[Ru]** mM	**v** V/s^{-1}	**Ep** V	**Eh** V	**ip** A	**Ah** C
awb1	1	0.1	0.462	0.404	8.634E-06	5.624E-06
awb2	1	0.2	0.468	0.408	1.232E-05	4.131E-06
awb3	1	0.5	0.477	0.416	2.037E-05	2.775E-06
awb4	1	1	0.490	0.423	2.993E-05	2.203E-06
awb5	1	2	0.502	0.433	4.455E-05	1.688E-06
awb6	1	5				
bwb1	0.5	0.1	0.463	0.403	4.495E-06	3.000E-06
bwb2	0.5	0.2	0.469	0.408	6.485E-06	2.209E-06
bwb3	0.5	0.5	0.475	0.415	1.066E-05	1.412E-06
bwb4	0.5	1	0.486	0.421	1.645E-05	1.173E-06
bwb5	0.5	2	0.498	0.427	2.544E-05	9.560E-07
bwb6	0.5	5				
cwb1	0.25	0.1	0.463	0.404	2.206E-06	1.426E-06
cwb2	0.25	0.2	0.470	0.407	3.215E-06	1.075E-06
cwb3	0.25	0.5	0.476	0.415	5.518E-06	7.336E-07
cwb4	0.25	1	0.481	0.420	8.859E-06	5.921E-07
cwb5	0.25	2	0.489	0.423	1.486E-05	4.935E-07
cwb6	0.25	5	0.521	0.434	2.617E-05	4.593E-07
dwb1	0.125	0.1	0.463	0.403	1.148E-06	7.252E-07
dwb2	0.125	0.2	0.462	0.408	1.710E-06	4.808E-07
dwb3	0.125	0.5	0.469	0.416	3.284E-06	3.826E-07
dwb4	0.125	1	0.474	0.421	5.582E-06	3.178E-07
dwb5	0.125	2	0.477	0.423	9.807E-06	2.544E-07
dwb6	0.125	5	0.511	0.441	1.944E-05	2.796E-07
ewb1	0.0625	0.1	0.460	0.403	5.593E-07	3.409E-07
ewb2	0.0625	0.2	0.466	0.406	1.006E-06	3.128E-07
ewb3	0.0625	0.5	0.475	0.414	2.136E-06	2.814E-07
ewb4	0.0625	1	0.474	0.419	4.026E-06	2.394E-07
ewb5	0.0625	2	0.489	0.419	8.062E-06	2.644E-07
ewb6	0.0625	5	0.500	0.434	1.521E-05	1.938E-07

Ru(Ad) in 0.1 M PO_4^{3-}(aq); pH 7; max E = 1.2 V

1.2 V	[Ru]	ν	Ep	Eh	ip	Ah
	mM	V/s^{-1}	V	V	A	C
axb1	1	0.1	0.464	0.405	8.468E-06	5.587E-06
axb2	1	0.2	0.468	0.410	1.195E-05	3.888E-06
axb3	1	0.5	0.479	0.418	1.902E-05	2.586E-06
axb4	1	1	0.491	0.425	2.677E-05	1.929E-06
axb5	1	2	0.502	0.434	3.796E-05	1.398E-06
axb6	1	5				
bxb1	0.5	0.1	0.465	0.404	4.299E-06	2.889E-06
bxb2	0.5	0.2	0.465	0.409	5.965E-06	1.850E-06
bxb3	0.5	0.5	0.475	0.416	9.706E-06	1.231E-06
bxb4	0.5	1	0.488	0.422	1.393E-05	1.012E-06
bxb5	0.5	2	0.493	0.431	2.137E-05	6.979E-07
bxb6	0.5	5				
cxb1	0.25	0.1	0.462	0.406	2.134E-06	1.328E-06
cxb2	0.25	0.2	0.465	0.409	2.990E-06	8.959E-07
cxb3	0.25	0.5	0.471	0.417	4.936E-06	5.769E-07
cxb4	0.25	1	0.476	0.422	7.566E-06	4.290E-07
cxb5	0.25	2	0.497	0.424	1.114E-05	4.035E-07
cxb6	0.25	5	0.510	0.439	2.009E-05	2.847E-07
dxb1	0.125	0.1	0.462	0.406	1.106E-06	6.696E-07
dxb2	0.125	0.2	0.459	0.410	1.622E-06	4.327E-07
dxb3	0.125	0.5	0.474	0.414	2.925E-06	3.638E-07
dxb4	0.125	1	0.473	0.420	5.039E-06	2.958E-07
dxb5	0.125	2	0.485	0.424	8.237E-06	2.396E-07
dxb6	0.125	5	0.513	0.444	1.515E-05	2.263E-07
exb1	0.0625	0.1	0.461	0.407	6.150E-07	3.662E-07
exb2	0.0625	0.2	0.465	0.405	1.022E-06	2.975E-07
exb3	0.0625	0.5	0.473	0.413	2.107E-06	2.593E-07
exb4	0.0625	1	0.481	0.426	3.641E-06	2.216E-07
exb5	0.0625	2	0.493	0.430	6.160E-06	2.013E-07
exb6	0.0625	5	0.506	0.445	1.242E-05	1.669E-07

Ru(Ad) in 0.1 M CO_3^{2-} (aq); pH 10; max E 1.2 V

	[Ru] mM	**v** V/s^{-1}	Ep V	Eh V	ip A	Ah C
ayb1	1	0.1	0.395	0.335	7.87E-06	5.28E-06
ayb2	1	0.2	0.398	0.336	1.09E-05	3.81E-06
ayb3	1	0.5	0.406	0.34	1.69E-05	2.54E-06
ayb4	1	1	0.411	0.345	2.47E-05	1.9E-06
ayb5	1	2	0.422	0.352	3.63E-05	1.45E-06
ayb6-2	1	5	0.443	0.37	4.93E-05	8.25E-07
byb1	0.5	0.1	0.398	0.334	4.39E-06	3.21E-06
byb2	0.5	0.2	0.399	0.335	6.2E-06	2.26E-06
byb3	0.5	0.5	0.406	0.339	9.56E-06	1.5E-06
byb4	0.5	1	0.41	0.343	1.36E-05	1.08E-06
byb5	0.5	2	0.418	0.351	2E-05	7.96E-07
byb6	0.5	5	0.437	0.368	2.9E-05	4.84E-07
cyb1	0.25	0.1	0.397	0.332	2.41E-06	1.84E-06
cyb2	0.25	0.2	0.396	0.334	3.46E-06	1.29E-06
cyb3	0.25	0.5	0.403	0.336	5.55E-06	9.02E-07
cyb4	0.25	1	0.41	0.341	7.93E-06	6.8E-07
cyb5	0.25	2	0.415	0.349	1.17E-05	4.81E-07
cyb6	0.25	5	0.431	0.366	1.85E-05	3.05E-07
dyb1	0.125	0.1	0.398	0.329	1.43E-06	1.18E-06
dyb2	0.125	0.2	0.396	0.332	2.17E-06	8.4E-07
dyb3	0.125	0.5	0.403	0.337	3.86E-06	6.21E-07
dyb4	0.125	1	0.411	0.345	5.76E-06	4.53E-07
dyb5	0.125	2	0.42	0.353	9.01E-06	3.69E-07
dyb6	0.125	5	0.433	0.374	1.34E-05	1.99E-07

1.6.4.3. 2D NMR Assignment Tables

Abbreviations	Meaning
ENT	Entry
INT	Integrations
MLT	Multiplicity
OVL	Overlapping peaks

Unless otherwise noted, actual reported values of chemical shifts was taken from 1D NMR values. Correlations for ambiguous 2D cross peaks are reported as lists of possible corresponding peaks. Where possible, 2D cross-peaks were assigned using MestreNova 14.0's snap-to-peak peak-picking feature. Cross-peaks that had to be manually assigned (i.e. due to low resolution in f1) may exhibit small deviations from the reported 1D chemical shifts.

For Ru(Me)

ENT	1D ^{1}H	^{13}C	^{1}H INT	^{1}H MLT	^{1}H J (Hz)	^{1}H COSY	^{1}H-^{13}C HSQC	^{1}H-^{13}C HMBC
	GROUP A							
A1	7.89	130.01	1	t	8.1	8.32	130.01	160.13
A2	8.32A	123.25/123.67	2/4 OVL	m	-	7.90/7.96	123.25/123.67	123.25/128.35/159.17/160.13
A3	-	160.13	-	-	-	-	-	-
	GROUP B							
B1	7.55	128.35	2	ddd	7.2, 5.8, 1.1	7.95, 8.37	128.35	123.25, 151.31
B2	7.96	137.46	2	ddd	8.1, 7.5, 1.6	7.55, 8.31	137.46	151.31, 159.17
B3	8.32B	123.25/123.67	2/4 OVL	m	-	7.90/7.96	123.25/123.67	123.25/128.35/159.17/160.13
B4	8.36	151.31	2	d	5.49	7.55	151.31	128.35, 137.46, 159.17
B5	-	159.17	-	-	-	-	-	-
	GROUP C							
C1	3.66	46.85	3	s	-	6.97, 7.71	46.25	133.75, 134.85, 136.09
C2	6.18	133.75	1	d	6.4	6.97	133.75	136.09, 146.85
C3	6.97	136.09	1	dd	6.4, 1.7	6.19, 7.71	136.09	134.85, 46.25
C4	7.72	134.85	1	d	1.7	6.97	134.85	46.25, 136.09
C5	-	146.85	-	-	-	-	-	-
C6	-	175.95	-	-	-	-	-	-
C7	-	230.87	-	-	-	-	-	-

For Ru(Ad)

ENT	^{1}H	^{13}C	^{1}H INT	^{1}H MLT	^{1}H J (Hz)	^{1}H COSY	^{1}H-^{13}C HSQC	^{1}H-^{13}C HMBC
	GROUP A							
A1	7.89	129.91	1	t	8.0	8.31	129.90	160.08,123.21
A2	8.31A	123.21/123.64	2/4 OVL	m	-	7.89/7.96	123.19/123.62	123.19/128.33/160.08
A3	-	160.14	-	-	-	-	-	-
	GROUP B							
B1	7.55	128.36	2	dd	1.3, 5.5, 7.3	8.36, 7.96	128.33	123.62, 151.41
B2	7.96	137.45	2	td	1.6, 7.8, 7.9	7.54	137.44	151.35, 159.10
B3	8.31B	123.21/123.64	2/4 OVL	m	-	7.89/7.96	123.19/123.62	123.19/128.33/160.08
B4	8.36	151.41	2	d	5.2	7.56	151.35	128.33, 137.44, 159.10
B5	-	159.15	-	-	-	-	-	-
	GROUP C							
C1	6.21	133.79	1	d	6.7	7.33	133.77	131.38, 146.67
C2	7.33	131.38	1	dd	2.0, 6.7	6.22	131.38	129.90
C3	8.00	129.86	1	d	2.0	7.33	129.90	131.38
C4	-	146.79	-	-	-	-	-	-
C5	-	176.10	-	-	-	-	-	-
C6	-	231.05[1]	-	-	-	-	-	-
	GROUP D							
D1	1.67	35.72	6	q	12.3, 12.5	1.98, 2.17	35.67	NCP
D2	1.97	42.41	6	d	3.0	1.67	42.35	30.88, 35.72, 42.41, 65.73
D3	2.17	30.88	OVL, >2.5	OVL	-	1.67	30.83	NCP
D4	-	65.73	-	-	-	-	-	-

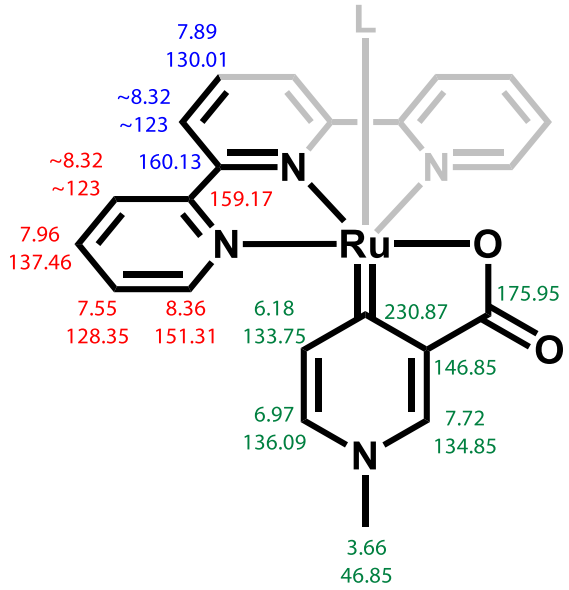
[1] HMBC cross-peak

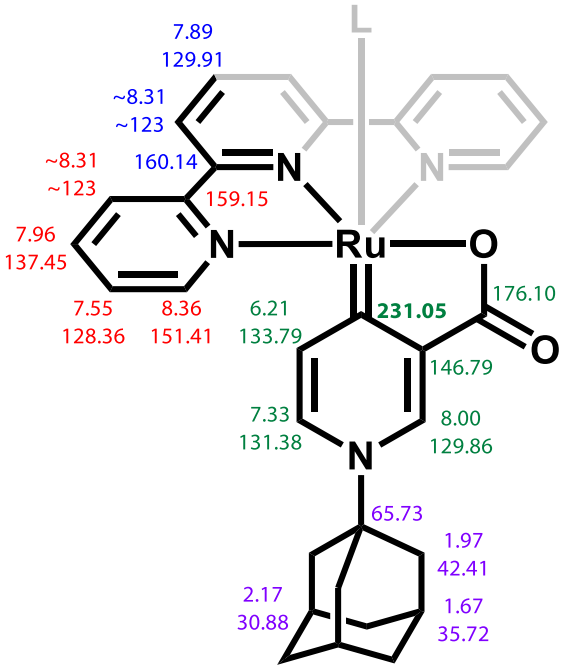
For Ru(Ar)

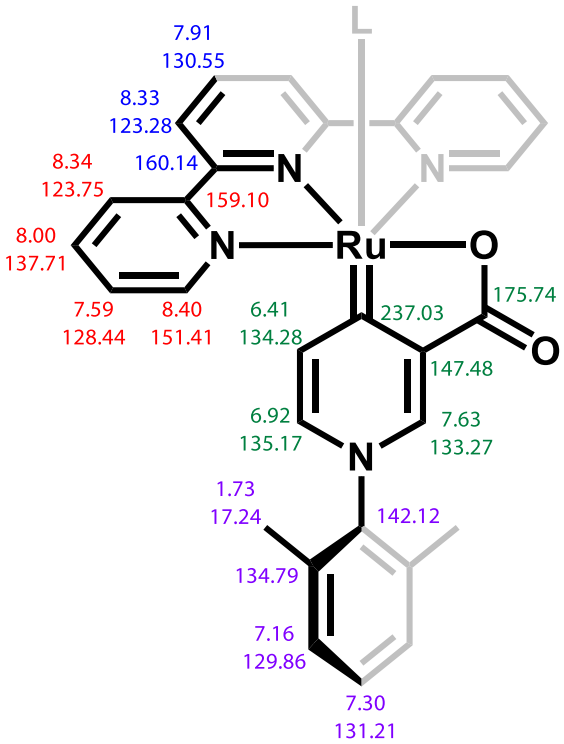
ENT	^{1}H	^{13}C	^{1}H INT	^{1}H MLT	^{1}H J (Hz)	^{1}H COSY	^{1}H-^{13}C HSQC	^{1}H-^{13}C HMBC
	GROUP A							
A1	7.91	130.55	1	t	8.1	8.33	130.55	123.28, 160.14
A2	8.33[2]	123.28	2/4 OVL	m	-	7.91	123.28	123.28, 160.14
A3	-	160.14	-	-	-	-	-	-
	GROUP B							
B1	7.59	128.44	2	ddd	7.7, 5.5, 1.2	8.00, 8.34, 8.40	128.44	123.75, 151.38
B2	8.00	137.71	2	ddd	1.5, 7.3, 8.2	7.59, 8.34, 8.40	137.71	151.41, 159.10
B3	8.34[3]	123.75	2/4 OVL	m	-	7.59, 8.00	123.75	128.44, 159.10
B4	8.40	151.41	2	dd	0.7, 5.5	7.59, 8.01	151.41	128.44, 137.71, 159.10
B5	-	159.10	-	-	-	-	-	-
	GROUP C							
C1	6.41	134.28	1	d	6.6	6.92	134.28	135.17, 147.48
C2	6.92	135.17	1	dd	6.4, 1.7	6.41, 7.63	135.17	133.27, 134.28
C3	7.63	133.27	1	d	1.6	6.92	133.27	135.17, 175.74
C4	-	147.48	-	-	-	-	-	-
C5	-	175.74	-	-	-	-	-	-
C6	-	237.03	-	-	-	-	-	-
	GROUP D							
D1	1.73	17.24	6	s	-	7.30, 7.15	17.24	129.86, 134.79, 142.12
D2	7.16	129.86	2	d	7.6	7.30, 1.73	129.86	17.24, 129.86, 142.12
D3	7.30	131.21	1	t	7.7	7.15, 1.73	131.21	134.79
D4	-	134.79	-	-	-	-	-	-
D5	-	142.12	-	-	-	-	-	-

[2] resolved w/ COSY
[3] resolved w/ COSY

Annotated schematic of Ru(R) NMR shifts







1.6.4.4. Summary of data for DFT optimized geometries of Ru(R)

Filenames

charge	multiplicity	L	R = Me	R = Ad	R = Ar
1	1	CH_3CN	rme2ni	rad2ni	rar2ni
1	1	OH_2	rme2aq	rad2aq	rad2aq
0	1	OH	rme2oh	rad2oh	rad2oh
2	2	OH_2	rme3aq	rad3aq	rar3aq
1	2	OH	rme3oh	rad3oh	rar3oh
3	1	OH_2	rme4aq	rad4aq	rar4aq
2	1	OH	rme4oh	rad4oh	rar4oh

Summary of energies (E_{solv} – E)

Species	R = Me	R = Ad	R = Ar
$Ru^{II}(CH_3CN)^+$	-43.6	-40.7	-41.5
$Ru^{II}(OH_2)^+$	-44.8	-41.5	-42.6
$Ru^{II}(OH)$	-26.0	-25.4	-24.9
$Ru^{III}(OH_2)^{2+}$	-133.7	-125.7	-128.1
$Ru^{III}(OH)^+$	-49.2	-45.5	-46.4
$Ru^{IV}(OH_2)^{3+}$	-288.7	-273.6	-275.4
$Ru^{IV}(OH)^{2+}$	-138.0	-129.3	-131.6

Computed thermodynamic parameters

	ZPE	TE	HE	GE	E	Esolv
rme2ni	-1445.156400	-1445.128190	-1445.127246	-1445.217952	-1445.553771	-1445.623224
rme2aq	-1388.834218	-1388.808292	-1388.807348	-1388.890604	-1389.210290	-1389.281674
rme2oh	-1388.395061	-1388.369677	-1388.368732	-1388.450859	-1388.757232	-1388.798743
rme3aq	-1388.517612	-1388.491485	-1388.490541	-1388.575440	-1388.894458	-1389.107456
rme3oh	-1388.206197	-1388.180740	-1388.179796	-1388.264690	-1388.570259	-1388.648683
rme4aq	-1388.022841	-1387.996792	-1387.995848	-1388.078645	-1388.399128	-1388.859277
rme4oh	-1387.864186	-1387.839452	-1387.838508	-1387.919737	-1388.230760	-1388.450750
rad2ni	-1795.246268	-1795.212439	-1795.211494	-1795.313596	-1795.838273	-1795.903063
rad2aq	-1738.924471	-1738.892907	-1738.891962	-1738.986809	-1739.495132	-1739.561340
rad2oh	-1738.480869	-1738.449828	-1738.448884	-1738.542992	-1739.037687	-1739.078176
rad3aq	-1738.615866	-1738.584119	-1738.583175	-1738.679044	-1739.187182	-1739.387561
rad3oh	-1738.297430	-1738.266459	-1738.265515	-1738.360372	-1738.856254	-1738.928716
rad4aq	-1738.134501	-1738.102498	-1738.101554	-1738.197090	-1738.704550	-1739.140573
rad4oh	-1737.964234	-1737.933887	-1737.932943	-1738.024999	-1738.525302	-1738.731327
rar2ni	-1715.459487	-1715.424782	-1715.423838	-1715.529811	-1715.963556	-1716.029725
rar2aq	-1659.137529	-1659.105094	-1659.104149	-1659.202768	-1659.620275	-1659.688216
rar2oh	-1658.697230	-1658.665398	-1658.664454	-1658.761954	-1659.166258	-1659.205897
rar3aq	-1658.824992	-1658.792381	-1658.791437	-1658.891029	-1659.308480	-1659.512700
rar3oh	-1658.509679	-1658.477805	-1658.476861	-1658.575815	-1658.980541	-1659.054485
rar4aq	-1658.341506	-1658.308548	-1658.307603	-1658.407001	-1658.823400	-1659.262213
rar4oh	-1658.172423	-1658.141280	-1658.140336	-1658.235721	-1658.645787	-1658.855474

Table 3. Selected bond lengths obtained optimized geometries of **Ru(R)**

$Ru^{II}(OH_2)$	Me	Ad	Ar
Ru-C	1.9604	1.9644	1.9610
Ru-OOC	2.0986	2.0999	2.0976
Ru-L^{trans}	2.2851	2.2887	2.2871
N-C	1.4713	1.5145	1.4518

				Δ $Ru^{II}(OH_2)$		
$Ru^{III}(OH_2)$	Me	Ad	Ar	Me	Ad	Ar
Ru-C	1.9921	1.9950	1.9930	0.0317	0.0306	0.0320
Ru-OOC	1.9679	1.9674	1.9962	-0.1307	-0.1325	-0.1014
Ru-L^{trans}	2.2586	2.2652	2.2630	-0.0265	-0.0235	-0.0241
N-C	1.4815	1.5330	1.4611	0.0102	0.0185	0.0093
				Δ $Ru^{II}(OH_2)$		
$Ru^{III}(OH)$	Me	Ad	Ar	Me	Ad	Ar
Ru-C	2.0690	2.0697	2.0683	0.1086	0.1053	0.1073
Ru- OOC	2.0794	2.0811	2.0785	-0.0192	-0.0188	-0.0191
Ru-L^{trans}	1.9683	1.9697	1.9694	-0.3168	-0.3190	-0.3177
N-C	1.4746	1.5195	1.4548	0.0033	0.0050	0.0030
				Δ $Ru^{II}(OH_2)$		
$Ru^{II}(CH_3CN)$	Me	Ad	Ar	Me	Ad	Ar
Ru-C	1.9956	1.9991	1.9960	0.0352	0.0347	0.0350
Ru- OOC	2.1102	2.1112	2.1088	0.0116	0.0113	0.0112
Ru-L^{trans}	2.1151	2.1140	2.1154	-0.1700	-0.1747	-0.1717
N-C	1.4712	1.5142	1.4517	-0.0001	-0.0003	-0.0001

1.6.4.5. DFT data for optimized geometries of Ru(Ad)

All structures used in this work were fully optimized in the gas phase at the B3LYP[54]/cc-PVDz level with Grimme D2 dispersion.[51] The formatted checkpoint files obtained using Gaussian 09 Rev. D.01[55] for the gas phase optimized geometries of the computed structures in this work were converted to .xyz (Cartesian coordinate) using Open Babel[56], and stored in the tables that follows this section.

1.6.4.6. Optimized geometries of Ru(Ad) used for TDDFT calculations

70			
adnc40-ooh | bs90-adnc40-oo.fchk			
Ru	2.09660	-0.03327	-0.67115
C	0.10189	-0.00344	-0.16147
C	-0.81801	-0.24310	-1.21847
C	-0.50989	0.22872	1.08980
C	-2.18980	-0.25099	-1.02718
C	-1.88871	0.21965	1.23717
N	-2.72524	-0.01690	0.19027
C	-0.31586	-0.52218	-2.58589
O	-0.92491	-0.77368	-3.58302
O	1.08325	-0.46267	-2.56167
C	-4.25507	-0.04394	0.33137
H	0.08915	0.42392	1.98135
H	-2.35935	0.40470	2.19871
H	-2.87272	-0.44864	-1.85132
N	2.80175	0.26490	1.13634
C	3.13535	-0.82316	1.88056
C	2.92211	1.53704	1.59621
C	3.60645	-0.64521	3.18244
C	3.39367	1.75747	2.89385
C	3.73192	0.65586	3.68574
H	3.50026	2.77108	3.27911
H	3.87827	-1.50429	3.79507
H	4.10244	0.81053	4.70041
N	2.45828	-2.01513	-0.10093
N	2.09508	2.07012	-0.59418
C	2.35145	-3.12398	-0.85060
C	1.76589	2.93156	-1.57011
C	2.97725	-2.10929	1.16579
C	2.53999	2.56065	0.60600
C	3.36632	-3.33867	1.69457
C	2.64073	3.93433	0.83353
C	3.23949	-4.49281	0.91316
C	2.29157	4.82506	-0.18478
C	2.73089	-4.38367	-0.38133
C	1.85061	4.31594	-1.40800
H	1.95631	-2.98185	-1.85625
H	1.43403	2.48513	-2.50858
H	2.62836	-5.25488	-1.02937
H	1.58043	4.97402	-2.23480
H	3.54622	-5.46152	1.31151
H	2.37254	5.90170	-0.02558
H	3.78136	-3.39552	2.70073
H	3.00153	4.30419	1.79328
C	-4.74704	-1.45766	-0.04576
C	-4.68534	0.27864	1.77160
C	-4.85160	1.00792	-0.62850
H	-4.30029	-2.19483	0.64267
H	-4.43349	-1.70970	-1.07241
C	-6.28823	-1.49419	0.04346
H	-4.32645	1.28142	2.05981
H	-4.26374	-0.46446	2.46964
C	-6.22846	0.23775	1.86265
H	-4.54345	0.80194	-1.66648
H	-4.47849	2.00842	-0.35121
C	-6.39190	0.95646	-0.53841
H	-6.62616	-2.50358	-0.23517
C	-6.72251	-1.17048	1.48456
C	-6.87840	-0.45329	-0.92792
H	-6.51298	0.47166	2.89925
C	-6.82731	1.28082	0.90197
H	-6.80328	1.70258	-1.23459
H	-6.31276	-1.91950	2.18363
H	-7.82043	-1.21100	1.56145
H	-6.57897	-0.68688	-1.96421
H	-7.97827	-0.48974	-0.88692
H	-7.92618	1.26142	0.97325
H	-6.49397	2.29455	1.18242
O	3.69888	0.15026	-1.75388
O	3.93387	-0.74732	-2.62122
H	1.48688	-0.69157	-3.42310

70			
adnc40 | bs90-adnc40.fchk			
Ru	2.17358	-0.07900	0.80601
C	0.16926	0.01274	0.30381
C	-0.77628	-0.28265	1.30798
C	-0.34668	0.32396	-0.96106
C	-2.13979	-0.27343	1.04394
C	-1.72557	0.30120	-1.17803
N	-2.60552	0.00822	-0.19089
C	-0.31578	-0.60251	2.67872
O	-0.94208	-0.77409	3.67507
O	1.08848	-0.68156	2.63659
C	-4.14410	-0.02400	-0.41982
H	0.29636	0.58179	-1.80343
H	-2.14991	0.52613	-2.15403
H	-2.86769	-0.50005	1.82222
N	3.08649	0.21727	-0.92004
C	3.28459	1.48738	-1.36894
C	3.56448	-0.87778	-1.57807
C	4.02135	1.70044	-2.53753
C	4.30463	-0.70652	-2.74574
C	4.53684	0.59418	-3.22006
H	4.69658	-1.56848	-3.28588
H	4.19602	2.71135	-2.90617
H	5.12109	0.74161	-4.13092
N	2.02941	2.01458	0.59368
N	2.39708	-2.05259	0.16743
C	1.42949	2.85925	1.45203
C	1.99503	-3.16741	0.81549
C	2.66987	2.50939	-0.51198
C	3.20235	-2.16245	-0.94408
C	2.70878	3.88232	-0.76389
C	3.62127	-3.40707	-1.39994
C	2.08653	4.76080	0.12965
C	3.21246	-4.56280	-0.71533
C	1.43653	4.24198	1.25327
C	2.38806	-4.44139	0.40626
H	0.95270	2.40823	2.32351
H	1.36021	-3.01299	1.68806
H	0.95078	4.89306	1.98224
H	2.05062	-5.31680	0.96358
H	2.11551	5.83788	-0.04855
H	3.53874	-5.54636	-1.06105
H	3.22317	4.26235	-1.64716
H	4.26781	-3.48501	-2.27440
C	-4.78579	1.01067	0.52854
C	-4.48735	0.31805	-1.87561
C	-4.63558	-1.44930	-0.08641
H	-4.40619	2.01777	0.28616
H	-4.53453	0.78459	1.57852
C	-6.32102	0.95078	0.35049
H	-4.02036	-0.41054	-2.56107
H	-4.12777	1.33121	-2.12619
C	-6.02640	0.26592	-2.04967
H	-4.38036	-1.71407	0.95362
H	-4.15004	-2.17354	-0.76221
C	-6.17181	-1.48982	-0.25862
H	-6.77017	1.68581	1.03463
C	-6.67819	1.29382	-1.10669
C	-6.81765	-0.46687	0.69575
H	-6.25386	0.51334	-3.09660
C	-6.52815	-1.15132	-1.71678
H	-6.51298	-2.50594	-0.01089
H	-6.33763	2.31321	-1.35544
H	-7.77117	1.27080	-1.23563
H	-6.57393	-0.71373	1.74350
H	-7.91290	-0.50903	0.59608
H	-7.61954	-1.19734	-1.85276
H	-6.07849	-1.88920	-2.40272
O	3.35738	0.40456	2.17402
H	3.79712	1.27817	2.14693
H	1.49271	-0.72694	3.52860

70			
adnc30 | bs90-adnc30.fchk			
Ru	-2.16701	-0.00712	-0.77978
C	-0.18064	-0.05162	-0.23133
C	0.77308	-0.12481	-1.28474
C	0.39667	-0.00032	1.05776
C	2.13952	-0.13256	-1.05767
C	1.77005	-0.01105	1.24177
N	2.63903	-0.07260	0.19552
C	0.31146	-0.20900	-2.69186
O	0.95534	-0.25039	-3.69959
O	-1.08440	-0.24107	-2.69494
C	4.16356	-0.08349	0.37589
H	-0.22783	0.05342	1.95164
H	2.21046	0.03418	2.23363
H	2.84737	-0.19121	-1.88261
N	-2.93747	0.14204	1.00746
C	-3.10988	1.37729	1.54725
C	-3.31320	-1.00108	1.64274
C	-3.67168	1.49883	2.82210
C	-3.87362	-0.92091	2.91783
C	-4.04763	0.33928	3.50601
H	-4.17976	-1.82355	3.44567
H	-3.81922	2.48080	3.27069
H	-4.48840	0.41537	4.50136
N	-2.17046	2.06749	-0.54947
N	-2.51239	-2.04391	-0.37705
C	-1.77445	2.99895	-1.43444
C	-2.32433	-3.09831	-1.18415
C	-2.67743	2.47084	0.66006
C	-3.09058	-2.23240	0.85089
C	-2.77964	3.82497	0.98682
C	-3.46742	-3.50359	1.28173
C	-2.36406	4.78614	0.06283
C	-3.26126	-4.60149	0.43905
C	-1.85497	4.36655	-1.16918
C	-2.68565	-4.39656	-0.81531
H	-1.39035	2.61802	-2.38178
H	-1.87704	-2.87972	-2.15464
H	-1.52740	5.08317	-1.92343
H	-2.51763	-5.22256	-1.50737
H	-2.44294	5.84834	0.30052
H	-3.55613	-5.60212	0.75997
H	-3.18877	4.12404	1.95191
H	-3.93007	-3.63739	2.25942
C	4.75269	1.12566	-0.38252
C	4.54475	0.01296	1.86164
C	4.71098	-1.40353	-0.20776
H	4.34023	2.05762	0.03990
H	4.47862	1.08074	-1.44933
C	6.29119	1.10249	-0.25131
H	4.12607	-0.84319	2.41740
H	4.14804	0.94657	2.29571
C	6.08516	-0.00118	1.99543
H	4.43485	-1.49512	-1.27113
H	4.26938	-2.25457	0.33789
C	6.24974	-1.41222	-0.07604
H	6.69777	1.96243	-0.80441
C	6.67657	1.19989	1.23541
C	6.83279	-0.21178	-0.84733
H	6.33349	0.06938	3.06483
C	6.63435	-1.31537	1.41119
H	6.62738	-2.35329	-0.50326
H	6.30366	2.14540	1.66505
H	7.77323	1.19918	1.33750
H	6.56955	-0.28202	-1.91684
H	7.93181	-0.22470	-0.77669
H	7.73060	-1.33762	1.51509
H	6.23016	-2.17876	1.96684
O	-3.75400	0.10112	-1.91581
H	-4.30268	0.90333	-1.86625
H	-1.45935	-0.26700	-3.59601

70			
adnc20 | bs90-adnc20.fchk			
Ru	2.15430	-0.02217	-0.75355
C	0.22025	0.06914	-0.23948
C	-0.75234	-0.00320	-1.29757
C	-0.38361	0.19133	1.04862
C	-2.11281	0.00897	-1.07245
C	-1.74709	0.20277	1.22982
N	-2.62448	0.10469	0.17852
C	-0.29855	-0.09955	-2.70576
O	-0.95895	-0.19712	-3.70790
O	1.08252	-0.05399	-2.72264
C	-4.13078	0.08486	0.35117
H	0.24294	0.26756	1.93962
H	-2.18730	0.28436	2.21875
H	-2.81443	-0.06161	-1.90153
N	2.85054	-0.02235	1.01586
C	3.08846	-1.22000	1.64789
C	3.16854	1.17022	1.62152
C	3.60062	-1.23468	2.94471
C	3.67966	1.18187	2.92018
C	3.88778	-0.02698	3.59237
H	3.92534	2.13075	3.39769
H	3.78263	-2.18662	3.44396
H	4.28802	-0.02970	4.60649
N	2.27870	-2.07082	-0.43176
N	2.46045	2.01473	-0.49642
C	2.00965	-3.06912	-1.29234
C	2.26610	3.00836	-1.38599
C	2.76441	-2.37921	0.81371
C	2.94539	2.32486	0.75119
C	2.94505	-3.71049	1.20796
C	3.21962	3.65187	1.10819
C	2.64553	-4.73732	0.31614
C	3.00616	4.67074	0.18402
C	2.17481	-4.41106	-0.96207
C	2.52291	4.34330	-1.09030
H	1.65906	-2.75602	-2.27647
H	1.89093	2.69189	-2.36037
H	1.94584	-5.18224	-1.69842
H	2.34828	5.10909	-1.84693
H	2.78745	-5.77925	0.60804
H	3.21884	5.70790	0.44879
H	3.32993	-3.93214	2.20348
H	3.60548	3.87404	2.10325
C	-4.67448	-1.25250	-0.19917
C	-4.52752	0.21145	1.83304
C	-4.74212	1.26742	-0.43290
H	-4.22375	-2.08527	0.36688
H	-4.39095	-1.36848	-1.25764
C	-6.21138	-1.27704	-0.07268
H	-4.14094	1.15774	2.24701
H	-4.09779	-0.62428	2.41002
C	-6.06553	0.18319	1.96510
H	-4.46147	1.20347	-1.49648
H	-4.33919	2.21293	-0.03207
C	-6.27897	1.23250	-0.30607
H	-6.58145	-2.23129	-0.47834
C	-6.60242	-1.14893	1.41054
C	-6.80712	-0.10097	-0.87149
H	-6.31976	0.27555	3.03214
C	-6.67113	1.35875	1.17684
H	-6.69715	2.07430	-0.87917
H	-6.18862	-1.99454	1.98651
H	-7.69936	-1.17990	1.51341
H	-6.53880	-0.19306	-1.93815
H	-7.90688	-0.12397	-0.80242
H	-7.76872	1.34777	1.27705
H	-6.30807	2.31760	1.58519
O	3.79920	-0.18565	-1.92222
H	4.41002	0.56473	-1.86086
H	1.46771	-0.14914	-3.61286

69			
adnb40 | bs90-adnb40.fchk			
Ru	2.19213	0.09129	-0.89246
C	0.24620	-0.04308	-0.29643
C	-0.66046	0.52231	-1.20648
C	-0.30253	-0.62099	0.85938
C	-2.02169	0.51526	-0.96898
C	-1.67993	-0.60166	1.05506
N	-2.52890	-0.04401	0.15493
C	-0.08228	1.14975	-2.43707
O	-0.73740	1.70548	-3.28829
O	1.24673	1.03718	-2.45010
C	-4.05264	-0.03168	0.34898
H	0.31310	-1.08983	1.62793
H	-2.12947	-1.03748	1.94249
H	-2.71124	0.96143	-1.68353
N	2.93252	-0.28221	0.97281
C	3.07527	-1.56608	1.39356
C	3.27267	0.77189	1.75931
C	3.61158	-1.83531	2.65540
C	3.80860	0.55194	3.02904
C	3.98321	-0.76411	3.47213
H	4.08708	1.39173	3.66451
H	3.73764	-2.86333	2.99365
H	4.40690	-0.95344	4.45997
N	2.13795	-2.02268	-0.74649
N	2.43402	2.04197	-0.09574
C	1.70111	-2.82957	-1.72533
C	2.19918	3.18776	-0.76319
C	2.61817	-2.55795	0.41170
C	3.02364	2.08732	1.14026
C	2.65853	-3.93940	0.60523
C	3.37084	3.30122	1.72695
C	2.19849	-4.78300	-0.41026
C	3.12037	4.49347	1.03623
C	1.71265	-4.22026	-1.59184
C	2.53100	4.43426	-0.22598
H	1.36142	-2.33648	-2.63552
H	1.75169	3.07639	-1.75114
H	1.35797	-4.84120	-2.41552
H	2.32444	5.33615	-0.80366
H	2.22930	-5.86629	-0.28054
H	3.39108	5.45240	1.48196
H	3.05336	-4.35084	1.53412
H	3.84344	3.32026	2.70870
C	-4.69020	-0.81511	-0.81884
C	-4.44879	-0.68938	1.68055
C	-4.53465	1.43585	0.34032
H	-4.32374	-1.85558	-0.80261
H	-4.40526	-0.36350	-1.78300
C	-6.22648	-0.77740	-0.66935
H	-3.98874	-0.14666	2.52408
H	-4.10805	-1.73861	1.70325
C	-5.98741	-0.65639	1.82823
H	-4.24811	1.92948	-0.60212
H	-4.05942	1.98073	1.17366
C	-6.07222	1.46058	0.48098
H	-6.66819	-1.33107	-1.51136
C	-6.62664	-1.43450	0.66377
C	-6.70339	0.68825	-0.69419
H	-6.24593	-1.13109	2.78642
C	-6.47227	0.80467	1.81453
H	-6.40207	2.51011	0.46186
H	-6.29862	-2.48800	0.68333
H	-7.72282	-1.42622	0.77016
H	-6.42798	1.16165	-1.65221
H	-7.80115	0.72233	-0.61253
H	-7.56708	0.83303	1.93150
H	-6.03310	1.36095	2.66029
O	3.19127	-0.44901	-2.40002
H	2.97633	0.13378	-3.15922

69			
adnb30 | bs90-adnb30.fchk			
Ru	2.11763	0.00391	-0.81517
C	0.16656	-0.00675	-0.12560
C	-0.75734	0.01558	-1.19745
C	-0.41321	-0.03498	1.16047
C	-2.11997	0.01542	-0.98749
C	-1.79005	-0.03892	1.32926
N	-2.64040	-0.01282	0.26698
C	-0.20977	0.03565	-2.61136
O	-0.95404	0.05935	-3.57985
O	1.10199	0.02208	-2.63151
C	-4.15236	-0.01048	0.41789
H	0.20459	-0.05570	2.06197
H	-2.24329	-0.06267	2.31551
H	-2.80415	0.03718	-1.83393
N	3.08964	-0.00416	0.88830
C	3.42211	-1.19554	1.45677
C	3.41799	1.18245	1.46919
C	4.12253	-1.22297	2.66500
C	4.11829	1.19956	2.67763
C	4.47475	-0.01426	3.27528
H	4.38221	2.14767	3.14615
H	4.38982	-2.17501	3.12355
H	5.02436	-0.01820	4.21729
N	2.24003	-2.04059	-0.44661
N	2.23278	2.04430	-0.42486
C	1.78763	-3.02127	-1.24780
C	1.77884	3.03194	-1.21659
C	2.95834	-2.35332	0.67663
C	2.95093	2.34712	0.70120
C	3.21216	-3.68636	1.01278
C	3.20259	3.67719	1.05029
C	2.73588	-4.70259	0.18471
C	2.72448	4.70070	0.23224
C	2.01483	-4.36669	-0.96679
C	2.00387	4.37491	-0.92238
H	1.24835	-2.68420	-2.13489
H	1.24082	2.70291	-2.10744
H	1.63678	-5.13215	-1.64531
H	1.62472	5.14627	-1.59356
H	2.93229	-5.74757	0.43103
H	2.91941	5.74355	0.48860
H	3.78834	-3.92021	1.90803
H	3.77885	3.90327	1.94748
C	-4.72294	-1.24974	-0.30779
C	-4.57558	-0.05914	1.89677
C	-4.70738	1.28256	-0.21992
H	-4.31179	-2.16125	0.15816
H	-4.42059	-1.24264	-1.36656
C	-6.26203	-1.23719	-0.21347
H	-4.17352	0.81659	2.43332
H	-4.18021	-0.97241	2.37240
C	-6.11671	-0.05433	1.99689
H	-4.40374	1.34374	-1.27668
H	-4.28501	2.15451	0.30781
C	-6.24657	1.28240	-0.12466
H	-6.65193	-2.11881	-0.74505
C	-6.68339	-1.28531	1.26615
C	-6.80183	0.05045	-0.86670
H	-6.39080	-0.09033	3.06245
C	-6.66720	1.23228	1.35526
H	-6.62583	2.20380	-0.59278
H	-6.31118	-2.21166	1.73673
H	-7.78282	-1.28985	1.34391
H	-6.50998	0.08626	-1.93039
H	-7.90316	0.05549	-0.82359
H	-7.76646	1.24606	1.43412
H	-6.28259	2.11823	1.88942
O	3.78918	0.01203	-1.85647
H	3.55681	0.01982	-2.80255

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adnb20 | bs90-adnb20.fchk

Ru	2.11007	-0.00040	-0.76902
C	0.21049	-0.00006	-0.16314
C	-0.73933	-0.00249	-1.23343
C	-0.38821	0.00282	1.13295
C	-2.09097	-0.00248	-1.01996
C	-1.75506	0.00329	1.30548
N	-2.62207	0.00063	0.24317
C	-0.18825	-0.00469	-2.64600
O	-0.94075	-0.00727	-3.61963
O	1.11271	-0.00327	-2.65723
C	-4.11476	0.00041	0.38956
H	0.23389	0.00496	2.03187
H	-2.20068	0.00582	2.29586
H	-2.77205	-0.00487	-1.86952
N	2.94539	0.00139	0.94647
C	3.26086	-1.19609	1.54746
C	3.25970	1.20006	1.54568
C	3.86045	-1.20813	2.80651
C	3.85927	1.21455	2.80472
C	4.15485	0.00383	3.44566
H	4.10347	2.16651	3.27834
H	4.10556	-2.15914	3.28155
H	4.62476	0.00478	4.42998
N	2.31028	-2.03066	-0.47923
N	2.30869	2.03053	-0.48246
C	1.97581	-3.01790	-1.33188
C	1.97329	3.01614	-1.33663
C	2.90377	-2.34832	0.71892
C	2.90158	2.35065	0.71534
C	3.13494	-3.68514	1.07199
C	3.13122	3.68825	1.06646
C	2.77143	-4.70090	0.19267
C	2.76677	4.70230	0.18557
C	2.18416	-4.36101	-1.03572
C	2.18011	4.35993	-1.04244
H	1.53241	-2.67651	-2.26949
H	1.53034	2.67284	-2.27374
H	1.89669	-5.12545	-1.75914
H	1.89190	5.12298	-1.76703
H	2.95001	-5.74582	0.45415
H	2.94412	5.74779	0.44553
H	3.60639	-3.91472	2.02836
H	3.60218	3.91977	2.02260
C	-4.68806	-1.26788	-0.28504
C	-4.54911	0.00613	1.86783
C	-4.68970	1.26251	-0.29530
H	-4.27014	-2.15715	0.21654
H	-4.37919	-1.30141	-1.34094
C	-6.22595	-1.26389	-0.19382
H	-4.14838	0.90126	2.37177
H	-4.14778	-0.88467	2.37890
C	-6.08877	0.00569	1.96806
H	-4.38098	1.28806	-1.35146
H	-4.27296	2.15636	0.19907
C	-6.22758	1.25727	-0.20424
H	-6.61378	-2.16785	-0.68995
C	-6.64964	-1.25577	1.28622
C	-6.77525	-0.00653	-0.89671
H	-6.36671	0.00994	3.03413
C	-6.65138	1.26069	1.27577
H	-6.61650	2.15663	-0.70781
H	-6.26992	-2.16031	1.79245
H	-7.75006	-1.26399	1.36460
H	-6.47978	-0.01075	-1.96008
H	-7.87777	-0.00704	-0.85539
H	-7.75181	1.26795	1.35401
H	-6.27302	2.16992	1.77454
O	3.85870	-0.00052	-1.81855
H	3.62552	-0.00235	-2.76040

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adna40 | bs90-adna40.fchk

Ru	2.06579	-0.00414	0.74046
C	0.14360	0.00675	0.20422
C	-0.79423	-0.01068	1.28087
C	-0.44046	0.02934	-1.08521
C	-2.16288	-0.00919	1.06586
C	-1.82062	0.03440	-1.25155
N	-2.67892	0.01482	-0.19044
C	-0.33191	-0.02895	2.69536
O	-0.98077	-0.04681	3.69102
O	1.08079	-0.01997	2.71914
C	-4.18861	0.01414	-0.35879
H	0.17298	0.04463	-1.98675
H	-2.26646	0.05457	-2.24289
H	-2.85973	-0.02666	1.90320
N	2.76714	0.00446	-1.10832
C	3.03284	1.19906	-1.69246
C	3.02828	-1.18533	-1.70428
C	3.52797	1.22808	-3.00620
C	3.52349	-1.20323	-3.01801
C	3.75214	0.01529	-3.67124
H	3.74771	-2.14716	-3.51682
H	3.75574	2.17602	-3.49569
H	4.13792	0.01952	-4.69336
N	2.40634	2.00939	0.48814
N	2.39654	-2.01548	0.46725
C	2.32128	2.97653	1.42836
C	2.30752	-2.99144	1.39805
C	2.82814	2.34373	-0.79265
C	2.81881	-2.33836	-0.81620
C	3.10945	3.66683	-1.13005
C	3.09641	-3.65896	-1.16612
C	2.99865	4.66395	-0.15351
C	2.98173	-4.66515	-0.19934
C	2.60369	4.31182	1.14679
C	2.58627	-4.32466	1.10398
H	1.99709	2.65642	2.41963
H	1.98299	-2.67975	2.39187
H	2.50858	5.06308	1.93371
H	2.48816	-5.08326	1.88346
H	3.23289	5.70289	-0.39929
H	3.21341	-5.70232	-0.45488
H	3.43981	3.91846	-2.13876
H	3.42715	-3.90189	-2.17682
C	-4.78381	1.25348	0.39473
C	-4.61036	0.06124	-1.83394
C	-4.76482	-1.28651	0.30455
H	-4.37283	2.16803	-0.06332
H	-4.50534	1.23613	1.45934
C	-6.30789	1.21596	0.26059
H	-4.21189	-0.81213	-2.37839
H	-4.21777	0.97201	-2.31848
C	-6.14518	0.05732	-1.95144
H	-4.48400	-1.33698	1.36750
H	-4.34039	-2.15925	-0.21782
C	-6.28903	-1.25823	0.17036
H	-6.72874	2.06353	0.84712
C	-6.75209	1.27237	-1.18682
C	-6.89679	-0.05637	0.95724
H	-6.42094	0.08965	-3.01338
C	-6.73247	-1.22599	-1.27802
H	-6.69684	-2.15611	0.69062
H	-6.38666	2.19318	-1.68281
H	-7.84815	1.25997	-1.26520
H	-6.61585	-0.08968	2.02019
H	-7.99220	-0.06047	0.87917
H	-7.82846	-1.22465	-1.35676
H	-6.35004	-2.09966	-1.84003
O	4.17558	-0.01361	1.52717
H	4.47900	-0.03524	2.45009
H	4.97962	0.01431	0.98174
H	1.39145	-0.02767	3.64777

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adna30 | bs90-adna30.fchk

Ru	-2.14014	-0.00413	-0.82275
C	-0.18697	0.00753	-0.27468
C	0.76013	-0.01265	-1.32764
C	0.35380	0.03483	1.01997
C	2.12841	-0.01064	-1.08293
C	1.73290	0.04062	1.21408
N	2.60754	0.01685	0.17728
C	0.30839	-0.03299	-2.73356
O	0.93025	-0.05585	-3.74667
O	-1.12009	-0.01840	-2.74731
C	4.14780	0.01457	0.37949
H	-0.28291	0.05314	1.90532
H	2.16573	0.06411	2.21118
H	2.85121	-0.03026	-1.89785
N	-2.97043	0.00149	0.97946
C	-3.26371	1.19528	1.55635
C	-3.25375	-1.18920	1.56775
C	-3.89053	1.22121	2.80622
C	-3.88030	-1.20836	2.81788
C	-4.19941	0.00807	3.43305
H	-4.11367	-2.15387	3.30769
H	-4.13189	2.16938	3.28694
H	-4.68872	0.01067	4.40910
N	-2.21127	2.04942	-0.42961
N	-2.19578	-2.05434	-0.41056
C	-1.77638	3.04420	-1.22864
C	-1.75493	-3.05349	-1.20082
C	-2.85218	2.35879	0.74725
C	-2.83365	-2.35723	0.76962
C	-3.07256	3.68493	1.11546
C	-3.04435	-3.68146	1.15030
C	-2.63352	4.71383	0.27339
C	-2.59881	-4.71504	0.31746
C	-1.97539	4.38915	-0.91651
C	-1.94417	-4.39681	-0.87610
H	-1.26752	2.73893	-2.14410
H	-1.24975	-2.75363	-2.12005
H	-1.61834	5.16186	-1.59925
H	-1.58260	-5.17325	-1.55221
H	-2.80345	5.75718	0.54771
H	-2.76122	-5.75697	0.60155
H	-3.58598	3.91713	2.04890
H	-3.55549	-3.90863	2.08621
C	4.72559	1.25337	-0.33769
C	4.49893	0.06743	1.87195
C	4.70353	-1.28394	-0.24255
H	4.30148	2.16870	0.10864
H	4.46904	1.23608	-1.41032
C	6.26488	1.23632	-0.18509
H	4.08208	-0.81065	2.39500
H	4.09135	0.98585	2.32899
C	6.04051	0.06120	2.02406
H	4.44458	-1.34061	-1.31338
H	4.26371	-2.15562	0.27109
C	6.24284	-1.28219	-0.08936
H	6.66735	2.11743	-0.70639
C	6.62810	1.29145	1.30921
C	6.82404	-0.05365	-0.81614
H	6.27221	0.10012	3.09827
C	6.60521	-1.23045	1.40555
H	6.63008	-2.20715	-0.54178
H	6.24320	2.22017	1.76362
H	7.72284	1.29707	1.42487
H	6.57758	-0.09244	-1.89118
H	7.92155	-0.05989	-0.73143
H	7.69969	-1.24767	1.52245
H	6.20299	-2.11462	1.92868
O	-4.21803	-0.01668	-1.61645
H	-4.52442	-0.01722	-2.53773
H	-5.01614	-0.01898	-1.06264
H	-1.43267	-0.02921	-3.67347

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adna20 | bs90-adna20.fchk

Ru	2.13809	0.00375	-0.78618
C	0.23655	-0.01096	-0.26412
C	-0.72646	0.00011	-1.32358
C	-0.34920	-0.02980	1.02934
C	-2.09050	-0.00207	-1.09188
C	-1.71824	-0.03470	1.21088
N	-2.59236	-0.01980	0.16231
C	-0.27862	0.01395	-2.73263
O	-0.92948	0.02830	-3.73852
O	1.12305	0.00642	-2.76620
C	-4.11278	-0.01661	0.34165
H	0.27646	-0.04088	1.92282
H	-2.15725	-0.05021	2.20408
H	-2.79858	0.01063	-1.91879
N	2.84148	0.00527	1.02922
C	3.09878	-1.18425	1.63959
C	3.08094	1.19646	1.64375
C	3.60170	-1.20404	2.94356
C	3.58357	1.21925	2.94774
C	3.83885	0.00831	3.59992
H	3.77749	2.16782	3.44805
H	3.80997	-2.15131	3.44057
H	4.23057	0.00949	4.61802
N	2.33559	-2.05732	-0.46804
N	2.30432	2.06607	-0.46048
C	2.05259	-3.07034	-1.30908
C	2.00585	3.07779	-1.29771
C	2.80504	-2.35418	0.78898
C	2.76955	2.36510	0.79753
C	2.99014	-3.67665	1.19866
C	2.93475	3.68868	1.21207
C	2.69438	-4.71905	0.31722
C	2.62319	4.72981	0.33454
C	2.21830	-4.41075	-0.95991
C	2.15141	4.41923	-0.94362
H	1.67819	-2.77707	-2.29126
H	1.63589	2.78263	-2.28101
H	1.97531	-5.19201	-1.68122
H	1.89663	5.19942	-1.66202
H	2.83514	-5.75667	0.62471
H	2.74853	5.76827	0.64582
H	3.36453	-3.88930	2.20005
H	3.30609	3.90328	2.21417
C	-4.69254	-1.26327	-0.36135
C	-4.49467	-0.05152	1.83042
C	-4.67612	1.27082	-0.29773
H	-4.27066	-2.17135	0.10170
H	-4.41850	-1.26315	-1.42910
C	-6.23084	-1.24970	-0.23038
H	-4.08223	0.83086	2.34852
H	-4.08941	-0.96158	2.30456
C	-6.03463	-0.04595	1.96533
H	-4.40046	1.31934	-1.36405
H	-4.24248	2.14892	0.21027
C	-6.21441	1.27069	-0.16605
H	-6.63021	-2.13696	-0.74431
C	-6.61507	-1.28484	1.25959
C	-6.78565	0.03156	-0.88328
H	-6.28221	-0.07178	3.03702
C	-6.59798	1.23523	1.32427
H	-6.60246	2.18804	-0.63384
H	-6.23265	-2.20678	1.73015
H	-7.71174	-1.28992	1.36244
H	-6.52252	0.05729	-1.95486
H	-7.88491	0.03681	-0.81319
H	-7.69446	1.25041	1.42802
H	-6.20258	2.12654	1.84091
O	4.18457	0.02192	-1.77973
H	4.76929	-0.74411	-1.66506
H	4.75310	0.80060	-1.66894
H	1.43470	0.01531	-3.68975

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Ru	1.69555	-0.99966	-0.53511
C	3.53898	-0.06505	-0.49716
C	3.60034	0.99643	0.43691
C	4.72178	-0.27952	-1.23568
C	4.73932	1.75285	0.61080
C	5.84620	0.50770	-1.03287
N	5.86156	1.51324	-0.11664
C	2.34235	1.30017	1.21633
O	2.29187	2.19579	2.05613
O	1.35733	0.51731	0.87496
C	7.08131	2.39031	0.12833
H	4.78741	-1.06916	-1.98826
H	6.76078	0.35024	-1.59631
H	4.75678	2.56718	1.33246
N	2.13428	-2.37924	-1.85145
C	2.66170	-3.55920	-1.41697
C	1.93763	-2.12432	-3.17695
C	2.99260	-4.55796	-2.33899
C	2.25818	-3.09370	-4.12648
C	2.78291	-4.32261	-3.70011
H	2.10662	-2.89440	-5.18737
H	3.41535	-5.50282	-1.99742
H	3.03744	-5.08977	-4.43251
N	2.51308	-2.44973	0.69639
N	1.25002	0.01091	-2.32148
C	2.68166	-2.36815	2.02819
C	0.77280	1.25765	-2.44585
C	2.86493	-3.59726	0.03620
C	1.39950	-0.77503	-3.43445
C	3.40977	-4.68382	0.73148
C	1.05472	-0.29699	-4.69893
C	3.58680	-4.59529	2.11066
C	0.54458	0.99988	-4.82204
C	3.21600	-3.41678	2.77213
C	0.39804	1.78861	-3.68060
H	2.36242	-1.42572	2.47632
H	0.66409	1.81127	-1.51664
H	3.33547	-3.30995	3.85100
H	-0.02955	2.78905	-3.72066
H	4.00943	-5.43474	2.66544
H	0.25952	1.38416	-5.80321
H	3.69067	-5.58759	0.19052
H	1.17642	-0.93434	-5.57491
C	7.50966	2.23159	1.60403
C	8.25774	1.99186	-0.78047
C	6.69870	3.85900	-0.15984
H	7.77213	1.17659	1.79215
H	6.67478	2.49927	2.27105
C	8.71432	3.15129	1.89112
H	7.96778	2.09257	-1.83991
H	8.54203	0.94287	-0.59245
C	9.46763	2.90775	-0.49247
H	5.84856	4.16135	0.47173
H	6.38975	3.95172	-1.21483
C	7.90709	4.77105	0.13580
H	8.99992	3.03354	2.94768
C	9.88917	2.75239	0.98007
C	8.31434	4.61408	1.61436
H	10.29262	2.60196	-1.15367
C	9.08243	4.37143	-0.77397
H	7.61404	5.81321	-0.06347
H	10.18949	1.70973	1.18170
H	10.75970	3.39555	1.18692
H	7.47730	4.90882	2.27069
H	9.16279	5.28031	1.83878
H	9.94686	5.02691	-0.58045
H	8.80158	4.49428	-1.83409
O	0.00001	-1.69313	0.00004

Ru	-1.69556	-0.99963	0.53510
C	-3.53902	-0.06505	0.49719
N	-2.13413	-2.37924	1.85145
C	-3.60043	0.99637	-0.43695
C	-4.72177	-0.27948	1.23578
C	-2.66148	-3.55923	1.41698
C	-1.93739	-2.12436	3.17694
C	-4.73942	1.75277	-0.61082
C	-2.34250	1.30004	-1.21649
C	-5.84621	0.50772	1.03298
H	-4.78736	-1.06907	1.98842
C	-2.99222	-4.55805	2.33899
C	-2.86483	-3.59727	-0.03618
C	-2.25778	-3.09379	4.12647
C	-1.39934	-0.77504	3.43443
N	-5.86162	1.51321	0.11669
H	-4.75693	2.56704	-1.33255
O	-2.29207	2.19566	-2.05630
O	-1.35745	0.51721	-0.87515
H	-6.76076	0.35028	1.59647
C	-2.78244	-4.32274	3.70010
H	-3.41492	-5.50293	1.99741
N	-2.51310	-2.44971	-0.69638
C	-3.40966	-4.68385	-0.73144
H	-2.10614	-2.89452	5.18736
N	-1.25000	0.01094	2.32147
C	-1.05453	-0.29699	4.69891
C	-7.08140	2.39023	-0.12829
H	-3.03685	-5.08994	4.43249
C	-2.68179	-2.36811	-2.02816
C	-3.58681	-4.59529	-2.11061
H	-3.69046	-5.58765	-0.19048
C	-0.77288	1.25771	2.44584
C	-0.54449	0.99992	4.82200
H	-1.17613	-0.93436	5.57488
C	-7.50970	2.23153	-1.60400
C	-8.25783	1.99173	0.78047
C	-6.69885	3.85894	0.15991
C	-3.21613	-3.41676	-2.77209
H	-2.36263	-1.42565	-2.47630
H	-4.00944	-5.43476	-2.66537
C	-0.39809	1.78869	3.68057
H	-0.66425	1.81136	1.51663
H	-0.25942	1.38421	5.80317
H	-7.77212	1.17651	-1.79215
H	-6.67481	2.49925	-2.27099
C	-8.71439	3.15118	-1.89111
H	-7.96790	2.09242	1.83992
H	-8.54208	0.94273	0.59242
C	-9.46775	2.90757	0.49246
H	-5.84871	4.16134	-0.47164
H	-6.38992	3.95166	1.21491
C	-7.90728	4.77094	-0.13574
H	-3.33570	-3.30991	-3.85094
H	0.02943	2.78916	3.72062
H	-8.99995	3.03343	-2.94768
C	-9.88925	2.75221	-0.98009
C	-8.31448	4.61398	-1.61431
H	-10.29275	2.60174	1.15363
C	-9.08262	4.37126	0.77400
H	-7.61427	5.81311	0.06356
H	-10.18953	1.70955	-1.18175
H	-10.75980	3.39534	-1.18696
H	-7.47744	4.90877	-2.27061
H	-9.16295	5.28018	-1.83874
H	-9.94708	5.02671	0.58046
H	-8.80180	4.49410	1.83413

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Ru	1.80086	-1.09261	-0.49901
C	3.72204	-0.45203	-0.29302
C	3.84434	0.80681	0.36621
C	4.95956	-0.99546	-0.72762
C	5.05242	1.43686	0.53763
C	6.15630	-0.33133	-0.53245
N	6.21525	0.88287	0.09010
C	2.56614	1.44246	0.86128
O	2.55156	2.52626	1.45381
O	1.53318	0.71137	0.58419
C	7.49713	1.66257	0.26737
H	4.99691	-1.96161	-1.23682
H	7.09931	-0.75035	-0.87032
H	5.09970	2.40540	1.03154
N	2.10983	-2.74604	-1.41819
C	2.20087	-3.90731	-0.68903
C	2.11779	-2.76736	-2.79126
C	2.38246	-5.12789	-1.34309
C	2.29523	-3.97122	-3.46987
C	2.44113	-5.16058	-2.74060
H	2.30392	-3.98595	-4.56017
H	2.46596	-6.04827	-0.76396
H	2.58007	-6.10836	-3.26165
N	1.91979	-2.36787	1.11599
N	1.74700	-0.42769	-2.46693
C	1.78404	-2.05279	2.41835
C	1.53702	0.82655	-2.90424
C	2.08490	-3.68315	0.75090
C	1.90581	-1.44128	-3.37834
C	2.13197	-4.69258	1.72455
C	1.85198	-1.18159	-4.75408
C	1.99549	-4.35907	3.06785
C	1.63192	0.11892	-5.19959
C	1.81417	-3.01213	3.42317
C	1.47248	1.14456	-4.25702
H	1.63526	-0.99007	2.61574
H	1.40967	1.57316	-2.12009
H	1.69548	-2.70946	4.46451
H	1.29254	2.17605	-4.56258
H	2.02639	-5.13702	3.83297
H	1.58020	0.33224	-6.26876
H	2.26716	-5.73012	1.41758
H	1.97190	-2.00128	-5.46268
C	7.71893	1.93941	1.77153
C	8.71461	0.89407	-0.27878
C	7.36618	2.99708	-0.50096
H	7.80979	0.97744	2.30387
H	6.85361	2.47673	2.18949
C	8.99165	2.78926	1.96119
H	8.57726	0.68669	-1.35293
H	8.81941	-0.06791	0.25026
C	9.99434	1.73531	-0.08428
H	6.49158	3.55634	-0.13319
H	7.20444	2.77943	-1.57033
C	8.64102	3.84017	-0.30366
H	9.12545	2.98723	3.03617
C	10.20543	2.01661	1.41442
C	8.83682	4.12039	1.19930
H	10.84633	1.16256	-0.48225
C	9.85439	3.06493	-0.84834
H	8.52526	4.78947	-0.84968
H	10.33012	1.06833	1.96504
H	11.12413	2.60962	1.55568
H	7.97331	4.68324	1.59420
H	9.73565	4.74106	1.34898
H	10.77143	3.66396	-0.72290
H	9.72593	2.87050	-1.92714
O	-0.15235	-1.31090	-0.49533
Ru	-1.81349	-0.43224	0.03276
C	-3.72660	0.20595	0.29092
N	-1.20984	0.24307	1.74952
C	-4.54905	-0.02270	-0.84679
C	-4.38835	0.84462	1.37111
C	-1.26413	-0.56942	2.84286
C	-0.74165	1.52068	1.81931
C	-5.86832	0.35631	-0.88619
C	-3.91657	-0.72236	-2.03452
C	-5.71710	1.21684	1.28922
H	-3.85849	1.07100	2.30011
C	-0.83329	-0.09304	4.08196
C	-1.75109	-1.92600	2.53291
C	-0.28534	2.02831	3.03542
C	-0.75837	2.20838	0.52275
N	-6.46365	0.98154	0.17077
H	-6.46582	0.15602	-1.77374
O	-4.56481	-0.94301	-3.05465
O	-2.67017	-1.03040	-1.81762
H	-6.21814	1.71681	2.11240
C	-0.33606	1.21447	4.17280
H	-0.87351	-0.73561	4.96211
N	-2.12048	-2.12871	1.23001
C	-1.80147	-2.97065	3.46159
H	0.13658	3.03032	3.08271
N	-1.25694	1.46505	-0.51768
C	-0.28636	3.50731	0.32065
C	-7.91927	1.36311	0.05195
H	0.01922	1.59645	5.13100
C	-2.51221	-3.34822	0.83173
C	-2.22900	-4.23319	3.04930
H	-1.49621	-2.79365	4.49290
C	-1.32223	2.01032	-1.74660
C	-0.35043	4.06536	-0.95490
H	0.16036	4.05025	1.15109
C	-8.75376	0.07810	-0.14749
C	-8.42404	2.09117	1.31189
C	-8.09613	2.29989	-1.16520
C	-2.58610	-4.42924	1.71106
H	-2.76520	-3.42570	-0.22761
H	-2.27511	-5.05763	3.76347
C	-0.88757	3.30779	-2.00460
H	-1.72633	1.35084	-2.51682
H	0.01917	5.07729	-1.13065
H	-8.61418	-0.57926	0.72748
H	-8.39822	-0.46443	-1.03749
C	-10.24063	0.44537	-0.32069
H	-7.83241	3.00675	1.47878
H	-8.31110	1.43940	2.19416
C	-9.91319	2.45985	1.14366
H	-7.73046	1.80586	-2.07830
H	-7.49220	3.20963	-1.00771
C	-9.58568	2.65757	-1.33690
H	-2.91780	-5.40263	1.34719
H	-0.95956	3.70893	-3.01686
H	-10.81783	-0.48040	-0.47085
C	-10.73741	1.17504	0.94100
C	-10.39938	1.36516	-1.54729
H	-10.24519	2.97786	2.05695
C	-10.08375	3.38449	-0.07508
H	-9.69142	3.31335	-2.21525
H	-10.63756	0.51793	1.82221
H	-11.80452	1.43026	0.83232
H	-10.05287	0.84515	-2.45690
H	-11.46381	1.61482	-1.69031
H	-11.14616	3.65617	-0.19040
H	-9.51374	4.31788	0.07413

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Ru	2.08989	-0.00860	-0.76933
C	0.22633	0.00845	-0.14699
C	-0.70154	-0.03339	-1.23050
C	-0.36548	0.05752	1.14043
C	-2.05864	-0.03355	-1.02085
C	-1.73946	0.05993	1.29768
N	-2.58998	0.01350	0.23351
C	-0.15053	-0.06925	-2.64308
O	-0.88689	-0.10811	-3.61750
O	1.16211	-0.04783	-2.65125
C	-4.09772	0.00858	0.37481
H	0.24966	0.09371	2.04190
H	-2.19500	0.09822	2.28254
H	-2.73822	-0.07041	-1.87041
N	2.92897	0.01852	0.98426
C	3.21562	-1.16614	1.60196
C	3.20748	1.21936	1.57398
C	3.79420	-1.16774	2.87285
C	3.78599	1.25654	2.84491
C	4.07680	0.05303	3.49787
H	4.00969	2.21218	3.31970
H	4.02451	-2.11013	3.37032
H	4.52774	0.06600	4.49079
N	2.28627	-2.04522	-0.43121
N	2.28553	2.03943	-0.48769
C	1.93390	-3.05343	-1.25095
C	1.91294	3.02665	-1.32688
C	2.85576	-2.33778	0.78490
C	2.84022	2.36765	0.72823
C	3.06973	-3.66242	1.17775
C	3.02717	3.70458	1.09429
C	2.70107	-4.70148	0.32299
C	2.64346	4.71923	0.21740
C	2.12373	-4.39220	-0.91338
C	2.07533	4.37482	-1.01482
H	1.48808	-2.74240	-2.19797
H	1.46901	2.68718	-2.26532
H	1.82284	-5.17369	-1.61223
H	1.75769	5.13701	-1.72755
H	2.86449	-5.73965	0.61717
H	2.78454	5.76593	0.49226
H	3.52589	-3.87333	2.14525
H	3.47112	3.94336	2.06106
C	-4.64776	-1.29715	-0.24157
C	-4.53127	0.08274	1.85009
C	-4.67144	1.23180	-0.37578
H	-4.22502	-2.15798	0.30391
H	-4.33732	-1.37696	-1.29513
C	-6.18710	-1.30121	-0.15504
H	-4.14064	1.00546	2.31121
H	-4.12873	-0.78151	2.40456
C	-6.07255	0.07462	1.94229
H	-4.36268	1.20692	-1.43246
H	-4.26549	2.15318	0.07523
C	-6.21061	1.21629	-0.29019
H	-6.56168	-2.23221	-0.60797
C	-6.61591	-1.22528	1.32144
C	-6.74295	-0.08501	-0.92223
H	-6.35329	0.12923	3.00545
C	-6.64021	1.28976	1.18600
H	-6.60151	2.08655	-0.83974
H	-6.23080	-2.09994	1.87364
H	-7.71565	-1.24139	1.39513
H	-6.44494	-0.13933	-1.98348
H	-7.84461	-0.09303	-0.88489
H	-7.74017	1.29176	1.25823
H	-6.27346	2.22593	1.64129
O	3.92382	-0.09488	-2.13418
H	3.46613	-0.14979	-2.99488
H	4.43564	0.72744	-2.18136

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Ru	1.93514	0.38408	0.04167
C	3.78596	-0.28568	0.22166
C	4.66960	0.24187	-0.76919
C	4.40088	-1.18873	1.13262
C	5.99580	-0.10276	-0.82104
C	5.74057	-1.50777	1.03988
N	6.54735	-0.97512	0.07428
C	4.09150	1.21116	-1.78205
O	4.78713	1.69835	-2.66802
O	2.82051	1.42852	-1.57602
C	8.01559	-1.29534	-0.04884
H	3.82152	-1.65787	1.93132
H	6.20720	-2.20019	1.73394
H	6.63684	0.32338	-1.59075
N	1.22753	-0.63866	1.51223
C	1.24135	-0.10529	2.77284
C	0.74430	-1.89776	1.27502
C	0.75812	-0.85073	3.85179
C	0.22561	-2.65542	2.32128
C	0.23881	-2.12919	3.62207
H	-0.21009	-3.63210	2.11867
H	0.77665	-0.42953	4.85779
H	-0.15909	-2.71583	4.45116
N	2.15444	1.75374	1.57438
N	1.34976	-1.32057	-0.96692
C	2.59131	3.02459	1.48360
C	1.40916	-1.54981	-2.29116
C	1.74952	1.26965	2.79552
C	0.80427	-2.27114	-0.14423
C	1.80365	2.07392	3.94021
C	0.30648	-3.47128	-0.65830
C	2.26729	3.38357	3.84036
C	0.37118	-3.70384	-2.03003
C	2.66499	3.87015	2.58727
C	0.93392	-2.72727	-2.86321
H	2.88633	3.33553	0.47946
H	1.85599	-0.74290	-2.87545
H	3.03079	4.89047	2.46360
H	1.00668	-2.87243	-3.94237
H	2.31573	4.02026	4.72580
H	-0.02181	-4.63262	-2.44798
H	1.47597	1.66864	4.89782
H	-0.17327	-4.18227	0.01052
C	8.82524	0.01168	0.11274
C	8.47573	-2.29628	1.02784
C	8.28059	-1.91096	-1.44154
H	8.62369	0.43554	1.11123
H	8.50210	0.74884	-0.63851
C	10.32852	-0.27979	-0.06068
H	7.90723	-3.23651	0.93347
H	8.29185	-1.87844	2.03161
C	9.98221	-2.58894	0.86321
H	7.94570	-1.21914	-2.22966
H	7.69574	-2.84144	-1.53792
C	9.78625	-2.19495	-1.60847
H	10.88595	0.66403	0.04557
C	10.78092	-1.28142	1.01684
C	10.57387	-0.87763	-1.46003
H	10.28161	-3.30494	1.64452
C	10.23931	-3.19428	-0.52881
H	9.95616	-2.62091	-2.60974
H	10.62040	-0.85436	2.02198
H	11.85869	-1.48873	0.90996
H	10.25894	-0.16011	-2.23729
H	11.65067	-1.06955	-1.60008
H	11.31310	-3.41561	-0.64641
H	9.68697	-4.14378	-0.63657
O	0.19694	1.46920	-0.58586
Ru	-1.88675	1.12672	-0.49808
C	-3.75771	0.45999	-0.33550
N	-2.27124	2.97483	-0.86627
C	-3.85529	-0.92076	0.02413
C	-5.01673	1.09912	-0.50927
C	-2.32639	3.86119	0.17720
C	-2.40189	3.39208	-2.16431
C	-5.05962	-1.55738	0.18350
C	-2.55316	-1.66229	0.21329
C	-6.20643	0.41948	-0.33873
H	-5.07291	2.15549	-0.78307
C	-2.58438	5.21098	-0.06868
C	-2.09454	3.22046	1.47808
C	-2.66345	4.73423	-2.44395
C	-2.19225	2.30321	-3.12958
N	-6.24429	-0.90287	0.00462
H	-5.08955	-2.61053	0.45660
O	-2.50958	-2.84473	0.56570
O	-1.53187	-0.90129	-0.03705
H	-7.16428	0.91322	-0.47078
C	-2.76576	5.64784	-1.38678
H	-2.63582	5.91727	0.76064
N	-1.88423	1.86319	1.42234
C	-2.08401	3.89660	2.70361
H	-2.77213	5.06697	-3.47670
N	-1.91608	1.08094	-2.56604
C	-2.22378	2.46205	-4.52008
C	-7.52812	-1.67892	0.17420
H	-2.96902	6.69959	-1.59130
C	-1.66608	1.18236	2.56151
C	-1.85342	3.18490	3.87957
H	-2.25150	4.97377	2.72699
C	-1.64854	0.03169	-3.36638
C	-1.95893	1.36824	-5.34204
H	-2.44293	3.44094	-4.94732
C	-7.58247	-2.25513	1.60728
C	-8.76642	-0.79020	-0.04813
C	-7.55055	-2.82909	-0.85728
C	-1.64047	1.80247	3.80658
H	-1.49775	0.11308	2.43298
H	-1.83803	3.70194	4.84067
C	-1.66093	0.13159	-4.75509
H	-1.41466	-0.89693	-2.84275
H	-1.97558	1.47965	-6.42764
H	-7.56248	-1.42168	2.32982
H	-6.69903	-2.88518	1.79408
C	-8.86137	-3.09796	1.78191
H	-8.74761	-0.36765	-1.06645
H	-8.76545	0.04325	0.67405
C	-10.05074	-1.62735	0.13154
H	-6.66458	-3.46931	-0.72305
H	-7.50768	-2.40013	-1.87280
C	-8.83004	-3.66913	-0.67427
H	-1.44831	1.20588	4.69896
H	-1.43679	-0.74600	-5.36291
H	-8.87586	-3.50961	2.80321
C	-10.09467	-2.20454	1.55797
C	-8.85911	-4.24717	0.75447
H	-10.91715	-0.96804	-0.03300
C	-10.06321	-2.77420	-0.89534
H	-8.82336	-4.48879	-1.40965
H	-10.10903	-1.38580	2.29805
H	-11.01672	-2.79386	1.69301
H	-7.98128	-4.89617	0.91698
H	-9.76149	-4.86646	0.88744
H	-10.98506	-3.36778	-0.77926
H	-10.05531	-2.36505	-1.92039
H	0.48368	1.92825	-1.39058

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Ru	2.09097	-0.06859	-0.71816
C	0.13172	0.03690	-0.12980
C	-0.75728	-0.30449	-1.16583
C	-0.44773	0.39341	1.09850
C	-2.12629	-0.29902	-0.97211
C	-1.83121	0.37707	1.24666
N	-2.65932	0.03700	0.22613
C	-0.17175	-0.69647	-2.49349
O	-0.82575	-1.00523	-3.46075
O	1.16606	-0.68077	-2.43847
C	-4.18930	0.01930	0.36845
H	0.15412	0.68136	1.96230
H	-2.30404	0.63859	2.18904
H	-2.80264	-0.56626	-1.78238
N	2.93779	0.16814	1.09707
C	3.28828	-0.94322	1.79239
C	3.13526	1.41952	1.58086
C	3.90971	-0.81616	3.03537
C	3.75738	1.59769	2.82041
C	4.15128	0.46763	3.54238
H	3.93035	2.59875	3.21471
H	4.20158	-1.69908	3.60319
H	4.64253	0.58471	4.50982
N	2.27086	-2.06645	-0.07906
N	2.03302	2.01170	-0.45411
C	1.91512	-3.15762	-0.78313
C	1.54199	2.87951	-1.35252
C	2.94106	-2.20871	1.10986
C	2.62886	2.47196	0.68617
C	3.25967	-3.47203	1.60121
C	2.72539	3.84089	0.94046
C	2.89112	-4.60678	0.86752
C	2.21149	4.74671	0.00825
C	2.21074	-4.44821	-0.34083
C	1.61125	4.26002	-1.15527
H	1.39977	-2.96394	-1.72444
H	1.10524	2.44254	-2.25157
H	1.91026	-5.30606	-0.94373
H	1.21271	4.93242	-1.91602
H	3.13932	-5.60259	1.23960
H	2.28829	5.82073	0.18667
H	3.79867	-3.57371	2.54296
H	3.20591	4.19396	1.85298
C	-4.68689	-1.40692	0.04588
C	-4.62332	0.39984	1.79304
C	-4.77655	1.03491	-0.63511
H	-4.24770	-2.11754	0.76649
H	-4.37273	-1.70464	-0.96743
C	-6.22828	-1.43228	0.12833
H	-4.27050	1.41590	2.03914
H	-4.19860	-0.31126	2.52205
C	-6.16709	0.36460	1.88101
H	-4.46137	0.78481	-1.66117
H	-4.39953	2.04368	-0.39509
C	-6.31736	0.99492	-0.54685
H	-6.56900	-2.44994	-0.11456
C	-6.66690	-1.05453	1.55386
C	-6.80936	-0.42631	-0.88461
H	-6.45424	0.63931	2.90687
C	-6.75681	1.37396	0.87899
H	-6.72326	1.71623	-1.27182
H	-6.26334	-1.77903	2.28181
H	-7.76528	-1.08641	1.62840
H	-6.50705	-0.70097	-1.90980
H	-7.90955	-0.45627	-0.84627
H	-7.85606	1.36256	0.94577
H	-6.41976	2.39583	1.12329
O	3.42440	0.49573	-1.96895
O	3.38915	0.20370	-3.30639
H	2.70090	-0.51231	-3.38623

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adn40-oo | bs90-adn40-oo.fchk

Ru	-2.10525	-0.00706	-0.79575
C	-0.14468	0.00827	-0.15656
C	0.76495	-0.03258	-1.22940
C	0.41991	0.05695	1.13031
C	2.12837	-0.03195	-1.01835
C	1.79859	0.06162	1.29787
N	2.64627	0.01617	0.23552
C	0.19813	-0.06821	-2.63728
O	0.94590	-0.11057	-3.60445
O	-1.10454	-0.04439	-2.63754
C	4.16077	0.01442	0.38653
H	-0.20248	0.09387	2.02732
H	2.25259	0.10146	2.28314
H	2.81058	-0.06843	-1.86597
N	-2.97992	0.01146	0.96403
C	-3.25957	1.20518	1.54772
C	-3.25578	-1.17110	1.57212
C	-3.90514	1.24123	2.78655
C	-3.90128	-1.18344	2.81138
C	-4.23880	0.03466	3.41129
H	-4.13126	-2.12822	3.30377
H	-4.13825	2.19521	3.25933
H	-4.74816	0.04370	4.37582
N	-2.07065	2.03663	-0.35843
N	-2.06349	-2.04012	-0.31523
C	-1.59367	3.00211	-1.15866
C	-1.58580	-3.02073	-1.09628
C	-2.77540	2.35764	0.76783
C	-2.76887	-2.33875	0.81666
C	-2.98734	3.69420	1.11574
C	-2.98039	-3.66823	1.19080
C	-2.47951	4.70085	0.29316
C	-2.47160	-4.69073	0.38849
C	-1.77355	4.35284	-0.86286
C	-1.76520	-4.36541	-0.77381
H	-1.08296	2.65187	-2.05741
H	-1.07625	-2.68806	-2.00227
H	-1.37604	5.11159	-1.53767
H	-1.36743	-5.13708	-1.43363
H	-2.64368	5.74958	0.54724
H	-2.63579	-5.73431	0.66292
H	-3.55632	3.93941	2.01252
H	-3.55024	-3.89607	2.09158
C	4.73095	1.23971	-0.36262
C	4.58388	0.08911	1.86400
C	4.71153	-1.29105	-0.22891
H	4.32172	2.16032	0.08690
H	4.42807	1.21359	-1.42092
C	6.27023	1.22622	-0.26931
H	4.18154	-0.77674	2.41629
H	4.19050	1.01161	2.32334
C	6.12541	0.08384	1.96241
H	4.40729	-1.37032	-1.28427
H	4.28839	-2.15286	0.31469
C	6.25099	-1.29132	-0.13473
H	6.66037	2.09749	-0.81734
C	6.69291	1.30061	1.20875
C	6.80726	-0.07393	-0.89968
H	6.40035	0.13876	3.02686
C	6.67277	-1.21532	1.34368
H	6.62776	-2.22171	-0.58659
H	6.32281	2.23596	1.66288
H	7.79233	1.30491	1.28532
H	6.51464	-0.12862	-1.96229
H	7.90851	-0.07983	-0.85734
H	7.77199	-1.22971	1.42179
H	6.28721	-2.09076	1.89421
O	-3.75411	0.65687	-1.77783
O	-3.75386	-0.69758	-1.76014

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adn40-o | bs90-adn40-o.fchk

Ru	2.28185	-0.04733	0.87306
C	0.26974	-0.02172	0.22725
C	-0.65148	-0.32333	1.24738
C	-0.29780	0.27719	-1.02862
C	-2.01218	-0.32256	1.02824
C	-1.67404	0.27516	-1.20958
N	-2.52771	-0.01870	-0.19182
C	-0.08951	-0.71898	2.59410
O	-0.82968	-1.04580	3.51146
O	1.21553	-0.69141	2.61117
C	-4.03849	-0.03451	-0.35655
H	0.32198	0.52192	-1.89516
H	-2.12364	0.51015	-2.16956
H	-2.69614	-0.57920	1.83508
N	2.94809	0.25242	-0.95466
C	3.03501	1.52419	-1.44570
C	3.22651	-0.83959	-1.73228
C	3.46736	1.73311	-2.76065
C	3.64944	-0.66873	-3.04494
C	3.78268	0.63341	-3.55866
H	3.87517	-1.53550	-3.66595
H	3.54669	2.74701	-3.15283
H	4.12289	0.78135	-4.58422
N	2.15714	2.03098	0.70520
N	2.51133	-2.02212	0.22820
C	1.73033	2.86289	1.67057
C	2.32438	-3.11245	0.98726
C	2.58707	2.53578	-0.49058
C	3.03305	-2.12735	-1.03144
C	2.55558	3.91265	-0.74096
C	3.36245	-3.37526	-1.55741
C	2.10365	4.77508	0.25568
C	3.16223	-4.51830	-0.77443
C	1.68938	4.24297	1.48379
C	2.64212	-4.38845	0.51452
H	1.44042	2.38430	2.60716
H	1.91813	-2.91660	1.98240
H	1.35477	4.88680	2.29800
H	2.47935	-5.25646	1.15413
H	2.08468	5.85241	0.08278
H	3.41966	-5.50205	-1.17128
H	2.89432	4.29798	-1.70293
H	3.78386	-3.45265	-2.55958
C	-4.64856	0.99563	0.61966
C	-4.45919	0.32514	-1.79255
C	-4.55374	-1.45277	-0.02319
H	-4.26467	1.99958	0.37054
H	-4.34595	0.76318	1.65262
C	-6.18602	0.95842	0.51118
H	-4.02679	-0.39793	-2.50441
H	-4.09418	1.33337	-2.05105
C	-5.99938	0.29417	-1.90434
H	-4.25064	-1.73724	0.99642
H	-4.10370	-2.17402	-0.72633
C	-6.09183	-1.47830	-0.12831
H	-6.60457	1.68999	1.21929
C	-6.60503	1.31731	-0.92600
C	-6.68741	-0.45686	0.86070
H	-6.27310	0.55481	-2.93826
C	-6.51032	-1.11827	-1.56472
H	-6.44213	-2.49116	0.12315
H	-6.26061	2.33486	-1.17892
H	-7.70386	1.30633	-1.01045
H	-6.39800	-0.71717	1.89332
H	-7.78779	-0.48540	0.80694
H	-7.60832	-1.14794	-1.65558
H	-6.09625	-1.85350	-2.27618
O	3.50405	0.29136	2.09252

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adn40 | bs90-adn40.fchk

Ru	2.01434	0.00412	-0.85124
C	0.09560	-0.02125	-0.17928
C	-0.82460	0.02937	-1.24470
C	-0.43713	-0.08089	1.11142
C	-2.19462	0.02658	-1.02278
C	-1.82263	-0.08581	1.28144
N	-2.68410	-0.03141	0.23472
C	-0.24783	0.08245	-2.61337
O	-0.80804	0.14016	-3.66484
O	1.15623	0.05509	-2.52639
C	-4.22830	-0.02716	0.42279
H	0.19028	-0.12468	2.00306
H	-2.26923	-0.13324	2.27178
H	-2.90789	0.06970	-1.84541
N	3.30251	-0.00104	0.80653
C	3.77258	-1.18026	1.27611
C	3.75012	1.17672	1.29969
C	4.76513	-1.21447	2.25994
C	4.74230	1.20981	2.28424
C	5.25977	-0.00231	2.75584
H	5.09736	2.16046	2.68350
H	5.13750	-2.16613	2.64068
H	6.03670	-0.00261	3.52316
N	2.10717	-1.94840	-0.21872
N	2.07282	1.94805	-0.18243
C	1.33406	-2.89009	-0.81002
C	1.28716	2.89094	-0.75502
C	3.08932	-2.31984	0.66277
C	3.04753	2.31637	0.70843
C	3.33358	-3.66459	0.93264
C	3.27088	3.65878	1.00717
C	2.55997	-4.64231	0.29773
C	2.48328	4.63806	0.39268
C	1.54614	-4.24773	-0.58226
C	1.47702	4.24628	-0.49698
H	0.55707	-2.53497	-1.48577
H	0.51869	2.54079	-1.44227
H	0.91765	-4.97822	-1.09468
H	0.83855	4.97739	-0.99606
H	2.74151	-5.70106	0.49586
H	2.64869	5.69502	0.61310
H	4.12038	-3.94246	1.63511
H	4.05271	3.93339	1.71635
C	-4.80351	-1.24423	-0.33187
C	-4.59545	-0.11626	1.90976
C	-4.77066	1.28948	-0.17150
H	-4.38918	-2.17288	0.09604
H	-4.53500	-1.20134	-1.40085
C	-6.34434	-1.22356	-0.19579
H	-4.18061	0.74641	2.45943
H	-4.19740	-1.04801	2.34787
C	-6.13876	-0.10632	2.04515
H	-4.50013	1.37256	-1.23771
H	-4.33287	2.14560	0.36961
C	-6.31164	1.29174	-0.03515
H	-6.74525	-2.08893	-0.74382
C	-6.72421	-1.31498	1.29265
C	-6.89021	0.08506	-0.79960
H	-6.38215	-0.17156	3.11549
C	-6.69039	1.20367	1.45401
H	-6.68954	2.22982	-0.46789
H	-6.34873	-2.25689	1.72742
H	-7.82016	-1.31827	1.39634
H	-6.63155	0.15017	-1.87048
H	-7.98853	0.09451	-0.72696
H	-7.78595	1.22380	1.55972
H	-6.28940	2.07200	2.00400
O	3.85490	0.03138	-2.09957
H	3.74314	0.05714	-3.06691
H	4.80775	0.02823	-1.91645

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adn30-ooh | bs90-adn30-ooh.fchk

Ru	2.03705	-0.00299	-0.66332
C	0.10573	0.00446	-0.04024
C	-0.79468	-0.01898	-1.14103
C	-0.51433	0.03043	1.22985
C	-2.16050	-0.01963	-0.96515
C	-1.89412	0.03281	1.35940
N	-2.71668	0.00745	0.27467
C	-0.22837	-0.04023	-2.54619
O	-0.94331	-0.06572	-3.53307
O	1.08899	-0.02552	-2.53381
C	-4.23155	0.00654	0.38015
H	0.07974	0.05055	2.14670
H	-2.37463	0.05493	2.33293
H	-2.82192	-0.04132	-1.82930
N	2.92334	0.01124	1.07630
C	3.22750	-1.17531	1.67373
C	3.22693	1.20686	1.65551
C	3.86315	-1.18647	2.91753
C	3.86265	1.23743	2.89906
C	4.18079	0.03036	3.53140
H	4.10982	2.19024	3.36725
H	4.11067	-2.13185	3.40037
H	4.67959	0.03785	4.50127
N	2.18909	-2.04885	-0.30774
N	2.18892	2.04791	-0.33977
C	1.78751	-3.04946	-1.11151
C	1.78564	3.03552	-1.15874
C	2.81864	-2.34413	0.87513
C	2.81683	2.36256	0.83902
C	3.04468	-3.67048	1.25420
C	3.03939	3.69502	1.19841
C	2.62676	-4.70459	0.41615
C	2.61967	4.71539	0.34471
C	1.98781	-4.39013	-0.78775
C	1.98247	4.38131	-0.85494
H	1.30210	-2.73487	-2.03709
H	1.30142	2.70545	-2.07954
H	1.65098	-5.16808	-1.47384
H	1.64427	5.14815	-1.55278
H	2.80205	-5.74435	0.69767
H	2.79203	5.75968	0.61083
H	3.55149	-3.88676	2.19473
H	3.54465	3.92651	2.13616
C	-4.76902	-1.28317	-0.27929
C	-4.70074	0.05016	1.84568
C	-4.77748	1.24983	-0.35759
H	-4.36527	-2.15772	0.25862
H	-4.43279	-1.34225	-1.32626
C	-6.31008	-1.28030	-0.23315
H	-4.31915	0.96118	2.33665
H	-4.31593	-0.82783	2.39118
C	-6.24436	0.04752	1.89715
H	-4.44212	1.24714	-1.40645
H	-4.37996	2.15851	0.12540
C	-6.31844	1.23956	-0.31218
H	-6.67625	-2.19909	-0.71656
C	-6.77703	-1.23528	1.23312
C	-6.83907	-0.04442	-0.98760
H	-6.55177	0.07979	2.95368
C	-6.78576	1.28252	1.15393
H	-6.69023	2.12406	-0.85195
H	-6.41092	-2.12426	1.77518
H	-7.87825	-1.24707	1.27763
H	-6.51243	-0.07649	-2.04136
H	-7.94120	-0.04770	-0.98097
H	-7.88706	1.28903	1.19763
H	-6.42637	2.20626	1.63936
O	3.77198	-0.01258	-1.72515
O	3.66617	-0.04020	-3.09473
H	2.68003	-0.04424	-3.26368

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adn30 | bs90-adn30.fchk

Ru	2.06140	0.00975	-0.82300
C	0.18160	-0.00542	-0.15448
C	-0.73603	0.04447	-1.23188
C	-0.39014	-0.06048	1.12974
C	-2.10049	0.04633	-1.02852
C	-1.77110	-0.06191	1.28380
N	-2.61871	-0.00788	0.22337
C	-0.16101	0.08715	-2.61782
O	-0.81096	0.13096	-3.63276
O	1.19529	0.06748	-2.58880
C	-4.14394	-0.00200	0.37717
H	0.22291	-0.10321	2.03187
H	-2.22927	-0.10605	2.26759
H	-2.79145	0.08993	-1.86856
N	2.98075	-0.03459	0.98649
C	3.25778	-1.23394	1.55597
C	3.28504	1.13807	1.59533
C	3.87375	-1.28889	2.80939
C	3.90156	1.13534	2.85006
C	4.19444	-0.09059	3.45609
H	4.14988	2.07315	3.34646
H	4.10076	-2.24839	3.27354
H	4.67566	-0.11251	4.43512
N	2.25533	-2.04129	-0.46472
N	2.28103	2.03871	-0.38393
C	1.85060	-3.00940	-1.30985
C	1.90737	3.04339	-1.19815
C	2.85170	-2.38010	0.72112
C	2.90468	2.32105	0.80164
C	3.04824	-3.71812	1.06615
C	3.15441	3.63973	1.18265
C	2.62994	-4.72191	0.18854
C	2.76484	4.68318	0.33843
C	2.02299	-4.36240	-1.01797
C	2.13359	4.38055	-0.87043
H	1.38660	-2.66632	-2.23611
H	1.42519	2.74591	-2.13061
H	1.68424	-5.11395	-1.73223
H	1.81798	5.16359	-1.56097
H	2.77922	-5.77232	0.44457
H	2.95709	5.71952	0.62155
H	3.52836	-3.97141	2.01142
H	3.65638	3.84764	2.12757
C	-4.71505	-1.21880	-0.38338
C	-4.55623	-0.08903	1.85568
C	-4.68542	1.31203	-0.22605
H	-4.30850	-2.14581	0.05539
H	-4.41918	-1.18216	-1.44427
C	-6.25540	-1.19968	-0.28390
H	-4.15088	0.77194	2.41399
H	-4.16560	-1.01823	2.30460
C	-6.09888	-0.07912	1.95845
H	-4.38736	1.39823	-1.28359
H	-4.25795	2.16791	0.32353
C	-6.22602	1.31636	-0.12583
H	-6.64842	-2.06472	-0.83893
C	-6.67138	-1.28741	1.19522
C	-6.78876	0.10841	-0.90058
H	-6.36874	-0.14300	3.02315
C	-6.64110	1.22873	1.35378
H	-6.59859	2.25283	-0.56754
H	-6.30415	-2.22855	1.63920
H	-7.76995	-1.28924	1.27524
H	-6.50216	0.17202	-1.96446
H	-7.88916	0.11805	-0.85384
H	-7.73938	1.24750	1.43556
H	-6.25118	2.09756	1.91133
O	3.96980	0.11832	-2.03823
H	3.73339	0.09745	-2.98270
H	4.71151	-0.49846	-1.93803

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adn20n | bs90-adn20n.fchk

Ru	1.97093	-0.00000	-0.53140
C	0.03054	0.00000	-0.04576
C	-0.82049	-0.00000	-1.18346
C	-0.64417	0.00001	1.19970
C	-2.18951	-0.00000	-1.06851
C	-2.02683	0.00002	1.26801
N	-2.80300	0.00001	0.14836
C	-0.16764	-0.00001	-2.55227
O	-0.84253	-0.00002	-3.57438
O	1.13647	-0.00001	-2.47134
C	-4.31685	0.00001	0.18816
H	-0.09045	0.00002	2.14173
H	-2.54830	0.00002	2.22041
H	-2.80896	-0.00001	-1.96361
N	2.60816	0.00000	1.30849
C	2.79521	-1.19224	1.94628
C	2.79521	1.19226	1.94627
C	3.19906	-1.21230	3.28330
C	3.19906	1.21232	3.28330
C	3.40352	0.00001	3.95324
H	3.35047	2.16186	3.79717
H	3.35047	-2.16184	3.79718
H	3.71934	0.00001	4.99719
N	2.10247	-2.04476	-0.18926
N	2.10247	2.04476	-0.18927
C	1.82807	-3.04017	-1.05251
C	1.82808	3.04016	-1.05253
C	2.52047	-2.35354	1.08203
C	2.52047	2.35355	1.08201
C	2.66258	-3.68434	1.48791
C	2.66258	3.68435	1.48789
C	2.37592	-4.71143	0.58855
C	2.37593	4.71143	0.58852
C	1.95157	-4.38427	-0.70424
C	1.95158	4.38427	-0.70426
H	1.50015	-2.71221	-2.04120
H	1.50016	2.71220	-2.04121
H	1.71666	-5.15646	-1.43800
H	1.71667	5.15645	-1.43803
H	2.48315	-5.75420	0.89233
H	2.48316	5.75420	0.89230
H	2.99750	-3.90877	2.50094
H	2.99750	3.90878	2.50092
C	-4.83051	-1.26641	-0.53319
C	-4.85015	0.00005	1.63279
C	-4.83052	1.26638	-0.53327
H	-4.45196	-2.15844	-0.00573
H	-4.44832	-1.29475	-1.56540
C	-6.37180	-1.26052	-0.55336
H	-4.48914	0.89473	2.16724
H	-4.48914	-0.89460	2.16730
C	-6.39401	0.00004	1.61886
H	-4.44833	1.29465	-1.56548
H	-4.45197	2.15844	-0.00586
C	-6.37180	1.26047	-0.55344
H	-6.71971	-2.16257	-1.08014
C	-6.90058	-1.25946	0.89257
C	-6.86676	-0.00005	-1.28969
H	-6.74700	0.00008	2.66172
C	-6.90059	1.25950	0.89249
H	-6.71973	2.16248	-1.08028
H	-6.55852	-2.16591	1.42133
H	-8.00289	-1.26948	0.89041
H	-6.49618	-0.00008	-2.32930
H	-7.96839	-0.00006	-1.32931
H	-8.00289	1.26951	0.89032
H	-6.55853	2.16599	1.42119
C	4.75949	-0.00001	-2.21922
C	5.88835	-0.00002	-3.14160
H	6.50714	0.89751	-2.98131
H	6.50714	-0.89754	-2.98131
H	5.51349	-0.00002	-4.17828
N	3.84590	-0.00001	-1.50626

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Ru	1.98205	0.35657	-0.05374
C	3.81807	-0.29744	0.18680
C	4.73675	0.21680	-0.78801
C	4.41792	-1.18977	1.12832
C	6.06156	-0.12271	-0.79664
C	5.75696	-1.50503	1.08108
N	6.59546	-0.98216	0.12960
C	4.18550	1.16611	-1.83643
O	4.91831	1.64757	-2.70149
O	2.91003	1.37252	-1.68688
C	8.05922	-1.29324	0.05313
H	3.81488	-1.64832	1.91602
H	6.20403	-2.18559	1.79976
H	6.72064	0.29522	-1.55589
N	1.23849	-0.60311	1.44815
C	1.22403	-0.00962	2.68004
C	0.74126	-1.86493	1.25330
C	0.73391	-0.70912	3.78465
C	0.21378	-2.57817	2.32581
C	0.22420	-2.00087	3.60492
H	-0.23954	-3.55350	2.15709
H	0.72544	-0.23574	4.76693
H	-0.18535	-2.55066	4.45371
N	2.12819	1.80685	1.41087
N	1.36129	-1.37204	-1.00444
C	2.48094	3.09740	1.25188
C	1.37295	-1.62458	-2.32677
C	1.68977	1.37862	2.64252
C	0.78104	-2.27793	-0.15214
C	1.64055	2.25675	3.73037
C	0.20757	-3.45893	-0.63754
C	2.01423	3.58720	3.56106
C	0.23220	-3.71769	-2.00376
C	2.43950	4.01728	2.29400
C	0.82660	-2.78330	-2.86807
H	2.79875	3.36030	0.24095
H	1.83550	-0.84536	-2.93580
H	2.72889	5.05346	2.11206
H	0.85670	-2.94183	-3.94738
H	1.96229	4.28474	4.39905
H	-0.22822	-4.62606	-2.39799
H	1.27120	1.89610	4.68949
H	-0.32097	-4.11544	0.05106
C	8.86291	0.01868	0.21456
C	8.49919	-2.27392	1.15757
C	8.37223	-1.93129	-1.32059
H	8.63095	0.45813	1.19954
H	8.55485	0.74167	-0.55606
C	10.37146	-0.26587	0.08782
H	7.93742	-3.21801	1.06411
H	8.28351	-1.84156	2.14855
C	10.01042	-2.56087	1.04055
H	8.05318	-1.25531	-2.12839
H	7.79504	-2.86643	-1.41733
C	9.88261	-2.20943	-1.44194
H	10.92269	0.68220	0.19353
C	10.79922	-1.24719	1.19393
C	10.66005	-0.88610	-1.29356
H	10.29318	-3.26239	1.84167
C	10.31161	-3.18752	-0.33325
H	10.08454	-2.65146	-2.43075
H	10.60710	-0.80397	2.18657
H	11.88117	-1.45092	1.12104
H	10.36226	-0.18340	-2.09088
H	11.74197	-1.07455	-1.40001
H	11.39020	-3.40444	-0.41639
H	9.76716	-4.14175	-0.44075
O	0.21602	1.31841	-0.68237
Ru	-1.90173	0.98810	-0.47403
C	-3.76433	0.43616	-0.26384
N	-2.13261	2.86321	-0.94092
C	-3.94339	-0.93151	0.15317
C	-5.00004	1.12788	-0.47536
C	-2.04808	3.79928	0.07824
C	-2.18735	3.22723	-2.25787
C	-5.17580	-1.49769	0.32076
C	-2.68362	-1.74245	0.35489
C	-6.21975	0.52022	-0.29107
H	-4.99346	2.17500	-0.78803
C	-2.12359	5.15939	-0.25532
C	-1.87168	3.21299	1.38490
C	-2.26310	4.57167	-2.61355
C	-2.10931	2.07667	-3.16476
N	-6.33262	-0.79145	0.10549
H	-5.25805	-2.54016	0.62443
O	-2.70682	-2.92183	0.73767
O	-1.62799	-1.05422	0.06929
H	-7.14934	1.05909	-0.44858
C	-2.24701	5.54584	-1.59216
H	-2.06838	5.91265	0.53280
N	-1.78901	1.81717	1.40660
C	-1.79176	3.93755	2.59314
H	-2.30756	4.86420	-3.66319
N	-1.95647	0.85502	-2.53882
C	-2.15344	2.16180	-4.56340
C	-7.64215	-1.50089	0.25930
H	-2.30121	6.60496	-1.84991
C	-1.67775	1.18798	2.59064
C	-1.65540	3.27313	3.80041
H	-1.84096	5.02757	2.56076
C	-1.82545	-0.25547	-3.29513
C	-2.02826	1.00930	-5.33350
H	-2.27596	3.13813	-5.03415
C	-7.76047	-2.05575	1.69828
C	-8.83938	-0.56578	-0.00127
C	-7.70147	-2.66691	-0.75489
C	-1.60712	1.85591	3.80419
H	-1.62821	0.10038	2.52293
H	-1.59078	3.83583	4.73421
C	-1.85656	-0.22678	-4.68353
H	-1.68239	-1.17760	-2.72900
H	-2.05479	1.06809	-6.42337
H	-7.71912	-1.21325	2.40923
H	-6.90885	-2.71842	1.91482
C	-9.07800	-2.83922	1.85674
H	-8.78089	-0.16013	-1.02460
H	-8.81218	0.28007	0.70549
C	-10.16378	-1.33993	0.16228
H	-6.84665	-3.34175	-0.59337
H	-7.61594	-2.25455	-1.77451
C	-9.02012	-3.44611	-0.59019
H	-1.51005	1.28691	4.72963
H	-1.74018	-1.15458	-5.24615
H	-9.13466	-3.23672	2.88282
C	-10.26612	-1.89650	1.59398
C	-9.10659	-4.00199	0.84500
H	-10.99747	-0.64570	-0.02982
C	-10.20746	-2.50051	-0.84893
H	-9.03782	-4.27687	-1.31384
H	-10.25910	-1.06801	2.32340
H	-11.21696	-2.44308	1.71505
H	-8.26143	-4.68612	1.03484
H	-10.03888	-4.57951	0.96677
H	-11.15847	-3.05028	-0.74517
H	-10.15776	-2.10592	-1.87869
H	0.43943	1.89228	-1.43048

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Ru	1.81578	1.07592	0.28331
C	3.54653	0.06227	0.26633
C	3.51347	-1.18073	-0.44425
C	4.82022	0.35160	0.84446
C	4.59548	-2.01123	-0.53655
C	5.88676	-0.51293	0.73550
N	5.79448	-1.70219	0.05418
C	2.20156	-1.53798	-1.10457
O	2.08120	-2.53637	-1.82334
O	1.28228	-0.67419	-0.82276
C	6.91826	-2.68569	-0.05601
H	4.97593	1.27810	1.40340
H	6.84765	-0.28713	1.18842
H	4.51575	-2.94556	-1.08946
N	2.43690	2.61899	1.20259
C	2.91203	3.69108	0.46904
C	2.28289	2.70913	2.57236
C	3.35804	4.83698	1.12511
C	2.71680	3.84947	3.24491
C	3.27778	4.91531	2.52367
H	2.60684	3.91158	4.32885
H	3.74660	5.67551	0.54468
H	3.62280	5.80953	3.04450
N	2.34006	2.23887	-1.33736
N	1.38498	0.52273	2.23360
C	2.12976	1.96301	-2.63722
C	0.82341	-0.62467	2.66492
C	2.83305	3.46916	-0.97135
C	1.66048	1.51979	3.14299
C	3.18051	4.41381	-1.95168
C	1.35221	1.35658	4.50338
C	2.98880	4.11190	-3.29534
C	0.74773	0.18008	4.93362
C	2.44139	2.86568	-3.64800
C	0.47840	-0.83161	3.99605
H	1.69153	0.98167	-2.83017
H	0.60966	-1.35742	1.89103
H	2.25017	2.59941	-4.68840
H	-0.01451	-1.76432	4.27206
H	3.24669	4.84322	-4.06449
H	0.48541	0.04937	5.98611
H	3.57689	5.38321	-1.64659
H	1.57659	2.16245	5.20360
C	7.24932	-2.91625	-1.54964
C	8.19238	-2.19019	0.65512
C	6.48306	-4.02106	0.59217
H	7.56041	-1.95703	-1.99715
H	6.35006	-3.25877	-2.08372
C	8.36594	-3.96843	-1.68813
H	7.98084	-2.01963	1.72350
H	8.51951	-1.23478	0.21264
C	9.31786	-3.23638	0.51689
H	5.56429	-4.38693	0.10888
H	6.25352	-3.84091	1.65605
C	7.60225	-5.06927	0.44710
H	8.57691	-4.12511	-2.75819
C	9.63241	-3.46387	-0.97323
C	7.90348	-5.29242	-1.04826
H	10.21254	-2.85409	1.03399
C	8.86977	-4.56242	1.15903
H	7.26754	-6.01378	0.90513
H	9.97632	-2.52208	-1.43528
H	10.44455	-4.20391	-1.07472
H	7.00022	-5.66333	-1.56275
H	8.69128	-6.05679	-1.16080
H	9.67675	-5.31007	1.07360
H	8.66362	-4.41138	2.23291
O	0.00011	1.74379	-0.00048
Ru	-1.81572	1.07593	-0.28355
C	-3.54648	0.06233	-0.26620
N	-2.43736	2.61902	-1.20240
C	-3.51328	-1.18075	0.44422
C	-4.82028	0.35173	-0.84407
C	-2.91233	3.69097	-0.46855
C	-2.28419	2.70920	-2.57226
C	-4.59525	-2.01129	0.53659
C	-2.20121	-1.53808	1.10416
C	-5.88677	-0.51286	-0.73510
H	-4.97610	1.27831	-1.40285
C	-3.35896	4.83679	-1.12433
C	-2.83254	3.46899	0.97179
C	-2.71875	3.84945	-3.24454
C	-1.66181	1.52001	-3.14326
N	-5.79435	-1.70221	-0.05396
H	-4.51543	-2.94568	1.08938
O	-2.08067	-2.53647	1.82289
O	-1.28195	-0.67434	0.82206
H	-6.84772	-0.28705	-1.18786
C	-3.27953	4.91516	-2.52294
H	-3.74738	5.67521	-0.54366
N	-2.33928	2.23870	1.33747
C	-3.17947	4.41358	1.95237
H	-2.60947	3.91160	-4.32854
N	-1.38557	0.52299	-2.23405
C	-1.35418	1.35692	-4.50380
C	-6.91805	-2.68581	0.05619
H	-3.62505	5.80932	-3.04355
C	-2.12816	1.96281	2.63719
C	-2.98690	4.11163	3.29590
H	-3.57607	5.38296	1.64755
C	-0.82375	-0.62418	-2.66564
C	-0.74955	0.18061	-4.93438
H	-1.57916	2.16273	-5.20390
C	-7.24908	-2.91645	1.54982
C	-8.19222	-2.19036	-0.65490
C	-6.48277	-4.02112	-0.59206
C	-2.43919	2.86544	3.64818
H	-1.68980	0.98147	2.82985
H	-3.24435	4.84291	4.06524
C	-0.47937	-0.83099	-3.99696
H	-0.60931	-1.35682	-1.89184
H	-0.48775	0.05000	-5.98701
H	-7.56023	-1.95727	1.99737
H	-6.34978	-3.25893	2.08386
C	-8.36563	-3.96871	1.68827
H	-7.98068	-2.01972	-1.72327
H	-8.51942	-1.23500	-0.21237
C	-9.31762	-3.23664	-0.51672
H	-5.56397	-4.38696	-0.10880
H	-6.25326	-3.84090	-1.65593
C	-7.60188	-5.06941	-0.44701
H	-2.24727	2.59915	4.68844
H	0.01370	-1.76353	-4.27327
H	-8.57658	-4.12545	2.75833
C	-9.63214	-3.46421	0.97340
C	-7.90308	-5.29264	1.04835
H	-10.21233	-2.85439	-1.03380
C	-8.86944	-4.56263	-1.15891
H	-7.26711	-6.01388	-0.90508
H	-9.97611	-2.52247	1.43549
H	-10.44423	-4.20431	1.07487
H	-6.99980	-5.66351	1.56280
H	-8.69083	-6.05706	1.16085
H	-9.67637	-5.31033	-1.07351
H	-8.66331	-4.41152	-2.23279

1.6.4.7. Optimized geometries of Ru(R)

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rme4oh rme4oh.fchk			
Ru	-0.13767	0.17671	-0.94961
N	-0.06350	1.75230	0.34436
C	-1.22701	2.21106	0.87584
C	1.13390	2.32477	0.63708
C	-1.21654	3.31179	1.73367
C	1.19269	3.43162	1.48778
C	0.00492	3.92599	2.03346
H	-2.14487	3.68838	2.16157
H	2.14880	3.90083	1.71780
H	0.02930	4.79191	2.69744
C	-2.41968	1.45274	0.45406
C	-3.72223	1.78919	0.81243
N	-2.16432	0.37799	-0.35714
C	-4.78773	1.01982	0.32791
H	-3.90931	2.64967	1.45441
C	-3.18928	-0.35692	-0.83011
C	-4.51668	-0.06336	-0.50719
H	-5.81447	1.27354	0.59822
H	-2.91731	-1.17978	-1.49145
H	-5.31488	-0.68517	-0.91479
C	2.27250	1.66847	-0.01868
C	3.60257	2.06868	0.11677
N	1.93357	0.60728	-0.80508
C	4.59834	1.36717	-0.56987
H	3.85615	2.92427	0.74267
C	2.88589	-0.06459	-1.46996
C	4.23518	0.28514	-1.37388
H	5.64316	1.67085	-0.48333
H	2.54115	-0.87986	-2.10538
H	4.97755	-0.28012	-1.93894
C	0.28257	-1.21742	0.47898
C	-0.03291	-2.52932	0.09321
C	0.85445	-1.04952	1.75701
C	0.19508	-3.60746	0.93150
C	1.06778	-2.15593	2.56456
H	1.13677	-0.07035	2.14532
N	0.74143	-3.41138	2.15208
H	-0.05920	-4.62592	0.63180
H	1.50403	-2.08182	3.56177
C	-0.64497	-2.70895	-1.26394
O	-0.76310	-1.53870	-1.88908
O	-1.00065	-3.77542	-1.70759
C	1.01042	-4.55914	3.05265
H	0.54290	-4.36494	4.02821
H	0.58412	-5.46662	2.60788
H	2.09786	-4.67479	3.17095
O	0.34755	0.47108	-2.74757
H	-0.12084	-0.16762	-3.32679

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rme4aq rme4aq.fchk			
Ru	0.11544	-0.11957	-0.88045
N	1.26023	-0.82389	0.70852
C	2.30784	-0.07739	1.15015
C	0.88760	-1.95487	1.34756
C	3.00020	-0.43864	2.30617
C	1.54674	-2.36597	2.51337
C	2.60051	-1.58919	3.00109
H	3.85304	0.15067	2.64592
H	1.24691	-3.28160	3.02377
H	3.12851	-1.89070	3.90825
C	2.61800	1.02356	0.23748
C	3.66441	1.93396	0.34372
N	1.79089	1.04111	-0.85541
C	3.86748	2.86357	-0.68724
H	4.32559	1.90952	1.21116
C	2.00669	1.90414	-1.87520
C	3.03228	2.84704	-1.80997
H	4.68925	3.58071	-0.62219
H	1.34070	1.82627	-2.73710
H	3.17609	3.53954	-2.64145
C	-0.18783	-2.66016	0.65041
C	-0.68000	-3.91661	1.00155
N	-0.63459	-2.01554	-0.47210
C	-1.62562	-4.53788	0.17957
H	-0.30564	-4.41487	1.89644
C	-1.53591	-2.62030	-1.28078
C	-2.04928	-3.88204	-0.97981
H	-2.01680	-5.52477	0.43686
H	-1.86435	-2.06150	-2.15591
H	-2.78557	-4.32648	-1.65252
C	-1.00612	0.89856	0.47703
C	-2.17126	1.41377	-0.12579
C	-0.80743	1.22157	1.83179
C	-3.06655	2.21991	0.56395
C	-1.73267	2.02373	2.48996
H	0.05507	0.87181	2.39939
N	-2.83578	2.51216	1.86132
H	-3.96364	2.63008	0.09495
H	-1.62194	2.30299	3.53957
C	-2.39415	1.05325	-1.55254
O	-1.37629	0.20053	-1.99647
O	-3.27725	1.39351	-2.27669
C	-3.78836	3.36513	2.62889
H	-3.23996	4.22872	3.03184
H	-4.58389	3.70426	1.95407
H	-4.21462	2.76689	3.44752
O	1.07988	-1.00441	-2.71949
H	0.52549	-1.13953	-3.50794
H	1.78110	-1.67584	-2.75631

48			
rme3oh rme3oh.fchk			
Ru	0.21766	-0.00020	-0.81075
N	1.78049	0.01715	0.37970
C	2.30522	1.21164	0.76559
C	2.32785	-1.16569	0.77035
C	3.43525	1.24669	1.58636
C	3.45800	-1.17604	1.59124
C	4.01430	0.04163	1.99815
H	3.85883	2.20133	1.89827
H	3.89962	-2.12118	1.90702
H	4.89868	0.05123	2.63635
C	1.56025	2.36503	0.23654
C	1.91578	3.70034	0.44738
N	0.45863	2.04520	-0.51137
C	1.14310	4.71177	-0.12346
H	2.79680	3.94028	1.04260
C	-0.28085	3.02099	-1.06742
C	0.02865	4.36863	-0.89710
H	1.41283	5.75859	0.02698
H	-1.12326	2.67877	-1.67124
H	-0.59212	5.12999	-1.37059
C	1.60594	-2.33565	0.24469
C	1.98828	-3.66278	0.45959
N	0.49867	-2.04058	-0.50500
C	1.23658	-4.69135	-0.10897
H	2.87354	-3.88324	1.05603
C	-0.22051	-3.03257	-1.05882
C	0.11609	-4.37327	-0.88441
H	1.52733	-5.73203	0.04485
H	-1.06942	-2.70900	-1.66387
H	-0.48891	-5.14847	-1.35586
C	-1.32619	-0.01092	0.56663
C	-2.58767	-0.02518	-0.07664
C	-1.36664	-0.00956	1.98267
C	-3.77202	-0.03606	0.63357
C	-2.57191	-0.02126	2.66106
H	-0.44864	-0.00155	2.57532
N	-3.75789	-0.03493	1.98919
H	-4.73784	-0.04814	0.12545
H	-2.64656	-0.02138	3.74959
C	-2.61573	-0.03227	-1.59364
O	-1.40869	-0.02247	-2.10620
O	-3.67156	-0.04615	-2.20629
C	-5.01954	-0.01600	2.75224
H	-5.15321	0.97202	3.21859
H	-5.85286	-0.21652	2.06722
H	-4.98603	-0.79175	3.53046
O	1.37342	0.01563	-2.40392
H	0.80427	-0.00267	-3.19441

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rme3aq rme3aq.fchk

Ru	0.14545	-0.00506	-0.82379
N	1.72494	0.12266	0.44830
C	2.15076	1.34614	0.84939
C	2.31496	-1.02068	0.87604
C	3.22666	1.45789	1.73464
C	3.39458	-0.96120	1.76235
C	3.84787	0.29050	2.19145
H	3.57620	2.43709	2.06118
H	3.87519	-1.87503	2.11091
H	4.68982	0.35681	2.88236
C	1.38110	2.45380	0.25199
C	1.63719	3.80663	0.47995
N	0.36865	2.06219	-0.58383
C	0.85025	4.77112	-0.15560
H	2.44870	4.10240	1.14492
C	-0.38962	2.99228	-1.19675
C	-0.17717	4.35804	-1.00816
H	1.04095	5.83268	0.01177
H	-1.17300	2.60972	-1.85325
H	-0.81185	5.07755	-1.52712
C	1.70642	-2.23765	0.30740
C	2.16226	-3.53384	0.54886
N	0.63818	-2.01167	-0.51863
C	1.52174	-4.61245	-0.06774
H	3.01617	-3.69729	1.20632
C	0.02359	-3.04982	-1.11601
C	0.43854	-4.36676	-0.91488
H	1.86994	-5.63168	0.10873
H	-0.81109	-2.79626	-1.77141
H	-0.08527	-5.17834	-1.42151
C	-1.29206	-0.06777	0.55394
C	-2.56834	-0.17274	-0.05124
C	-1.27862	-0.02810	1.96667
C	-3.72969	-0.23588	0.69478
C	-2.46555	-0.09451	2.67592
H	-0.34738	0.05293	2.52991
N	-3.66973	-0.19740	2.04678
H	-4.71168	-0.31680	0.22530
H	-2.50326	-0.06924	3.76611
C	-2.61027	-0.20992	-1.55311
O	-1.36376	-0.13938	-2.07946
O	-3.61825	-0.29120	-2.20884
C	-4.90480	-0.26910	2.86186
H	-4.97717	0.63292	3.48646
H	-5.77078	-0.32735	2.19111
H	-4.86523	-1.16504	3.49832
O	1.39994	-0.05290	-2.70134
H	0.81366	-0.05599	-3.47884
H	2.11000	0.57512	-2.90649

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rme2oh rme2oh.fchk

Ru	0.20953	0.00230	-0.79467
N	1.67477	0.04388	0.42875
C	2.17618	1.25603	0.84339
C	2.23855	-1.13828	0.84987
C	3.23754	1.29989	1.74708
C	3.30062	-1.12191	1.75365
C	3.79991	0.10407	2.21370
H	3.62973	2.26294	2.07689
H	3.74238	-2.06142	2.08863
H	4.63126	0.12764	2.91936
C	1.48408	2.38874	0.22588
C	1.80950	3.73463	0.44358
N	0.46187	2.04193	-0.62394
C	1.09865	4.72945	-0.22167
H	2.62356	3.98796	1.12377
C	-0.21043	3.00853	-1.27699
C	0.07166	4.35980	-1.10329
H	1.34541	5.78132	-0.06448
H	-0.98827	2.64435	-1.95122
H	-0.50044	5.10726	-1.65491
C	1.60668	-2.30881	0.23838
C	2.00142	-3.63474	0.46373
N	0.56853	-2.02028	-0.61395
C	1.34392	-4.66881	-0.19651
H	2.82685	-3.84166	1.14592
C	-0.05179	-3.02412	-1.26230
C	0.30007	-4.35788	-1.08099
H	1.64482	-5.70557	-0.03325
H	-0.84684	-2.70461	-1.93908
H	-0.23183	-5.13708	-1.62889
C	-1.26770	-0.03304	0.53962
C	-2.57684	-0.07110	-0.04239
C	-1.26116	-0.03313	1.97152
C	-3.71796	-0.10277	0.71449
C	-2.42875	-0.06610	2.69670
H	-0.31658	-0.01164	2.52102
N	-3.65329	-0.10592	2.08100
H	-4.70436	-0.13232	0.24822
H	-2.45503	-0.06716	3.78802
C	-2.65619	-0.07965	-1.55717
O	-1.47516	-0.04625	-2.10291
O	-3.74167	-0.11414	-2.13362
C	-4.87887	-0.05679	2.87669
H	-5.16351	0.98778	3.09110
H	-5.69133	-0.54281	2.31843
H	-4.72311	-0.59081	3.82553
O	1.37863	0.03038	-2.46380
H	0.78573	0.01347	-3.23172

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rme2ni rme2ni.fchk

Ru	0.29570	0.00177	0.56149
N	1.29517	0.02040	-1.11193
C	1.62660	-1.16572	-1.69939
C	1.59274	1.21842	-1.69332
C	2.29300	-1.17334	-2.92720
C	2.25855	1.25125	-2.92102
C	2.61020	0.04528	-3.53908
H	2.56044	-2.11768	-3.40184
H	2.49902	2.20522	-3.39082
H	3.13009	0.05510	-4.49784
C	1.20431	-2.33579	-0.90851
C	1.45465	-3.66171	-1.27569
N	0.53150	-2.04054	0.25164
C	1.01552	-4.69757	-0.45068
H	1.99259	-3.87590	-2.19952
C	0.11199	-3.04377	1.04425
C	0.33307	-4.38394	0.72994
H	1.20495	-5.73679	-0.72504
H	-0.41419	-2.72584	1.94682
H	-0.02685	-5.16339	1.40279
C	1.13752	2.37194	-0.89643
C	1.35026	3.70628	-1.25684
N	0.47346	2.05183	0.26219
C	0.88222	4.72511	-0.42656
H	1.88178	3.94027	-2.17957
C	0.02601	3.03883	1.05990
C	0.20914	4.38631	0.75247
H	1.04221	5.77066	-0.69561
H	-0.49082	2.70180	1.96095
H	-0.17243	5.15183	1.42938
C	-1.50316	-0.02098	-0.30223
C	-2.56835	-0.04027	0.64200
C	-1.90394	-0.02608	-1.66564
C	-3.88687	-0.06091	0.25242
C	-3.23996	-0.04714	-2.01444
H	-1.16550	-0.01767	-2.47043
N	-4.22040	-0.06668	-1.06729
H	-4.69288	-0.07722	0.98823
H	-3.58483	-0.05217	-3.04938
C	-2.20209	-0.04227	2.11488
O	-0.90859	-0.02169	2.29415
O	-3.06821	-0.06130	2.97931
C	-5.63662	-0.02703	-1.46383
H	-6.23057	-0.58835	-0.72992
H	-5.98782	1.01656	-1.49844
H	-5.74920	-0.48712	-2.45480
N	1.94595	0.02225	1.88434
C	2.71120	0.03122	2.75438
C	3.65064	0.04210	3.86895
H	4.27084	0.95208	3.83075
H	3.09178	0.02517	4.81898
H	4.30555	-0.84265	3.81911

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rme2aq rme2aq.fchk

Ru	0.18642	-0.00069	-0.80210
N	1.69159	0.06736	0.43025
C	2.15672	1.28113	0.84958
C	2.24690	-1.10195	0.86549
C	3.21520	1.34802	1.75880
C	3.30658	-1.07477	1.77478
C	3.78948	0.15984	2.22562
H	3.58950	2.31442	2.09733
H	3.75285	-2.00526	2.12629
H	4.61622	0.19572	2.93601
C	1.43662	2.41087	0.23680
C	1.72845	3.75569	0.48612
N	0.42962	2.05622	-0.63098
C	0.98856	4.75106	-0.15266
H	2.53192	4.01602	1.17556
C	-0.28260	3.02435	-1.24145
C	-0.03516	4.37965	-1.03200
H	1.20765	5.80385	0.03354
H	-1.07054	2.66445	-1.90679
H	-0.63923	5.12603	-1.54949
C	1.61447	-2.29180	0.26933
C	2.01924	-3.60496	0.52650
N	0.57747	-2.02859	-0.59291
C	1.36355	-4.66266	-0.10430
H	2.84562	-3.79267	1.21238
C	-0.04892	-3.05420	-1.19955
C	0.31234	-4.38309	-0.98400
H	1.67132	-5.69223	0.08620
H	-0.86083	-2.76652	-1.87064
H	-0.22497	-5.17978	-1.49997
C	-1.22551	-0.03544	0.55744
C	-2.53042	-0.10443	-0.02198
C	-1.19348	-0.01196	1.97961
C	-3.66428	-0.14812	0.75312
C	-2.35948	-0.05847	2.71535
H	-0.24576	0.03614	2.51947
N	-3.58117	-0.12945	2.11228
H	-4.65527	-0.20240	0.29900
H	-2.37319	-0.04542	3.80607
C	-2.63841	-0.12909	-1.53579
O	-1.45696	-0.07695	-2.10493
O	-3.72083	-0.18776	-2.09773
C	-4.80979	-0.11580	2.92152
H	-5.15818	0.92025	3.05954
H	-5.58589	-0.69688	2.40536
H	-4.60434	-0.56921	3.90066
O	1.25927	-0.05055	-2.81911
H	0.48064	-0.10649	-3.40538
H	1.70497	0.77053	-3.07888

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rar4oh rar4oh.fchk

Ru	-1.67712	-0.08910	0.92164
N	-2.48055	-0.18233	-0.95286
C	-2.88765	0.97176	-1.54300
C	-2.60614	-1.38611	-1.57038
C	-3.47405	0.93985	-2.80905
C	-3.19102	-1.46775	-2.83671
C	-3.63000	-0.29297	-3.45300
H	-3.80675	1.86008	-3.28775
H	-3.30318	-2.43187	-3.33173
H	-4.09270	-0.33573	-4.44057
C	-2.65116	2.17840	-0.72844
C	-3.05595	3.45818	-1.09836
N	-2.01092	1.95557	0.46236
C	-2.81045	4.53219	-0.23359
H	-3.56857	3.61833	-2.04655
C	-1.78219	2.98677	1.29790
C	-2.16960	4.29136	0.98108
H	-3.12493	5.54059	-0.50894
H	-1.29338	2.73400	2.23902
H	-1.96508	5.09542	1.68925
C	-2.07870	-2.50636	-0.78062
C	-2.08892	-3.83966	-1.19273
N	-1.56272	-2.14750	0.42922
C	-1.56147	-4.81847	-0.34516
H	-2.51243	-4.11081	-2.15977
C	-1.06066	-3.08485	1.24737
C	-1.03946	-4.43575	0.89184
H	-1.56828	-5.86751	-0.64644
H	-0.69471	-2.73163	2.21091
H	-0.63201	-5.16808	1.59007
C	0.25084	-0.05836	0.25749
C	1.16979	0.38590	1.22200
C	0.76825	-0.43831	-0.99612
C	2.52380	0.46390	0.94702
C	2.13435	-0.35702	-1.22558
H	0.13276	-0.80404	-1.80327
N	2.98866	0.08909	-0.26655
H	3.24641	0.82532	1.67976
H	2.60111	-0.64664	-2.16696
C	0.61277	0.78807	2.55331
O	-0.71043	0.62479	2.58460
O	1.27865	1.22231	3.46388
C	4.42269	0.15280	-0.54494
C	4.87722	1.14366	-1.43107
C	5.25644	-0.77606	0.09994
C	6.25637	1.18620	-1.67309
C	6.62618	-0.69324	-0.18319
C	7.12096	0.27687	-1.05829
H	6.65057	1.94902	-2.34731
H	7.30651	-1.40289	0.29152
H	8.19236	0.32658	-1.26140
C	3.93997	2.12946	-2.08634
H	3.37055	1.66511	-2.91137
H	3.21020	2.53882	-1.36721
H	4.50757	2.96886	-2.51229
C	4.71938	-1.81648	1.05301
H	4.47394	-1.37715	2.03623
H	3.80379	-2.29452	0.66484
H	5.46992	-2.60126	1.22319
O	-2.60745	-0.90558	2.34592
H	-2.38727	-0.44968	3.18627

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rar4aq rar4aq.fchk

Ru	-1.50875	-0.10248	0.85535
N	-2.77103	0.06808	-0.80085
C	-3.22462	1.29117	-1.16483
C	-3.21606	-1.05481	-1.41400
C	-4.18578	1.42667	-2.17105
C	-4.17678	-0.98323	-2.42701
C	-4.66948	0.27298	-2.79836
H	-4.54591	2.41289	-2.46531
H	-4.52950	-1.88833	-2.92232
H	-5.42210	0.35376	-3.58528
C	-2.57755	2.36916	-0.41148
C	-2.83383	3.73118	-0.56010
N	-1.63533	1.92572	0.47821
C	-2.11411	4.65201	0.20828
H	-3.59010	4.06711	-1.27036
C	-0.91847	2.81457	1.20435
C	-1.14280	4.18566	1.10064
H	-2.30709	5.72225	0.10715
H	-0.18100	2.40456	1.89328
H	-0.56098	4.86956	1.72109
C	-2.55991	-2.26159	-0.90299
C	-2.80352	-3.56462	-1.33375
N	-1.62132	-2.00588	0.06107
C	-2.07513	-4.61909	-0.77341
H	-3.55638	-3.75153	-2.10027
C	-0.89592	-3.01996	0.58668
C	-1.10821	-4.34112	0.19884
H	-2.25770	-5.64617	-1.09694
H	-0.16107	-2.75483	1.34616
H	-0.52003	-5.13465	0.66302
C	0.38258	-0.02013	0.13788
C	1.32912	-0.09913	1.18091
C	0.88687	0.09572	-1.16864
C	2.69369	-0.05273	0.93587
C	2.26138	0.12060	-1.37326
H	0.23456	0.15700	-2.04118
N	3.14198	0.05233	-0.33564
H	3.43918	-0.09339	1.73142
H	2.71261	0.18909	-2.36333
C	0.78455	-0.22933	2.56205
O	-0.60807	-0.25137	2.51774
O	1.39088	-0.30969	3.58907
C	4.58341	0.08222	-0.59710
C	5.13492	1.25799	-1.14126
C	5.33608	-1.06128	-0.27683
C	6.52626	1.26140	-1.37014
C	6.72119	-1.00135	-0.53342
C	7.30897	0.14627	-1.07152
H	6.98698	2.16138	-1.78216
H	7.33355	-1.87698	-0.30898
H	8.38418	0.16969	-1.25793
C	4.31524	2.47824	-1.47009
H	3.90686	2.41920	-2.49611
H	3.47009	2.61609	-0.77610
H	4.94404	3.37968	-1.43035
C	4.73136	-2.31034	0.31063
H	4.67398	-2.24626	1.41303
H	3.71547	-2.50251	-0.07222
H	5.35801	-3.18276	0.07506
O	-3.33290	-0.24458	2.11252
H	-3.21642	-0.33412	3.07499
H	-4.28610	-0.24068	1.93290

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rar3oh rar3oh.fchk

Ru	-1.60653	-0.04779	0.82498
N	-2.61995	0.03787	-0.85469
C	-2.97511	1.25342	-1.35290
C	-2.96778	-1.12090	-1.47809
C	-3.71806	1.33584	-2.53315
C	-3.71039	-1.08351	-2.66048
C	-4.08917	0.15624	-3.18727
H	-4.00413	2.30755	-2.93570
H	-3.99067	-2.00924	-3.16302
H	-4.67188	0.20286	-4.10801
C	-2.48972	2.37440	-0.53312
C	-2.75280	3.72141	-0.79890
N	-1.73978	2.01045	0.55334
C	-2.25330	4.69827	0.06237
H	-3.35368	3.99653	-1.66570
C	-1.26495	2.95285	1.38689
C	-1.50013	4.30964	1.17612
H	-2.45672	5.75339	-0.12885
H	-0.70172	2.57507	2.24218
H	-1.10383	5.04277	1.87948
C	-2.47679	-2.31951	-0.77964
C	-2.73452	-3.63245	-1.18421
N	-1.72879	-2.06805	0.33944
C	-2.23174	-4.69170	-0.42843
H	-3.33397	-3.81843	-2.07535
C	-1.25081	-3.08986	1.07118
C	-1.48083	-4.41837	0.72044
H	-2.43105	-5.72196	-0.72858
H	-0.68933	-2.80004	1.96126
H	-1.08212	-5.21927	1.34401
C	0.33225	-0.00142	0.10609
C	1.27375	-0.05513	1.16370
C	0.87731	0.06993	-1.19819
C	2.63424	-0.03530	0.93019
C	2.24694	0.08323	-1.39569
H	0.23283	0.11228	-2.07965
N	3.10662	0.03297	-0.33992
H	3.36190	-0.07197	1.74198
H	2.72012	0.12994	-2.37693
C	0.74650	-0.13847	2.58350
O	-0.56520	-0.14634	2.62107
O	1.50461	-0.19225	3.53875
C	4.54196	0.04423	-0.57679
C	5.15578	1.27392	-0.86016
C	5.23248	-1.17492	-0.49863
C	6.53942	1.25924	-1.08116
C	6.61434	-1.13971	-0.72906
C	7.26107	0.06453	-1.01773
H	7.04983	2.19968	-1.29886
H	7.18196	-2.07120	-0.67956
H	8.33886	0.07255	-1.19218
C	4.36273	2.55639	-0.91397
H	3.67553	2.57208	-1.77819
H	3.74675	2.68499	-0.00766
H	5.03537	3.42152	-1.00159
C	4.52045	-2.46471	-0.17360
H	4.17523	-2.47836	0.87512
H	3.63018	-2.60623	-0.80983
H	5.19203	-3.32282	-0.31936
O	-3.26421	-0.09961	1.88698
H	-3.02139	-0.16144	2.82843

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rph3aq rar3aq.fchk

Ru	-1.55984	-0.06729	0.83287
N	-2.50048	0.08696	-0.96076
C	-2.78778	1.31842	-1.45061
C	-2.80827	-1.04647	-1.63815
C	-3.41878	1.44943	-2.69090
C	-3.43944	-0.96777	-2.88311
C	-3.74358	0.29266	-3.40761
H	-3.65451	2.43522	-3.09123
H	-3.69078	-1.87373	-3.43411
H	-4.23689	0.37395	-4.37747
C	-2.37773	2.41180	-0.54937
C	-2.58447	3.76771	-0.80760
N	-1.76882	2.00234	0.60752
C	-2.16501	4.71672	0.12860
H	-3.07397	4.07723	-1.73106
C	-1.36411	2.91768	1.50975
C	-1.54709	4.28538	1.30559
H	-2.32263	5.78027	-0.05920
H	-0.89186	2.52091	2.41008
H	-1.20812	4.99219	2.06409
C	-2.41752	-2.27548	-0.92313
C	-2.66883	-3.56868	-1.38232
N	-1.78443	-2.06567	0.27246
C	-2.27311	-4.66138	-0.60585
H	-3.17723	-3.71920	-2.33467
C	-1.40615	-3.11775	1.02227
C	-1.63479	-4.43265	0.61552
H	-2.46685	-5.67869	-0.95039
H	-0.91851	-2.87693	1.96819
H	-1.31561	-5.25617	1.25552
C	0.30879	-0.00652	0.14248
C	1.24262	-0.10485	1.20404
C	0.84861	0.11143	-1.15618
C	2.60534	-0.08335	0.97918
C	2.22242	0.12032	-1.33777
H	0.21092	0.18942	-2.03842
N	3.07955	0.02661	-0.28494
H	3.33578	-0.14895	1.78669
H	2.69757	0.19626	-2.31612
C	0.68497	-0.22861	2.59293
O	-0.67172	-0.22861	2.57965
O	1.34787	-0.31826	3.59559
C	4.52159	0.03792	-0.51983
C	5.12667	1.26500	-0.83524
C	5.21364	-1.17852	-0.40769
C	6.51092	1.24878	-1.05079
C	6.59550	-1.14104	-0.63680
C	7.23704	0.05883	-0.95429
H	7.01923	2.18469	-1.29074
H	7.16794	-2.06787	-0.56492
H	8.31499	0.06713	-1.12634
C	4.33327	2.54563	-0.92933
H	3.69525	2.56476	-1.83101
H	3.67361	2.67909	-0.05468
H	5.00875	3.41096	-0.98392
C	4.51217	-2.46751	-0.05477
H	4.21689	-2.48878	1.00948
H	3.59735	-2.61146	-0.65503
H	5.17647	-3.32540	-0.23027
O	-3.45552	-0.26160	2.05335
H	-3.21924	-0.29201	2.99757
H	-4.21249	0.34131	1.98916

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rar2oh rar2oh.fchk

Ru	-1.61160	-0.06051	0.78022
N	-2.45490	0.05464	-0.92885
C	-2.77573	1.28967	-1.44310
C	-2.76447	-1.09965	-1.61023
C	-3.37756	1.38828	-2.69735
C	-3.36585	-1.02847	-2.86652
C	-3.66818	0.22313	-3.41981
H	-3.62690	2.36945	-3.10380
H	-3.60608	-1.94580	-3.40582
H	-4.13996	0.28952	-4.40096
C	-2.42321	2.38282	-0.53533
C	-2.66447	3.73956	-0.79193
N	-1.82584	1.98525	0.63626
C	-2.30837	4.69228	0.15837
H	-3.13835	4.03374	-1.72917
C	-1.49890	2.91055	1.55810
C	-1.71834	4.26994	1.35933
H	-2.49530	5.75182	-0.02735
H	-1.05253	2.50593	2.46876
H	-1.43697	4.98271	2.13591
C	-2.40354	-2.30511	-0.86191
C	-2.63437	-3.61507	-1.30407
N	-1.81098	-2.06883	0.35484
C	-2.27313	-4.68733	-0.49332
H	-3.10438	-3.78036	-2.27427
C	-1.47991	-3.11018	1.14141
C	-1.68903	-4.43066	0.75631
H	-2.45177	-5.71237	-0.82414
H	-1.03879	-2.83231	2.10084
H	-1.40437	-5.24184	1.42808
C	0.27695	-0.01119	0.15760
C	1.24118	-0.07508	1.21699
C	0.84380	0.07583	-1.15499
C	2.59026	-0.04960	0.98523
C	2.20372	0.09565	-1.35059
H	0.19755	0.12424	-2.03512
N	3.07708	0.03618	-0.29273
H	3.31386	-0.09264	1.80008
H	2.67457	0.15333	-2.33292
C	0.70232	-0.17369	2.63138
O	-0.59915	-0.18199	2.65322
O	1.46256	-0.23708	3.59541
C	4.50024	0.05369	-0.52653
C	5.11058	1.27341	-0.86231
C	5.21473	-1.14903	-0.39890
C	6.49424	1.26775	-1.08534
C	6.59692	-1.10994	-0.62799
C	7.23164	0.08674	-0.96988
H	6.99241	2.20534	-1.34287
H	7.17389	-2.03324	-0.53801
H	8.30986	0.09967	-1.14461
C	4.30278	2.54352	-0.96357
H	3.62958	2.52572	-1.83824
H	3.66256	2.67698	-0.07570
H	4.96476	3.41703	-1.05822
C	4.51472	-2.43229	-0.02685
H	4.16811	-2.40901	1.02071
H	3.61980	-2.59344	-0.65077
H	5.19108	-3.29159	-0.14656
O	-3.35583	-0.14223	1.83142
H	-3.12449	-0.19414	2.77234

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rar2ni rar2ni.fchk

Ru	-1.49402	0.04260	-0.53311
N	-2.10833	-0.09546	1.31094
C	-2.28934	-1.33208	1.85898
C	-2.28364	1.04566	2.03862
C	-2.67165	-1.45245	3.19720
C	-2.66588	0.96546	3.37986
C	-2.86157	-0.29375	3.95974
H	-2.81773	-2.43760	3.64078
H	-2.80731	1.87348	3.96647
H	-3.15970	-0.37207	5.00595
C	-2.03344	-2.42557	0.90443
C	-2.17922	-3.78259	1.20944
N	-1.63216	-2.02312	-0.34581
C	-1.91404	-4.73936	0.22935
H	-2.50113	-4.08214	2.20713
C	-1.37932	-2.95059	-1.28751
C	-1.50762	-4.31679	-1.04128
H	-2.02466	-5.80166	0.45393
H	-1.06513	-2.54952	-2.25348
H	-1.29050	-5.03194	-1.83580
C	-2.02167	2.26888	1.25924
C	-2.16182	3.56542	1.76437
N	-1.62070	2.05680	-0.03699
C	-1.89125	4.65719	0.93906
H	-2.48378	3.71330	2.79548
C	-1.36210	3.11386	-0.82862
C	-1.48482	4.42817	-0.38028
H	-1.99765	5.67426	1.32038
H	-1.04832	2.86058	-1.84354
H	-1.26358	5.25347	-1.05837
C	0.44840	0.00142	-0.07580
C	1.28725	0.08522	-1.22271
C	1.12504	-0.09340	1.17031
C	2.65891	0.07231	-1.12183
C	2.50436	-0.09912	1.22937
H	0.57049	-0.15967	2.10909
N	3.25971	-0.01889	0.09654
H	3.30115	0.13268	-2.00134
H	3.07013	-0.16292	2.15936
C	0.61419	0.19260	-2.57813
O	-0.68858	0.18963	-2.47651
O	1.27361	0.27181	-3.60604
C	4.70831	-0.02227	0.19068
C	5.35789	-1.25047	0.38889
C	5.38227	1.20274	0.06836
C	6.75643	-1.22890	0.47415
C	6.78039	1.17594	0.16058
C	7.46079	-0.02746	0.36227
H	7.29177	-2.16897	0.62332
H	7.33396	2.11315	0.07259
H	8.55063	-0.02948	0.42993
C	4.58176	-2.54001	0.49447
H	3.97815	-2.57481	1.41841
H	3.88294	-2.65588	-0.35134
H	5.26469	-3.40164	0.50286
C	4.63207	2.49160	-0.15963
H	4.17811	2.51769	-1.16568
H	3.81096	2.61346	0.56710
H	5.30900	3.35337	-0.06995
N	-3.38926	0.11829	-1.46967
C	-4.32297	0.17085	-2.15389
C	-5.47919	0.23845	-3.03910
H	-6.08663	1.12598	-2.79935
H	-5.13643	0.30675	-4.08457
H	-6.09880	-0.66495	-2.92027

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rph2aq rar2aq.fchk

Ru	-1.59668	-0.04944	0.78021
N	-2.44124	0.05958	-0.96915
C	-2.71764	1.28669	-1.50195
C	-2.72563	-1.09416	-1.64271
C	-3.29249	1.38433	-2.77137
C	-3.30025	-1.03597	-2.91421
C	-3.58160	0.21303	-3.48134
H	-3.51430	2.36146	-3.20111
H	-3.52818	-1.95387	-3.45649
H	-4.02992	0.27304	-4.47372
C	-2.35389	2.39429	-0.60159
C	-2.54647	3.74651	-0.90246
N	-1.79920	2.01009	0.59746
C	-2.17027	4.71885	0.02442
H	-2.98991	4.03022	-1.85721
C	-1.43487	2.95634	1.48585
C	-1.60414	4.31748	1.24011
H	-2.31648	5.77705	-0.19900
H	-0.99241	2.57361	2.40824
H	-1.29345	5.04534	1.99077
C	-2.36920	-2.30328	-0.88021
C	-2.58653	-3.60759	-1.33421
N	-1.80181	-2.06892	0.34928
C	-2.22540	-4.68611	-0.52629
H	-3.04000	-3.77229	-2.31187
C	-1.45750	-3.11477	1.12398
C	-1.65223	-4.43607	0.72526
H	-2.39194	-5.70907	-0.86813
H	-1.01356	-2.84933	2.08567
H	-1.35805	-5.24994	1.38913
C	0.25713	-0.00615	0.14227
C	1.19822	-0.07950	1.21557
C	0.81951	0.08330	-1.16134
C	2.55373	-0.06288	0.98806
C	2.18699	0.09233	-1.34117
H	0.18161	0.14082	-2.04552
N	3.04264	0.02166	-0.28040
H	3.27366	-0.11342	1.80584
H	2.66616	0.15128	-2.31889
C	0.65954	-0.17146	2.63094
O	-0.65346	-0.16642	2.65011
O	1.40454	-0.23846	3.59599
C	4.47697	0.03179	-0.50439
C	5.09905	1.26265	-0.76504
C	5.16607	-1.18915	-0.43848
C	6.48437	1.24821	-0.97533
C	6.55011	-1.15520	-0.65577
C	7.20273	0.05100	-0.92229
H	6.99886	2.19038	-1.17576
H	7.11478	-2.08898	-0.61431
H	8.28206	0.05854	-1.08744
C	4.30909	2.54749	-0.80616
H	3.62520	2.57491	-1.67269
H	3.68810	2.66381	0.09832
H	4.98348	3.41275	-0.87922
C	4.44657	-2.48106	-0.13977
H	4.08135	-2.50430	0.90191
H	3.56684	-2.61232	-0.79255
H	5.11869	-3.33932	-0.28284
O	-3.41586	-0.19995	2.15810
H	-2.94956	-0.27685	3.01246
H	-3.94563	0.60820	2.23892

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Ru	2.18774	0.09281	-0.89311
N	2.94151	-0.27514	0.96805
C	3.28393	0.78141	1.75042
C	3.09674	-1.55772	1.38817
C	3.83412	0.56533	3.01465
C	3.64783	-1.82314	2.64449
C	4.02136	-0.74932	3.45671
H	4.11481	1.40693	3.64674
H	3.78379	-2.85028	2.98160
H	4.45672	-0.93534	4.44008
C	3.02187	2.09522	1.13334
C	3.36314	3.31139	1.71903
N	2.42558	2.04627	-0.09925
C	3.09867	4.50224	1.03110
H	3.84130	3.33328	2.69798
C	2.17879	3.19075	-0.76468
C	2.50318	4.43939	-0.22807
H	3.36352	5.46299	1.47647
H	1.72753	3.07684	-1.75054
H	2.28619	5.34012	-0.80374
C	2.63550	-2.55263	0.41147
C	2.68589	-3.93386	0.60457
N	2.13896	-2.02043	-0.74118
C	2.21867	-4.78001	-0.40546
H	3.09383	-4.34305	1.52877
C	1.69414	-2.82965	-1.71440
C	1.71468	-4.22014	-1.58085
H	2.25760	-5.86311	-0.27638
H	1.34025	-2.33805	-2.61999
H	1.35318	-4.84318	-2.39995
C	0.24305	-0.04936	-0.29556
C	-0.66530	0.51757	-1.20298
C	-0.30455	-0.63803	0.85562
C	-2.02639	0.50549	-0.96559
C	-1.68260	-0.62793	1.04900
H	0.31237	-1.10946	1.62154
N	-2.53255	-0.06599	0.15259
H	-2.71662	0.95756	-1.67580
H	-2.13240	-1.07446	1.93108
C	-0.09018	1.15021	-2.43220
O	1.23838	1.03469	-2.45077
O	-0.74753	1.71084	-3.27859
C	-4.05608	-0.04859	0.34984
C	-4.70482	-0.78985	-0.83937
C	-4.45645	-0.74172	1.66209
C	-4.51992	1.42374	0.38608
H	-4.35148	-1.83489	-0.85383
H	-4.41637	-0.31543	-1.79118
C	-6.24042	-0.73699	-0.68676
H	-3.99251	-0.22711	2.52095
H	-4.12199	-1.79326	1.65400
C	-5.99510	-0.69717	1.81276
H	-4.22805	1.94080	-0.54227
H	-4.03627	1.93736	1.23430
C	-6.05675	1.46251	0.53137
H	-6.68980	-1.25909	-1.54471
C	-6.64594	-1.43080	0.62604
C	-6.69916	0.73435	-0.66566
H	-6.25777	-1.19784	2.75651
C	-6.46209	0.76946	1.84469
H	-6.37479	2.51576	0.54606
H	-6.33127	-2.48836	0.61156
H	-7.74171	-1.41227	0.73545
H	-6.42009	1.23362	-1.60942
H	-7.79629	0.77897	-0.58086
H	-7.55629	0.80693	1.96442
H	-6.01531	1.29409	2.70658
O	3.18348	-0.45229	-2.40135
H	2.96351	0.12464	-3.16365

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Ru	2.01308	-0.00001	-0.85010
N	3.30521	0.00003	0.80407
C	3.76636	1.17864	1.28317
C	3.76641	-1.17856	1.28318
C	4.76372	1.21234	2.26224
C	4.76377	-1.21221	2.26225
C	5.27242	0.00008	2.74332
H	5.12949	2.16363	2.65018
H	5.12958	-2.16348	2.65020
H	6.05350	0.00010	3.50642
C	3.07061	2.31830	0.68392
C	3.30429	3.66195	0.96826
N	2.08966	1.94831	-0.19945
C	2.52111	4.64039	0.34657
H	4.09049	3.93838	1.67188
C	1.30858	2.89050	-0.77932
C	1.50908	4.24710	-0.53599
H	2.69436	5.69830	0.55619
H	0.53532	2.53752	-1.45997
H	0.87389	4.97781	-1.03981
C	3.07071	-2.31825	0.68395
C	3.30444	-3.66189	0.96830
N	2.08974	-1.94831	-0.19943
C	2.52130	-4.64037	0.34662
H	4.09066	-3.93828	1.67192
C	1.30871	-2.89054	-0.77928
C	1.50925	-4.24713	-0.53594
H	2.69460	-5.69828	0.55625
H	0.53542	-2.53760	-1.45993
H	0.87409	-4.97787	-1.03975
C	0.09476	-0.00001	-0.17528
C	-0.82607	-0.00001	-1.24139
C	-0.43790	-0.00001	1.11705
C	-2.19583	-0.00002	-1.01931
C	-1.82366	-0.00001	1.28759
H	0.18947	-0.00000	2.00978
N	-2.68519	-0.00002	0.23965
H	-2.90869	-0.00003	-1.84331
H	-2.27083	-0.00001	2.27892
C	-0.25087	-0.00002	-2.61169
O	1.15319	-0.00002	-2.52502
O	-0.81243	-0.00002	-3.66406
C	-4.22930	-0.00002	0.42632
C	-4.78688	-1.26966	-0.25062
C	-4.60015	-0.00001	1.91567
C	-4.78689	1.26961	-0.25064
H	-4.36216	-2.16351	0.23715
H	-4.51466	-1.29090	-1.31933
C	-6.32803	-1.26027	-0.11967
H	-4.19480	0.89898	2.41168
H	-4.19480	-0.89899	2.41169
C	-6.14395	-0.00001	2.04610
H	-4.51467	1.29084	-1.31934
H	-4.36216	2.16347	0.23712
C	-6.32803	1.26022	-0.11968
H	-6.71630	-2.16398	-0.61219
C	-6.71104	-1.26207	1.37116
C	-6.88850	-0.00003	-0.80715
H	-6.38978	-0.00000	3.11788
C	-6.71104	1.26203	1.37114
H	-6.71630	2.16392	-0.61222
H	-6.32344	-2.16901	1.86561
H	-7.80710	-1.27409	1.47291
H	-6.62649	-0.00004	-1.87923
H	-7.98710	-0.00003	-0.73885
H	-7.80711	1.27405	1.47289
H	-6.32344	2.16898	1.86557
O	3.85453	0.00003	-2.09782
H	3.74378	0.00001	-3.06561
H	4.80721	-0.00008	-1.91394

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Ru	2.11250	0.00000	-0.81262
N	3.09844	-0.00006	0.88328
C	3.44047	1.18894	1.45088
C	3.44039	-1.18909	1.45084
C	4.16362	1.21124	2.64574
C	4.16354	-1.21148	2.64570
C	4.52887	-0.00014	3.24306
H	4.43922	2.16130	3.10351
H	4.43908	-2.16158	3.10344
H	5.09642	-0.00018	4.17438
C	2.96406	2.35018	0.68333
C	3.21777	3.68205	1.02401
N	2.23319	2.04213	-0.43305
C	2.72836	4.70154	0.20752
H	3.80357	3.91278	1.91378
C	1.76791	3.02574	-1.22301
C	1.99442	4.37021	-0.93714
H	2.92456	5.74568	0.45758
H	1.21926	2.69149	-2.10546
H	1.60608	5.13842	-1.60667
C	2.96389	-2.35027	0.68326
C	3.21750	-3.68218	1.02390
N	2.23306	-2.04213	-0.43311
C	2.72800	-4.70160	0.20738
H	3.80327	-3.91298	1.91367
C	1.76769	-3.02568	-1.22311
C	1.99409	-4.37017	-0.93728
H	2.92411	-5.74576	0.45740
H	1.21909	-2.69135	-2.10556
H	1.60570	-5.13832	-1.60684
C	0.16196	0.00001	-0.12062
C	-0.76266	0.00004	-1.19222
C	-0.41817	0.00002	1.16572
C	-2.12519	0.00005	-0.98227
C	-1.79520	0.00003	1.33490
H	0.19965	0.00000	2.06731
N	-2.64572	0.00004	0.27242
H	-2.80878	0.00007	-1.82936
H	-2.24873	0.00003	2.32132
C	-0.21689	0.00009	-2.60671
O	1.09480	0.00011	-2.62794
O	-0.96213	0.00012	-3.57479
C	-4.15774	0.00004	0.42282
C	-4.72027	-1.26665	-0.25991
C	-4.58184	0.00004	1.90251
C	-4.72028	1.26672	-0.25992
H	-4.30370	-2.15901	0.23742
H	-4.41626	-1.29385	-1.31791
C	-6.25955	-1.26052	-0.16662
H	-4.18376	0.89529	2.40901
H	-4.18376	-0.89520	2.40901
C	-6.12311	0.00004	2.00098
H	-4.41627	1.29391	-1.31792
H	-4.30372	2.15909	0.23741
C	-6.25957	1.26057	-0.16663
H	-6.64362	-2.16272	-0.66705
C	-6.68104	-1.25974	1.31388
C	-6.80728	0.00002	-0.86476
H	-6.39806	0.00004	3.06691
C	-6.68105	1.25980	1.31387
H	-6.64364	2.16277	-0.66707
H	-6.30217	-2.16624	1.81672
H	-7.78043	-1.26967	1.39170
H	-6.51589	0.00002	-1.92917
H	-7.90858	0.00002	-0.82156
H	-7.78044	1.26972	1.39169
H	-6.30220	2.16631	1.81671
O	3.78347	-0.00014	-1.85538
H	3.55196	0.00010	-2.80167

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rad3aq rad3aq.fchk

Ru	2.06040	-0.00608	-0.82305
N	2.98019	0.02831	0.98674
C	3.25839	1.22434	1.56228
C	3.28512	-1.14766	1.58882
C	3.87736	1.27242	2.81453
C	3.90450	-1.15202	2.84211
C	4.19970	0.07058	3.45392
H	4.10560	2.22944	3.28316
H	4.15357	-2.09273	3.33258
H	4.68386	0.08708	4.43159
C	2.85192	2.37523	0.73422
C	3.04804	3.71116	1.08753
N	2.25642	2.04336	-0.45395
C	2.63109	4.72024	0.21537
H	3.52689	3.95861	2.03497
C	1.85360	3.01663	-1.29416
C	2.02607	4.36786	-0.99420
H	2.78019	5.76911	0.47776
H	1.39140	2.67981	-2.22361
H	1.68892	5.12360	-1.70478
C	2.90385	-2.32614	0.78892
C	3.15181	-3.64711	1.16312
N	2.28211	-2.03690	-0.39589
C	2.76385	-4.68550	0.31199
H	3.65130	-3.86068	2.10809
C	1.91054	-3.03668	-1.21713
C	2.13608	-4.37576	-0.89694
H	2.95493	-5.72354	0.58964
H	1.43067	-2.73309	-2.14881
H	1.82241	-5.15475	-1.59293
C	0.18108	0.00252	-0.15372
C	-0.73716	-0.02427	-1.23141
C	-0.39041	0.02916	1.13162
C	-2.10148	-0.02606	-1.02792
C	-1.77150	0.02521	1.28628
H	0.22279	0.05144	2.03436
N	-2.61939	-0.00250	0.22511
H	-2.79224	-0.04638	-1.86894
H	-2.22983	0.04359	2.27085
C	-0.16289	-0.04862	-2.61791
O	1.19349	-0.04722	-2.58862
O	-0.81309	-0.06657	-3.63351
C	-4.14462	-0.00722	0.37865
C	-4.69480	-1.29041	-0.28094
C	-4.55763	0.01863	1.85963
C	-4.70665	1.24494	-0.32873
H	-4.27402	-2.17195	0.23195
H	-4.39682	-1.33461	-1.34095
C	-6.23547	-1.28834	-0.18338
H	-4.16488	0.92699	2.34753
H	-4.15531	-0.86645	2.38133
C	-6.10047	0.01306	1.96061
H	-4.40874	1.25162	-1.38972
H	-4.29402	2.14907	0.15039
C	-6.24722	1.23226	-0.23051
H	-6.61367	-2.20200	-0.66613
C	-6.65162	-1.26277	1.29833
C	-6.78934	-0.04363	-0.90436
H	-6.37088	0.03170	3.02692
C	-6.66320	1.25821	1.25131
H	-6.63399	2.12365	-0.74695
H	-6.26863	-2.15819	1.81722
H	-7.75008	-1.27701	1.37853
H	-6.50265	-0.06220	-1.96996
H	-7.88980	-0.04793	-0.85857
H	-7.76175	1.26544	1.33120
H	-6.28843	2.17585	1.73632
O	3.96993	-0.11441	-2.03668
H	3.73703	-0.08171	-2.98169
H	4.71925	0.49168	-1.92830

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rad2oh rad2oh.fchk

Ru	2.11142	0.00004	-0.76866
N	2.93673	-0.00012	0.95115
C	3.24686	1.19780	1.55397
C	3.24668	-1.19813	1.55387
C	3.83726	1.21105	2.81731
C	3.83706	-1.21159	2.81720
C	4.12812	-0.00032	3.45937
H	4.07794	2.16272	3.29328
H	4.07759	-2.16334	3.29309
H	4.59143	-0.00040	4.44680
C	2.89709	2.34931	0.72137
C	3.12827	3.68630	1.07377
N	2.31298	2.03058	-0.48100
C	2.77609	4.70098	0.18861
H	3.59149	3.91672	2.03395
C	1.98991	3.01666	-1.33939
C	2.19986	4.35986	-1.04466
H	2.95525	5.74601	0.44924
H	1.55439	2.67432	-2.28032
H	1.92187	5.12340	-1.77273
C	2.89684	-2.34952	0.72110
C	3.12797	-3.68657	1.07330
N	2.31284	-2.03058	-0.48126
C	2.77585	-4.70109	0.18792
H	3.59112	-3.91716	2.03346
C	1.98986	-3.01648	-1.33986
C	2.19975	-4.35974	-1.04535
H	2.95497	-5.74616	0.44839
H	1.55445	-2.67396	-2.28077
H	1.92182	-5.12316	-1.77357
C	0.21122	0.00003	-0.16546
C	-0.73782	0.00026	-1.23606
C	-0.38773	-0.00018	1.13047
C	-2.08957	0.00025	-1.02316
C	-1.75470	-0.00018	1.30255
H	0.23410	-0.00035	2.02961
N	-2.62125	0.00004	0.23986
H	-2.76999	0.00042	-1.87312
H	-2.20095	-0.00034	2.29262
C	-0.18579	0.00048	-2.64808
O	1.11514	0.00041	-2.65848
O	-0.93754	0.00071	-3.62228
C	-4.11407	-0.00000	0.38642
C	-4.68835	-1.26469	-0.29379
C	-4.54815	-0.00023	1.86501
C	-4.68839	1.26488	-0.29341
H	-4.27056	-2.15666	0.20319
H	-4.37953	-1.29359	-1.34987
C	-6.22631	-1.26052	-0.20230
H	-4.14749	0.89299	2.37229
H	-4.14748	-0.89360	2.37202
C	-6.08775	-0.00027	1.96514
H	-4.37956	1.29412	-1.34947
H	-4.27063	2.15670	0.20385
C	-6.22634	1.26063	-0.20192
H	-6.61454	-2.16224	-0.70218
C	-6.64913	-1.25875	1.27800
C	-6.77595	0.00015	-0.89900
H	-6.36568	-0.00043	3.03122
C	-6.64917	1.25840	1.27837
H	-6.61460	2.16248	-0.70153
H	-6.26882	-2.16530	1.78018
H	-7.74950	-1.26774	1.35705
H	-6.48255	0.00031	-1.96293
H	-7.87834	0.00013	-0.85563
H	-7.74954	1.26733	1.35742
H	-6.26890	2.16481	1.78082
O	3.86334	-0.00024	-1.81280
H	3.63622	0.00082	-2.75611

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rad2ni rad2ni.fchk

Ru	1.96944	0.00001	-0.53334
N	2.60353	-0.00002	1.30785
C	2.78750	1.19231	1.94641
C	2.78751	-1.19237	1.94637
C	3.18376	1.21226	3.28575
C	3.18377	-1.21236	3.28571
C	3.38402	-0.00006	3.95682
H	3.33237	2.16165	3.80076
H	3.33239	-2.16176	3.80069
H	3.69336	-0.00007	5.00271
C	2.51762	2.35366	1.08056
C	2.66309	3.68442	1.48539
N	2.10241	2.04499	-0.19167
C	2.38292	4.71138	0.58382
H	2.99636	3.90888	2.49895
C	1.83441	3.04016	-1.05712
C	1.96162	4.38423	-0.70999
H	2.49313	5.75414	0.88662
H	1.50883	2.71172	-2.04644
H	1.73200	5.15646	-1.44538
C	2.51765	-2.35369	1.08048
C	2.66312	-3.68446	1.48527
N	2.10243	-2.04498	-0.19174
C	2.38296	-4.71140	0.58367
H	2.99639	-3.90895	2.49883
C	1.83445	-3.04013	-1.05722
C	1.96166	-4.38421	-0.71013
H	2.49318	-5.75416	0.88644
H	1.50887	-2.71166	-2.04653
H	1.73205	-5.15642	-1.44555
C	0.02959	-0.00002	-0.05004
C	-0.82168	0.00003	-1.18795
C	-0.64574	-0.00009	1.19500
C	-2.19090	0.00001	-1.07331
C	-2.02828	-0.00010	1.26305
H	-0.09327	-0.00012	2.13762
N	-2.80462	-0.00006	0.14342
H	-2.81067	0.00005	-1.96818
H	-2.54879	-0.00015	2.21585
C	-0.16763	0.00009	-2.55609
O	1.13627	0.00007	-2.47320
O	-0.84101	0.00013	-3.57915
C	-4.31829	-0.00005	0.18451
C	-4.83403	-1.26600	-0.53610
C	-4.84851	-0.00021	1.62994
C	-4.83396	1.26610	-0.53581
H	-4.45321	-2.15842	-0.01090
H	-4.45471	-1.29331	-1.56942
C	-6.37574	-1.26051	-0.55228
H	-4.48665	0.89457	2.16360
H	-4.48670	-0.89514	2.16338
C	-6.39243	-0.00016	1.61971
H	-4.45462	1.29362	-1.56913
H	-4.45309	2.15837	-0.01040
C	-6.37567	1.26070	-0.55198
H	-6.72460	-2.16248	-1.07859
C	-6.90107	-1.25958	0.89463
C	-6.87312	0.00019	-1.28698
H	-6.74296	-0.00027	2.66342
C	-6.90099	1.25946	0.89493
H	-6.72448	2.16281	-1.07809
H	-6.55831	-2.16610	1.42281
H	-8.00341	-1.26939	0.89486
H	-6.50659	0.00031	-2.32794
H	-7.97493	0.00023	-1.32179
H	-8.00333	1.26934	0.89516
H	-6.55817	2.16584	1.42332
N	3.85018	0.00004	-1.49859
C	4.77558	0.00004	-2.19614
C	5.92104	0.00005	-3.09786
H	6.53685	-0.89742	-2.92604
H	5.56576	-0.00001	-4.14138
H	6.53678	0.89759	-2.92612

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rad2aq rad2aq.fchk

Ru	2.09350	-0.00435	-0.76930
N	2.91932	0.01048	0.99057
C	3.18947	1.20740	1.59193
C	3.19810	-1.17786	1.60453
C	3.75238	1.23656	2.86999
C	3.76096	-1.18773	2.88247
C	4.03629	0.02897	3.51863
H	3.96899	2.18936	3.35368
H	3.98440	-2.13353	3.37657
H	4.47559	0.03567	4.51681
C	2.83233	2.36140	0.74976
C	3.01927	3.69573	1.12517
N	2.28921	2.04159	-0.47340
C	2.64889	4.71628	0.24938
H	3.45361	3.92780	2.09789
C	1.93000	3.03437	-1.31190
C	2.09387	4.38033	-0.99114
H	2.79064	5.76105	0.53119
H	1.49599	2.70142	-2.25731
H	1.78747	5.14733	-1.70363
C	2.84851	-2.34397	0.77554
C	3.06026	-3.67105	1.16137
N	2.29261	-2.04334	-0.44481
C	2.70477	-4.70445	0.29438
H	3.50488	-3.88803	2.13289
C	1.95299	-3.04626	-1.27645
C	2.14230	-4.38710	-0.94685
H	2.86694	-5.74444	0.58275
H	1.51729	-2.72916	-2.22614
H	1.85209	-5.16401	-1.65528
C	0.22946	0.00360	-0.14937
C	-0.69755	-0.01449	-1.23402
C	-0.36274	0.02348	1.13866
C	-2.05478	-0.01517	-1.02511
C	-1.73685	0.02107	1.29529
H	0.25202	0.03886	2.04102
N	-2.58677	0.00131	0.22986
H	-2.73377	-0.02864	-1.87576
H	-2.19315	0.03409	2.28043
C	-0.14584	-0.02816	-2.64659
O	1.16697	-0.02064	-2.65370
O	-0.88167	-0.04161	-3.62204
C	-4.09465	-0.00120	0.37073
C	-4.65321	-1.27755	-0.29761
C	-4.52815	0.01666	1.84799
C	-4.66005	1.25445	-0.33030
H	-4.23646	-2.16228	0.21308
H	-4.34308	-1.31816	-1.35342
C	-6.19267	-1.27498	-0.21248
H	-4.13486	0.91939	2.34487
H	-4.12906	-0.87029	2.36810
C	-6.06948	0.01345	1.93951
H	-4.35014	1.26916	-1.38688
H	-4.24783	2.15427	0.15722
C	-6.19944	1.24594	-0.24467
H	-6.57282	-2.18442	-0.70296
C	-6.62145	-1.25621	1.26582
C	-6.74080	-0.02492	-0.92896
H	-6.35025	0.02627	3.00398
C	-6.62807	1.26264	1.23375
H	-6.58454	2.14051	-0.75813
H	-6.24244	-2.15525	1.78185
H	-7.72129	-1.26787	1.33883
H	-6.44404	-0.03768	-1.99186
H	-7.84245	-0.02741	-0.89100
H	-7.72796	1.27046	1.30655
H	-6.25374	2.17652	1.72664
O	3.92206	-0.07927	-2.14360
H	3.45590	-0.11225	-3.00094
H	4.44378	0.73731	-2.17944

1.6.5. X-ray diffraction

1.6.5.1. Ru(Ad) dimer

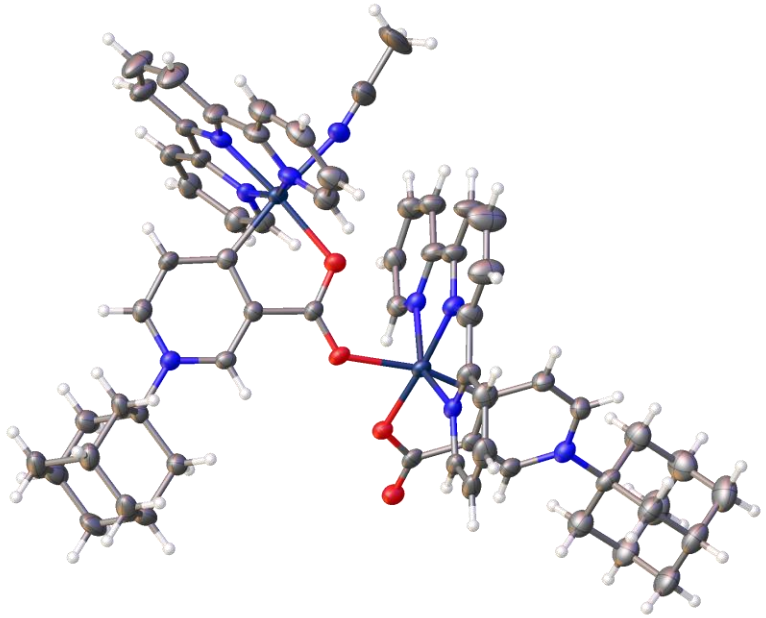


Table 1. Crystal data and structure refinement for grot531_a_sq_sq.

Identification code	grot531	
Empirical formula	C66 H66 F18 N9 O4.50 P3 Ru2	
Formula weight	1694.32	
Temperature	273.15 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 16.1525(16) Å	□= 74.135(3)°.
	b = 21.958(3) Å	□= 74.331(3)°.
	c = 22.521(3) Å	□ = 80.428(3)°.
Volume	7361.0(14) Å^3	
Z	4	
Density (calculated)	1.529 Mg/m^3	
Absorption coefficient	0.574 mm^{-1}	
F(000)	3424	
Crystal size	0.35 x 0.17 x 0.08 mm^3	
Theta range for data collection	1.316 to 25.000°.	
Index ranges	-18<=h<=19, -23<=k<=26, -26<=l<=26	
Reflections collected	88505	
Independent reflections	25819 [R(int) = 0.0512]	
Completeness to theta = 25.000°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.0928 and 0.0682	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	25819 / 0 / 1841	
Goodness-of-fit on F^2	1.023	
Final R indices [I>2sigma(I)]	R1 = 0.0825, wR2 = 0.1942	
R indices (all data)	R1 = 0.1250, wR2 = 0.2284	

Extinction coefficient	n/a
Largest diff. peak and hole	3.975 and -3.871 e.Å^{-3}

Table 2. Atomic coordinates (x 104) and equivalent isotropic displacement parameters (Å2x 103)
for grot531_a_sq_sq. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ru(1)	1826(1)	3918(1)	10650(1)	26(1)
Ru(2)	3183(1)	5221(1)	11879(1)	30(1)
O(1)	2728(3)	3786(3)	8823(2)	34(1)
O(2)	2306(3)	4156(2)	9701(2)	28(1)
O(3)	2028(3)	4886(2)	10586(2)	28(1)
O(4)	2523(3)	4757(2)	11452(2)	30(1)
N(1)	1753(4)	2061(3)	9959(3)	31(1)
N(2)	507(4)	4117(3)	10747(3)	28(1)
N(3)	1369(4)	3755(3)	11587(3)	32(1)
N(4)	2917(4)	3508(3)	10981(3)	28(1)
N(5)	2661(4)	6762(3)	10020(3)	28(1)
N(6)	2151(4)	5565(3)	12513(3)	37(2)
N(7)	3775(4)	5705(3)	12204(3)	35(2)
N(8)	4427(4)	5033(3)	11387(3)	32(2)
N(9)	3310(4)	4405(3)	12648(3)	41(2)
C(1)	1745(5)	1490(4)	9703(4)	36(2)
C(2)	2193(6)	1608(4)	8994(4)	46(2)
C(3)	2227(6)	902(4)	10067(5)	48(2)
C(4)	2203(7)	319(5)	9814(5)	56(2)
C(5)	2643(6)	443(5)	9126(5)	57(3)
C(6)	810(5)	1372(4)	9791(4)	43(2)
C(7)	2178(6)	1017(4)	8751(5)	48(2)
C(8)	1235(6)	919(5)	8840(5)	56(3)
C(9)	797(6)	786(4)	9537(5)	50(2)
C(10)	1266(7)	209(5)	9917(5)	61(3)
C(11)	1449(5)	2024(4)	10593(4)	35(2)
C(12)	1438(5)	2524(4)	10846(4)	33(2)
C(13)	1745(4)	3095(3)	10460(3)	27(2)
C(14)	2049(4)	3115(4)	9811(3)	29(2)
C(15)	2051(4)	2608(4)	9575(4)	31(2)
C(16)	104(5)	4242(3)	10267(4)	34(2)
C(17)	-775(5)	4439(4)	10367(4)	41(2)
C(18)	-1245(5)	4508(4)	10955(5)	49(2)
C(19)	-841(5)	4345(4)	11454(4)	41(2)
C(20)	35(5)	4150(4)	11339(4)	36(2)
C(21)	532(5)	3938(4)	11827(4)	39(2)
C(22)	218(6)	3898(5)	12470(4)	58(3)
C(23)	778(6)	3656(6)	12868(5)	68(3)
C(24)	1628(6)	3460(5)	12623(4)	55(3)
C(25)	1919(5)	3517(4)	11978(4)	37(2)
C(26)	2801(5)	3361(4)	11628(4)	34(2)
C(27)	3485(5)	3086(4)	11905(4)	42(2)
C(28)	4288(5)	2968(4)	11526(4)	43(2)
C(29)	4396(5)	3104(4)	10872(4)	37(2)
C(30)	3699(4)	3371(3)	10612(4)	30(2)
C(31)	2379(5)	7271(4)	9481(3)	32(2)
C(32)	3180(5)	7552(4)	8992(4)	44(2)
C(33)	1890(5)	6983(4)	9140(4)	37(2)
C(34)	1593(6)	7515(4)	8612(4)	46(2)
C(35)	2388(6)	7795(5)	8130(4)	57(3)
C(36)	1494(6)	8308(4)	9235(4)	47(2)
C(37)	2875(6)	8080(5)	8474(4)	53(3)
C(38)	2294(6)	8597(5)	8758(5)	55(3)
C(39)	998(6)	8028(4)	8899(5)	52(3)
C(40)	1782(5)	7793(4)	9760(4)	39(2)
C(41)	3139(5)	6925(4)	10363(4)	33(2)
C(42)	3323(5)	6524(4)	10899(4)	33(2)
C(43)	3030(4)	5913(3)	11133(3)	27(2)
C(44)	2352(4)	5087(3)	10936(3)	27(2)
C(45)	2594(4)	5750(3)	10739(3)	27(2)
C(46)	2407(4)	6170(3)	10210(3)	26(2)
C(47)	2396(4)	3715(4)	9389(4)	29(2)
C(48)	4716(5)	4664(4)	10972(4)	37(2)
C(49)	5557(5)	4610(4)	10633(4)	42(2)
C(50)	6142(5)	4955(4)	10723(4)	42(2)
C(51)	5860(5)	5335(4)	11151(4)	44(2)
C(52)	5000(5)	5371(4)	11485(4)	34(2)
C(53)	4632(5)	5745(4)	11953(4)	39(2)
C(54)	5051(6)	6128(5)	12153(4)	54(3)
C(55)	4594(7)	6436(6)	12612(5)	70(3)
C(56)	3732(7)	6380(6)	12871(4)	65(3)
C(57)	3318(6)	6004(4)	12658(4)	44(2)
C(58)	2399(6)	5901(4)	12857(4)	42(2)
C(59)	1810(6)	6117(4)	13340(4)	50(2)
C(60)	946(6)	6021(4)	13468(4)	49(2)
C(61)	697(5)	5699(5)	13108(4)	49(2)
C(62)	1310(5)	5480(4)	12639(4)	42(2)
C(63)	3406(7)	4060(5)	13097(5)	65(3)
C(64)	3568(11)	3605(8)	13689(7)	146(8)
Ru(1')	2020(1)	1094(1)	15069(1)	78(1)
Ru(2')	2520(1)	2853(1)	16141(1)	66(1)
O(1')	2658(5)	2558(4)	13534(3)	68(2)
O(2')	2146(4)	1979(4)	14523(3)	71(2)
O(3')	1420(6)	1400(5)	15917(3)	97(3)
O(4')	2393(5)	2053(4)	15813(3)	77(2)
N(1')	3346(5)	786(4)	13000(3)	53(2)
N(2')	743(6)	1025(6)	15087(4)	75(3)
N(3')	1869(6)	224(6)	15589(4)	87(4)
N(4')	3222(6)	814(6)	15285(4)	90(4)
N(5')	-200(5)	2111(4)	17384(3)	52(2)
N(6')	3197(6)	2430(4)	16829(3)	55(2)
N(7')	2465(5)	3564(4)	16499(4)	62(2)
N(8')	1897(7)	3550(6)	15546(4)	91(4)
N(9')	3729(7)	2973(5)	15454(4)	77(3)
C(1')	3831(6)	702(5)	12340(4)	51(2)
C(2')	3266(7)	366(7)	12099(4)	77(4)
C(3')	4019(6)	1335(5)	11877(4)	50(2)
C(4')	4508(6)	1230(5)	11224(4)	49(2)
C(5')	3948(7)	899(6)	10981(4)	67(3)
C(6')	4687(6)	297(5)	12393(4)	54(2)
C(7')	3754(8)	268(7)	11444(5)	78(4)
C(8')	4578(10)	-143(5)	11507(5)	80(4)
C(9')	5161(7)	180(5)	11739(4)	61(3)
C(10')	5349(6)	814(5)	11279(4)	54(2)
C(11')	3149(7)	255(6)	13467(4)	64(3)
C(12')	2759(7)	289(7)	14080(4)	75(4)
C(13')	2526(6)	879(6)	14236(5)	62(3)

C(14')	2721(6)	1419(6)	13745(4)	61(3)
C(15')	3128(5)	1354(6)	13140(4)	52(2)
C(16')	202(8)	1483(9)	14850(9)	111(6)
C(17')	-667(9)	1465(8)	14966(9)	121(6)
C(18')	-1003(9)	930(9)	15329(8)	104(5)
C(19')	-488(8)	435(7)	15615(5)	80(4)
C(20')	431(8)	484(8)	15465(5)	81(4)
C(21')	1062(9)	18(8)	15728(5)	90(5)
C(22')	934(10)	-557(8)	16107(6)	113(6)
C(23')	1613(10)	-930(9)	16326(8)	138(8)
C(24')	2426(10)	-705(9)	16188(7)	127(7)
C(25')	2526(9)	-103(7)	15807(5)	90(5)
C(26')	3314(8)	226(8)	15637(5)	91(5)
C(27')	4061(8)	-16(9)	15832(5)	108(6)
C(28')	4719(9)	374(9)	15672(6)	110(6)
C(29')	4625(8)	967(9)	15324(5)	105(6)
C(30')	3861(7)	1194(8)	15129(5)	89(5)
C(31')	-1056(6)	1861(5)	17755(5)	54(2)
C(32')	-1768(7)	2408(5)	17741(5)	69(3)
C(33')	-1265(8)	1359(6)	17478(5)	74(3)
C(34')	-2135(8)	1110(6)	17878(5)	74(4)
C(35')	-2842(9)	1662(8)	17858(7)	98(5)
C(36')	-1860(6)	1311(5)	18836(5)	54(2)
C(37')	-2630(7)	2154(6)	18144(6)	70(3)
C(38')	-2554(7)	1864(5)	18813(5)	65(3)
C(39')	-2058(7)	810(5)	18557(5)	63(3)
C(40')	-982(6)	1548(4)	18444(4)	47(2)
C(41')	77(6)	2586(4)	17550(5)	53(2)
C(42')	851(6)	2825(5)	17231(5)	58(3)
C(43')	1406(7)	2607(5)	16715(4)	57(3)
C(44')	1660(8)	1837(6)	16069(5)	77(4)
C(45')	1098(7)	2109(5)	16580(4)	64(3)
C(46')	319(7)	1888(6)	16898(4)	68(3)
C(47')	2503(6)	2047(6)	13906(5)	59(3)
C(48')	1676(10)	3476(9)	15030(6)	121(7)
C(49')	1288(16)	3999(12)	14656(8)	172(12)
C(50')	1149(15)	4594(13)	14802(10)	181(13)
C(51')	1367(11)	4656(8)	15337(7)	128(7)
C(52')	1764(9)	4127(8)	15694(6)	96(5)
C(53')	2032(8)	4143(6)	16264(5)	75(4)
C(54')	1898(8)	4635(6)	16562(6)	79(4)
C(55')	2176(7)	4523(6)	17110(6)	71(3)
C(56')	2577(6)	3950(5)	17365(5)	57(3)
C(57')	2739(6)	3465(5)	17037(4)	54(3)
C(58')	3195(6)	2829(4)	17210(4)	49(2)
C(59')	3608(6)	2634(4)	17696(4)	49(2)
C(60')	4077(7)	2048(5)	17776(5)	59(3)
C(61')	4103(8)	1654(5)	17382(4)	66(3)
C(62')	3653(8)	1862(5)	16915(4)	61(3)
C(63')	4373(9)	3025(6)	15115(5)	83(4)
C(64')	5230(8)	3074(8)	14663(6)	115(6)
P(4)	5318(2)	1861(3)	13378(2)	110(2)
F(25)	4584(6)	2160(6)	13824(4)	143(4)
F(26)	4808(5)	1213(5)	13628(4)	126(3)
F(27)	5745(5)	1591(5)	13989(3)	124(3)
F(28)	6065(4)	1489(4)	13003(3)	97(2)
F(29)	5819(7)	2435(4)	13170(4)	137(4)
F(30)	4836(6)	2081(5)	12827(4)	123(3)
P(6)	4668(1)	2314(1)	9368(1)	41(1)
F(13)	3924(3)	2245(2)	10008(2)	42(1)
F(14)	4673(4)	3053(3)	9349(3)	71(2)
F(15)	3965(3)	2515(3)	8961(2)	61(2)
F(16)	5406(3)	2398(3)	8726(2)	63(2)
F(17)	4682(4)	1596(3)	9383(3)	76(2)
F(18)	5380(3)	2143(4)	9776(3)	80(2)
P(5)	3616(2)	-1640(3)	13978(2)	107(2)
F(19)	3409(8)	-1130(5)	14452(5)	154(4)
F(20)	4201(6)	-1142(5)	13466(6)	203(7)
F(21)	2812(5)	-1274(5)	13748(5)	140(4)
F(22)	3795(7)	-2090(6)	13520(5)	147(4)
F(23)	4424(7)	-1959(5)	14225(6)	187(6)
F(24)	3055(7)	-2104(5)	14530(4)	146(4)
P(1)	-51(1)	6422(1)	11204(1)	44(1)
F(1)	-671(3)	7043(2)	11330(2)	56(1)
F(2)	-837(3)	6109(2)	11147(2)	45(1)
F(3)	-247(3)	6118(3)	11946(3)	58(1)
F(4)	572(3)	5805(3)	11076(4)	81(2)
F(5)	747(3)	6739(3)	11259(3)	72(2)
F(6)	143(4)	6742(3)	10455(3)	81(2)
P(2)	-943(4)	3443(3)	14676(4)	176(3)
F(7)	-1364(13)	2885(7)	15062(13)	440(20)
F(8)	-845	3091	14151	388
F(9)	30(8)	3062(6)	14608(6)	164(4)
F(10)	-578(7)	4041(6)	14134(4)	152(4)
F(11)	-848(14)	3756(6)	15144(5)	247(9)
F(12)	-1870(8)	3810(10)	14683(13)	329(13)
P(3)	807(2)	1769(2)	12746(2)	101(1)
F(31)	1761(4)	1831(3)	12384(3)	80(2)
F(32)	982(7)	2094(5)	13265(4)	142(4)
F(33)	1084(7)	1100(5)	13136(4)	173(5)
F(34)	-155(6)	1747(6)	13150(7)	222(8)
F(35)	692(10)	1489(6)	12195(6)	199(6)
F(36)	512(5)	2464(4)	12353(3)	98(2)
O(5)	-1603(6)	19(3)	12360(4)	75(2)
C(65)	-149(11)	294(6)	11982(11)	152(9)
C(66)	-774(12)	-165(11)	12445(8)	144(8)
C(67)	-2250(11)	-373(10)	12722(7)	131(7)
C(68)	-3080(8)	-140(6)	12628(6)	78(3)

Table 3. Bond lengths [Å] and angles [°] for grot531_a_sq_sq.

Ru(1)-O(2)	2.019(5)
Ru(1)-O(3)	2.162(5)
Ru(1)-N(2)	2.067(6)
Ru(1)-N(3)	1.989(6)
Ru(1)-N(4)	2.069(6)
Ru(1)-C(13)	2.000(7)
Ru(2)-O(4)	2.132(5)
Ru(2)-N(6)	2.067(7)
Ru(2)-N(7)	1.929(6)
Ru(2)-N(8)	2.052(6)
Ru(2)-N(9)	2.150(7)
Ru(2)-C(43)	1.975(7)
O(1)-C(47)	1.220(9)
O(2)-C(47)	1.312(9)

O(3)-C(44) 1.258(8)
O(4)-C(44) 1.263(8)
N(1)-C(1) 1.519(10)
N(1)-C(11) 1.364(10)
N(1)-C(15) 1.349(9)
N(2)-C(16) 1.352(9)
N(2)-C(20) 1.360(10)
N(3)-C(21) 1.351(10)
N(3)-C(25) 1.361(9)
N(4)-C(26) 1.370(9)
N(4)-C(30) 1.350(9)
N(5)-C(31) 1.521(9)
N(5)-C(41) 1.375(9)
N(5)-C(46) 1.348(9)
N(6)-C(58) 1.371(10)
N(6)-C(62) 1.345(10)
N(7)-C(53) 1.355(10)
N(7)-C(57) 1.348(11)
N(8)-C(48) 1.342(10)
N(8)-C(52) 1.372(9)
N(9)-C(63) 1.116(11)
C(1)-C(2) 1.535(12)
C(1)-C(3) 1.540(12)
C(1)-C(6) 1.527(10)
C(2)-H(2A) 0.9700
C(2)-H(2B) 0.9700
C(2)-C(7) 1.547(12)
C(3)-H(3A) 0.9700
C(3)-H(3B) 0.9700
C(3)-C(4) 1.547(13)
C(4)-H(4) 0.9800
C(4)-C(5) 1.490(14)
C(4)-C(10) 1.519(14)
C(5)-H(5A) 0.9700
C(5)-H(5B) 0.9700
C(5)-C(7) 1.520(13)
C(6)-H(6A) 0.9700
C(6)-H(6B) 0.9700
C(6)-C(9) 1.549(12)
C(7)-H(7) 0.9800
C(7)-C(8) 1.525(13)
C(8)-H(8A) 0.9700
C(8)-H(8B) 0.9700
C(8)-C(9) 1.505(13)
C(9)-H(9) 0.9800
C(9)-C(10) 1.532(14)
C(10)-H(10A) 0.9700
C(10)-H(10B) 0.9700
C(11)-H(11) 0.9300
C(11)-C(12) 1.363(11)
C(12)-H(12) 0.9300
C(12)-C(13) 1.398(10)
C(13)-C(14) 1.400(10)
C(14)-C(15) 1.358(10)
C(14)-C(47) 1.494(10)
C(15)-H(15) 0.9300
C(16)-H(16) 0.9300
C(16)-C(17) 1.388(11)
C(17)-H(17) 0.9300
C(17)-C(18) 1.372(13)
C(18)-H(18) 0.9300
C(18)-C(19) 1.383(12)
C(19)-H(19) 0.9300
C(19)-C(20) 1.384(10)
C(20)-C(21) 1.462(11)
C(21)-C(22) 1.384(12)
C(22)-H(22) 0.9300
C(22)-C(23) 1.385(13)
C(23)-H(23) 0.9300
C(23)-C(24) 1.378(13)
C(24)-H(24) 0.9300
C(24)-C(25) 1.377(12)
C(25)-C(26) 1.466(11)
C(26)-C(27) 1.386(10)
C(27)-H(27) 0.9300
C(27)-C(28) 1.373(12)
C(28)-H(28) 0.9300
C(28)-C(29) 1.389(11)
C(29)-H(29) 0.9300
C(29)-C(30) 1.379(10)
C(30)-H(30) 0.9300
C(31)-C(32) 1.547(10)
C(31)-C(33) 1.539(10)
C(31)-C(40) 1.529(12)
C(32)-H(32A) 0.9700
C(32)-H(32B) 0.9700
C(32)-C(37) 1.526(12)
C(33)-H(33A) 0.9700
C(33)-H(33B) 0.9700
C(33)-C(34) 1.539(11)
C(34)-H(34) 0.9800
C(34)-C(35) 1.534(12)
C(34)-C(39) 1.521(14)
C(35)-H(35A) 0.9700
C(35)-H(35B) 0.9700
C(35)-C(37) 1.538(13)
C(36)-H(36) 0.9800
C(36)-C(38) 1.541(12)
C(36)-C(39) 1.529(12)
C(36)-C(40) 1.511(11)
C(37)-H(37) 0.9800
C(37)-C(38) 1.515(14)
C(38)-H(38A) 0.9700
C(38)-H(38B) 0.9700
C(39)-H(39A) 0.9700
C(39)-H(39B) 0.9700
C(40)-H(40A) 0.9700
C(40)-H(40B) 0.9700
C(41)-H(41) 0.9300
C(41)-C(42) 1.360(10)
C(42)-H(42) 0.9300
C(42)-C(43) 1.410(10)
C(43)-C(45) 1.415(10)
C(44)-C(45) 1.486(10)
C(45)-C(46) 1.366(10)
C(46)-H(46) 0.9300

C(48)-H(48)	0.9300
C(48)-C(49)	1.370(11)
C(49)-H(49)	0.9300
C(49)-C(50)	1.390(11)
C(50)-H(50)	0.9300
C(50)-C(51)	1.380(13)
C(51)-H(51)	0.9300
C(51)-C(52)	1.391(11)
C(52)-C(53)	1.453(12)
C(53)-C(54)	1.389(11)
C(54)-H(54)	0.9300
C(54)-C(55)	1.369(14)
C(55)-H(55)	0.9300
C(55)-C(56)	1.369(14)
C(56)-H(56)	0.9300
C(56)-C(57)	1.390(12)
C(57)-C(58)	1.468(12)
C(58)-C(59)	1.374(12)
C(59)-H(59)	0.9300
C(59)-C(60)	1.387(13)
C(60)-H(60)	0.9300
C(60)-C(61)	1.381(13)
C(61)-H(61)	0.9300
C(61)-C(62)	1.372(12)
C(62)-H(62)	0.9300
C(63)-C(64)	1.489(13)
C(64)-H(64A)	0.9600
C(64)-H(64B)	0.9600
C(64)-H(64C)	0.9600
Ru(1')-O(2')	2.004(8)
Ru(1')-O(3')	2.126(7)
Ru(1')-N(2')	2.082(9)
Ru(1')-N(3')	1.964(11)
Ru(1')-N(4')	2.081(11)
Ru(1')-C(13')	1.983(10)
Ru(2')-O(4')	2.141(7)
Ru(2')-N(6')	2.061(8)
Ru(2')-N(7')	1.923(9)
Ru(2')-N(8')	2.060(11)
Ru(2')-N(9')	2.143(11)
Ru(2')-C(43')	1.971(10)
O(1')-C(47')	1.222(13)
O(2')-C(47')	1.329(12)
O(3')-C(44')	1.251(12)
O(4')-C(44')	1.276(12)
N(1')-C(1')	1.527(11)
N(1')-C(11')	1.357(12)
N(1')-C(15')	1.336(13)
N(2')-C(16')	1.314(19)
N(2')-C(20')	1.342(16)
N(3')-C(21')	1.379(13)
N(3')-C(25')	1.311(17)
N(4')-C(26')	1.326(18)
N(4')-C(30')	1.347(13)
N(5')-C(31')	1.512(11)
N(5')-C(41')	1.374(11)
N(5')-C(46')	1.344(13)
N(6')-C(58')	1.385(12)
N(6')-C(62')	1.332(13)
N(7')-C(53')	1.388(15)
N(7')-C(57')	1.350(11)
N(8')-C(48')	1.361(14)
N(8')-C(52')	1.365(19)
N(9')-C(63')	1.114(15)
C(1')-C(2')	1.542(12)
C(1')-C(3')	1.512(13)
C(1')-C(6')	1.530(14)
C(2')-H(2'A)	0.9700
C(2')-H(2'B)	0.9700
C(2')-C(7')	1.527(14)
C(3')-H(3'A)	0.9700
C(3')-H(3'B)	0.9700
C(3')-C(4')	1.529(12)
C(4')-H(4')	0.9800
C(4')-C(5')	1.533(12)
C(4')-C(10')	1.521(13)
C(5')-H(5'A)	0.9700
C(5')-H(5'B)	0.9700
C(5')-C(7')	1.511(16)
C(6')-H(6'A)	0.9700
C(6')-H(6'B)	0.9700
C(6')-C(9')	1.533(13)
C(7')-H(7')	0.9800
C(7')-C(8')	1.498(18)
C(8')-H(8'A)	0.9700
C(8')-H(8'B)	0.9700
C(8')-C(9')	1.535(15)
C(9')-H(9')	0.9800
C(9')-C(10')	1.511(13)
C(10')-H(10C)	0.9700
C(10')-H(10D)	0.9700
C(11')-H(11')	0.9300
C(11')-C(12')	1.370(13)
C(12')-H(12')	0.9300
C(12')-C(13')	1.400(16)
C(13')-C(14')	1.396(15)
C(14')-C(15')	1.378(13)
C(14')-C(47')	1.485(16)
C(15')-H(15')	0.9300
C(16')-H(16')	0.9300
C(16')-C(17')	1.362(17)
C(17')-H(17')	0.9300
C(17')-C(18')	1.34(2)
C(18')-H(18')	0.9300
C(18')-C(19')	1.377(19)
C(19')-H(19')	0.9300
C(19')-C(20')	1.446(16)
C(20')-C(21')	1.44(2)
C(21')-C(22')	1.329(18)
C(22')-H(22')	0.9300
C(22')-C(23')	1.37(2)
C(23')-H(23')	0.9300
C(23')-C(24')	1.406(18)
C(24')-H(24')	0.9300
C(24')-C(25')	1.372(19)
C(25')-C(26')	1.478(15)

C(26')-C(27')	1.369(18)
C(27')-H(27')	0.9300
C(27')-C(28')	1.386(17)
C(28')-H(28')	0.9300
C(28')-C(29')	1.33(2)
C(29')-H(29')	0.9300
C(29')-C(30')	1.389(19)
C(30')-H(30')	0.9300
C(31')-C(32')	1.518(15)
C(31')-C(33')	1.528(13)
C(31')-C(40')	1.543(12)
C(32')-H(32C)	0.9700
C(32')-H(32D)	0.9700
C(32')-C(37')	1.540(15)
C(33')-H(33C)	0.9700
C(33')-H(33D)	0.9700
C(33')-C(34')	1.545(14)
C(34')-H(34')	0.9800
C(34')-C(35')	1.520(18)
C(34')-C(39')	1.523(15)
C(35')-H(35C)	0.9700
C(35')-H(35D)	0.9700
C(35')-C(37')	1.522(16)
C(36')-H(36')	0.9800
C(36')-C(38')	1.510(14)
C(36')-C(39')	1.521(13)
C(36')-C(40')	1.542(13)
C(37')-H(37')	0.9800
C(37')-C(38')	1.498(15)
C(38')-H(38C)	0.9700
C(38')-H(38D)	0.9700
C(39')-H(39C)	0.9700
C(39')-H(39D)	0.9700
C(40')-H(40C)	0.9700
C(40')-H(40D)	0.9700
C(41')-H(41')	0.9300
C(41')-C(42')	1.371(13)
C(42')-H(42')	0.9300
C(42')-C(43')	1.409(15)
C(43')-C(45')	1.406(13)
C(44')-C(45')	1.462(16)
C(45')-C(46')	1.363(13)
C(46')-H(46')	0.9300
C(48')-H(48')	0.9300
C(48')-C(49')	1.39(3)
C(49')-H(49')	0.9300
C(49')-C(50')	1.40(3)
C(50')-H(50')	0.9300
C(50')-C(51')	1.39(2)
C(51')-H(51')	0.9300
C(51')-C(52')	1.388(19)
C(52')-C(53')	1.472(16)
C(53')-C(54')	1.380(17)
C(54')-H(54')	0.9300
C(54')-C(55')	1.371(16)
C(55')-H(55')	0.9300
C(55')-C(56')	1.367(14)
C(56')-H(56')	0.9300
C(56')-C(57')	1.408(14)
C(57')-C(58')	1.470(14)
C(58')-C(59')	1.368(12)
C(59')-H(59')	0.9300
C(59')-C(60')	1.373(14)
C(60')-H(60')	0.9300
C(60')-C(61')	1.386(14)
C(61')-H(61')	0.9300
C(61')-C(62')	1.373(14)
C(62')-H(62')	0.9300
C(63')-C(64')	1.480(18)
C(64')-H(64D)	0.9600
C(64')-H(64E)	0.9600
C(64')-H(64F)	0.9600
P(4)-F(25)	1.518(10)
P(4)-F(26)	1.650(11)
P(4)-F(27)	1.629(8)
P(4)-F(28)	1.528(8)
P(4)-F(29)	1.509(11)
P(4)-F(30)	1.564(8)
P(6)-F(13)	1.595(5)
P(6)-F(14)	1.612(6)
P(6)-F(15)	1.580(5)
P(6)-F(16)	1.596(5)
P(6)-F(17)	1.565(6)
P(6)-F(18)	1.596(6)
P(5)-F(19)	1.688(12)
P(5)-F(20)	1.577(9)
P(5)-F(21)	1.545(9)
P(5)-F(22)	1.557(11)
P(5)-F(23)	1.542(9)
P(5)-F(24)	1.552(8)
P(1)-F(1)	1.596(6)
P(1)-F(2)	1.590(5)
P(1)-F(3)	1.587(6)
P(1)-F(4)	1.594(6)
P(1)-F(5)	1.610(5)
P(1)-F(6)	1.605(6)
P(2)-F(7)	1.447(13)
P(2)-F(8)	1.541(5)
P(2)-F(9)	1.641(13)
P(2)-F(10)	1.599(12)
P(2)-F(11)	1.458(12)
P(2)-F(12)	1.576(18)
P(3)-F(31)	1.545(7)
P(3)-F(32)	1.630(10)
P(3)-F(33)	1.554(10)
P(3)-F(34)	1.576(10)
P(3)-F(35)	1.590(11)
P(3)-F(36)	1.608(8)
O(5)-C(66)	1.381(18)
O(5)-C(67)	1.398(16)
C(65)-H(65A)	0.9600
C(65)-H(65B)	0.9600
C(65)-H(65C)	0.9600
C(65)-C(66)	1.52(2)
C(66)-H(66A)	0.9700
C(66)-H(66B)	0.9700

C(67)-H(67A)	0.9700
C(67)-H(67B)	0.9700
C(67)-C(68)	1.404(19)
C(68)-H(68A)	0.9600
C(68)-H(68B)	0.9600
C(68)-H(68C)	0.9600

O(2)-Ru(1)-O(3)	83.53(19)
O(2)-Ru(1)-N(2)	103.4(2)
O(2)-Ru(1)-N(4)	102.3(2)
N(2)-Ru(1)-O(3)	94.1(2)
N(2)-Ru(1)-N(4)	153.5(2)
N(3)-Ru(1)-O(2)	175.3(2)
N(3)-Ru(1)-O(3)	91.8(2)
N(3)-Ru(1)-N(2)	77.0(2)
N(3)-Ru(1)-N(4)	77.9(2)
N(3)-Ru(1)-C(13)	103.4(3)
N(4)-Ru(1)-O(3)	95.3(2)
C(13)-Ru(1)-O(2)	81.3(3)
C(13)-Ru(1)-O(3)	164.8(2)
C(13)-Ru(1)-N(2)	88.5(2)
C(13)-Ru(1)-N(4)	88.9(2)
O(4)-Ru(2)-N(9)	94.3(2)
N(6)-Ru(2)-O(4)	100.4(2)
N(6)-Ru(2)-N(9)	86.7(3)
N(7)-Ru(2)-O(4)	175.0(2)
N(7)-Ru(2)-N(6)	80.1(3)
N(7)-Ru(2)-N(8)	80.2(3)
N(7)-Ru(2)-N(9)	90.7(3)
N(7)-Ru(2)-C(43)	94.8(3)
N(8)-Ru(2)-O(4)	99.3(2)
N(8)-Ru(2)-N(6)	160.2(2)
N(8)-Ru(2)-N(9)	92.0(2)
C(43)-Ru(2)-O(4)	80.1(2)
C(43)-Ru(2)-N(6)	95.4(3)
C(43)-Ru(2)-N(8)	87.8(3)
C(43)-Ru(2)-N(9)	174.4(3)
C(47)-O(2)-Ru(1)	117.7(4)
C(44)-O(3)-Ru(1)	128.5(5)
C(44)-O(4)-Ru(2)	114.8(4)
C(11)-N(1)-C(1)	119.4(6)
C(15)-N(1)-C(1)	121.9(6)
C(15)-N(1)-C(11)	118.7(7)
C(16)-N(2)-Ru(1)	124.9(5)
C(16)-N(2)-C(20)	119.4(6)
C(20)-N(2)-Ru(1)	115.6(4)
C(21)-N(3)-Ru(1)	119.5(5)
C(21)-N(3)-C(25)	120.4(7)
C(25)-N(3)-Ru(1)	119.8(5)
C(26)-N(4)-Ru(1)	115.3(5)
C(30)-N(4)-Ru(1)	125.1(5)
C(30)-N(4)-C(26)	119.6(6)
C(41)-N(5)-C(31)	118.7(6)
C(46)-N(5)-C(31)	123.1(6)
C(46)-N(5)-C(41)	118.0(6)
C(58)-N(6)-Ru(2)	112.8(5)
C(62)-N(6)-Ru(2)	128.8(6)
C(62)-N(6)-C(58)	118.4(7)
C(53)-N(7)-Ru(2)	118.4(6)
C(57)-N(7)-Ru(2)	119.0(5)
C(57)-N(7)-C(53)	122.6(7)
C(48)-N(8)-Ru(2)	128.3(5)
C(48)-N(8)-C(52)	118.8(7)
C(52)-N(8)-Ru(2)	112.7(5)
C(63)-N(9)-Ru(2)	167.4(8)
N(1)-C(1)-C(2)	110.9(6)
N(1)-C(1)-C(3)	109.4(6)
N(1)-C(1)-C(6)	108.9(6)
C(2)-C(1)-C(3)	108.7(7)
C(6)-C(1)-C(2)	108.8(7)
C(6)-C(1)-C(3)	110.1(7)
C(1)-C(2)-H(2A)	109.8
C(1)-C(2)-H(2B)	109.8
C(1)-C(2)-C(7)	109.5(7)
H(2A)-C(2)-H(2B)	108.2
C(7)-C(2)-H(2A)	109.8
C(7)-C(2)-H(2B)	109.8
C(1)-C(3)-H(3A)	109.8
C(1)-C(3)-H(3B)	109.8
C(1)-C(3)-C(4)	109.3(7)
H(3A)-C(3)-H(3B)	108.3
C(4)-C(3)-H(3A)	109.8
C(4)-C(3)-H(3B)	109.8
C(3)-C(4)-H(4)	109.5
C(5)-C(4)-C(3)	109.2(8)
C(5)-C(4)-H(4)	109.5
C(5)-C(4)-C(10)	110.7(9)
C(10)-C(4)-C(3)	108.5(8)
C(10)-C(4)-H(4)	109.5
C(4)-C(5)-H(5A)	109.6
C(4)-C(5)-H(5B)	109.6
C(4)-C(5)-C(7)	110.4(8)
H(5A)-C(5)-H(5B)	108.1
C(7)-C(5)-H(5A)	109.6
C(7)-C(5)-H(5B)	109.6
C(1)-C(6)-H(6A)	109.8
C(1)-C(6)-H(6B)	109.8
C(1)-C(6)-C(9)	109.2(7)
H(6A)-C(6)-H(6B)	108.3
C(9)-C(6)-H(6A)	109.8
C(9)-C(6)-H(6B)	109.8
C(2)-C(7)-H(7)	109.6
C(5)-C(7)-C(2)	109.1(8)
C(5)-C(7)-H(7)	109.6
C(5)-C(7)-C(8)	111.2(8)
C(8)-C(7)-C(2)	107.8(7)
C(8)-C(7)-H(7)	109.6
C(7)-C(8)-H(8A)	109.8
C(7)-C(8)-H(8B)	109.8
H(8A)-C(8)-H(8B)	108.2
C(9)-C(8)-C(7)	109.4(8)
C(9)-C(8)-H(8A)	109.8
C(9)-C(8)-H(8B)	109.8
C(6)-C(9)-H(9)	109.4
C(8)-C(9)-C(6)	109.0(8)
C(8)-C(9)-H(9)	109.4

C(8)-C(9)-C(10)	111.3(8)
C(10)-C(9)-C(6)	108.3(7)
C(10)-C(9)-H(9)	109.4
C(4)-C(10)-C(9)	109.9(8)
C(4)-C(10)-H(10A)	109.7
C(4)-C(10)-H(10B)	109.7
C(9)-C(10)-H(10A)	109.7
C(9)-C(10)-H(10B)	109.7
H(10A)-C(10)-H(10B)	108.2
N(1)-C(11)-H(11)	119.1
C(12)-C(11)-N(1)	121.7(7)
C(12)-C(11)-H(11)	119.1
C(11)-C(12)-H(12)	119.6
C(11)-C(12)-C(13)	120.8(7)
C(13)-C(12)-H(12)	119.6
C(12)-C(13)-Ru(1)	132.2(6)
C(12)-C(13)-C(14)	115.8(7)
C(14)-C(13)-Ru(1)	112.0(5)
C(13)-C(14)-C(47)	116.9(7)
C(15)-C(14)-C(13)	122.0(7)
C(15)-C(14)-C(47)	121.1(7)
N(1)-C(15)-C(14)	121.1(7)
N(1)-C(15)-H(15)	119.4
C(14)-C(15)-H(15)	119.4
N(2)-C(16)-H(16)	119.7
N(2)-C(16)-C(17)	120.5(8)
C(17)-C(16)-H(16)	119.7
C(16)-C(17)-H(17)	119.8
C(18)-C(17)-C(16)	120.3(8)
C(18)-C(17)-H(17)	119.8
C(17)-C(18)-H(18)	120.5
C(17)-C(18)-C(19)	119.0(8)
C(19)-C(18)-H(18)	120.5
C(18)-C(19)-H(19)	120.4
C(18)-C(19)-C(20)	119.2(8)
C(20)-C(19)-H(19)	120.4
N(2)-C(20)-C(19)	121.4(7)
N(2)-C(20)-C(21)	113.8(6)
C(19)-C(20)-C(21)	124.8(8)
N(3)-C(21)-C(20)	112.4(7)
N(3)-C(21)-C(22)	121.0(7)
C(22)-C(21)-C(20)	126.6(8)
C(21)-C(22)-H(22)	120.7
C(21)-C(22)-C(23)	118.6(9)
C(23)-C(22)-H(22)	120.7
C(22)-C(23)-H(23)	119.9
C(24)-C(23)-C(22)	120.2(9)
C(24)-C(23)-H(23)	119.9
C(23)-C(24)-H(24)	120.3
C(25)-C(24)-C(23)	119.4(8)
C(25)-C(24)-H(24)	120.3
N(3)-C(25)-C(24)	120.4(7)
N(3)-C(25)-C(26)	112.2(7)
C(24)-C(25)-C(26)	127.4(7)
N(4)-C(26)-C(25)	114.6(6)
N(4)-C(26)-C(27)	120.6(7)
C(27)-C(26)-C(25)	124.8(7)
C(26)-C(27)-H(27)	120.2
C(28)-C(27)-C(26)	119.5(8)
C(28)-C(27)-H(27)	120.2
C(27)-C(28)-H(28)	120.2
C(27)-C(28)-C(29)	119.6(7)
C(29)-C(28)-H(28)	120.2
C(28)-C(29)-H(29)	120.4
C(30)-C(29)-C(28)	119.3(7)
C(30)-C(29)-H(29)	120.4
N(4)-C(30)-C(29)	121.3(7)
N(4)-C(30)-H(30)	119.4
C(29)-C(30)-H(30)	119.4
N(5)-C(31)-C(32)	109.9(6)
N(5)-C(31)-C(33)	110.3(6)
N(5)-C(31)-C(40)	108.6(6)
C(33)-C(31)-C(32)	108.6(6)
C(40)-C(31)-C(32)	110.2(7)
C(40)-C(31)-C(33)	109.2(6)
C(31)-C(32)-H(32A)	110.0
C(31)-C(32)-H(32B)	110.0
H(32A)-C(32)-H(32B)	108.4
C(37)-C(32)-C(31)	108.6(7)
C(37)-C(32)-H(32A)	110.0
C(37)-C(32)-H(32B)	110.0
C(31)-C(33)-H(33A)	109.9
C(31)-C(33)-H(33B)	109.9
C(31)-C(33)-C(34)	108.9(7)
H(33A)-C(33)-H(33B)	108.3
C(34)-C(33)-H(33A)	109.9
C(34)-C(33)-H(33B)	109.9
C(33)-C(34)-H(34)	109.1
C(35)-C(34)-C(33)	109.1(7)
C(35)-C(34)-H(34)	109.1
C(39)-C(34)-C(33)	109.8(7)
C(39)-C(34)-H(34)	109.1
C(39)-C(34)-C(35)	110.5(8)
C(34)-C(35)-H(35A)	110.0
C(34)-C(35)-H(35B)	110.0
C(34)-C(35)-C(37)	108.6(7)
H(35A)-C(35)-H(35B)	108.4
C(37)-C(35)-H(35A)	110.0
C(37)-C(35)-H(35B)	110.0
C(38)-C(36)-H(36)	109.2
C(39)-C(36)-H(36)	109.2
C(39)-C(36)-C(38)	110.2(8)
C(40)-C(36)-H(36)	109.2
C(40)-C(36)-C(38)	109.2(7)
C(40)-C(36)-C(39)	109.7(7)
C(32)-C(37)-C(35)	109.2(8)
C(32)-C(37)-H(37)	108.9
C(35)-C(37)-H(37)	108.9
C(38)-C(37)-C(32)	110.5(8)
C(38)-C(37)-C(35)	110.2(8)
C(38)-C(37)-H(37)	108.9
C(36)-C(38)-H(38A)	109.9
C(36)-C(38)-H(38B)	109.9
C(37)-C(38)-C(36)	109.0(7)
C(37)-C(38)-H(38A)	109.9
C(37)-C(38)-H(38B)	109.9

H(38A)-C(38)-H(38B)	108.3
C(34)-C(39)-C(36)	108.8(7)
C(34)-C(39)-H(39A)	109.9
C(34)-C(39)-H(39B)	109.9
C(36)-C(39)-H(39A)	109.9
C(36)-C(39)-H(39B)	109.9
H(39A)-C(39)-H(39B)	108.3
C(31)-C(40)-H(40A)	109.7
C(31)-C(40)-H(40B)	109.7
C(36)-C(40)-C(31)	109.9(7)
C(36)-C(40)-H(40A)	109.7
C(36)-C(40)-H(40B)	109.7
H(40A)-C(40)-H(40B)	108.2
N(5)-C(41)-H(41)	118.9
C(42)-C(41)-N(5)	122.3(7)
C(42)-C(41)-H(41)	118.9
C(41)-C(42)-H(42)	119.3
C(41)-C(42)-C(43)	121.3(7)
C(43)-C(42)-H(42)	119.3
C(42)-C(43)-Ru(2)	131.8(5)
C(42)-C(43)-C(45)	114.3(6)
C(45)-C(43)-Ru(2)	113.8(5)
O(3)-C(44)-O(4)	124.7(7)
O(3)-C(44)-C(45)	120.0(6)
O(4)-C(44)-C(45)	115.3(6)
C(43)-C(45)-C(44)	115.8(6)
C(46)-C(45)-C(43)	122.5(7)
C(46)-C(45)-C(44)	121.7(6)
N(5)-C(46)-C(45)	121.3(6)
N(5)-C(46)-H(46)	119.3
C(45)-C(46)-H(46)	119.3
O(1)-C(47)-O(2)	124.0(7)
O(1)-C(47)-C(14)	124.1(7)
O(2)-C(47)-C(14)	111.9(6)
N(8)-C(48)-H(48)	118.3
N(8)-C(48)-C(49)	123.4(7)
C(49)-C(48)-H(48)	118.3
C(48)-C(49)-H(49)	120.8
C(48)-C(49)-C(50)	118.4(8)
C(50)-C(49)-H(49)	120.8
C(49)-C(50)-H(50)	120.4
C(51)-C(50)-C(49)	119.2(8)
C(51)-C(50)-H(50)	120.4
C(50)-C(51)-H(51)	119.9
C(50)-C(51)-C(52)	120.1(7)
C(52)-C(51)-H(51)	119.9
N(8)-C(52)-C(51)	120.1(8)
N(8)-C(52)-C(53)	114.8(7)
C(51)-C(52)-C(53)	125.1(7)
N(7)-C(53)-C(52)	113.4(7)
N(7)-C(53)-C(54)	118.8(8)
C(54)-C(53)-C(52)	127.8(8)
C(53)-C(54)-H(54)	120.4
C(55)-C(54)-C(53)	119.2(9)
C(55)-C(54)-H(54)	120.4
C(54)-C(55)-H(55)	119.4
C(54)-C(55)-C(56)	121.3(9)
C(56)-C(55)-H(55)	119.4
C(55)-C(56)-H(56)	120.6
C(55)-C(56)-C(57)	118.8(10)
C(57)-C(56)-H(56)	120.6
N(7)-C(57)-C(56)	119.3(8)
N(7)-C(57)-C(58)	113.5(7)
C(56)-C(57)-C(58)	127.2(9)
N(6)-C(58)-C(57)	114.3(7)
N(6)-C(58)-C(59)	120.9(8)
C(59)-C(58)-C(57)	124.8(8)
C(58)-C(59)-H(59)	120.0
C(58)-C(59)-C(60)	120.0(9)
C(60)-C(59)-H(59)	120.0
C(59)-C(60)-H(60)	120.6
C(61)-C(60)-C(59)	118.7(8)
C(61)-C(60)-H(60)	120.6
C(60)-C(61)-H(61)	120.4
C(62)-C(61)-C(60)	119.2(8)
C(62)-C(61)-H(61)	120.4
N(6)-C(62)-C(61)	122.7(8)
N(6)-C(62)-H(62)	118.6
C(61)-C(62)-H(62)	118.6
N(9)-C(63)-C(64)	177.8(11)
C(63)-C(64)-H(64A)	109.5
C(63)-C(64)-H(64B)	109.5
C(63)-C(64)-H(64C)	109.5
H(64A)-C(64)-H(64B)	109.5
H(64A)-C(64)-H(64C)	109.5
H(64B)-C(64)-H(64C)	109.5
O(2')-Ru(1')-O(3')	94.2(3)
O(2')-Ru(1')-N(2')	99.3(4)
O(2')-Ru(1')-N(4')	103.1(4)
N(2')-Ru(1')-O(3')	81.9(3)
N(3')-Ru(1')-O(2')	178.1(3)
N(3')-Ru(1')-O(3')	86.5(4)
N(3')-Ru(1')-N(2')	79.0(5)
N(3')-Ru(1')-N(4')	78.6(4)
N(3')-Ru(1')-C(13')	97.7(5)
N(4')-Ru(1')-O(3')	95.3(4)
N(4')-Ru(1')-N(2')	157.5(5)
C(13')-Ru(1')-O(2')	81.5(4)
C(13')-Ru(1')-O(3')	174.8(5)
C(13')-Ru(1')-N(2')	95.9(3)
C(13')-Ru(1')-N(4')	88.5(4)
O(4')-Ru(2')-N(9')	89.0(3)
N(6')-Ru(2')-O(4')	101.5(3)
N(6')-Ru(2')-N(9')	88.6(3)
N(7')-Ru(2')-O(4')	171.8(3)
N(7')-Ru(2')-N(6')	80.5(3)
N(7')-Ru(2')-N(8')	79.9(4)
N(7')-Ru(2')-N(9')	99.0(4)
N(7')-Ru(2')-C(43')	91.3(4)
N(8')-Ru(2')-O(4')	98.4(4)
N(8')-Ru(2')-N(6')	160.1(4)
N(8')-Ru(2')-N(9')	90.9(4)
C(43')-Ru(2')-O(4')	80.7(4)
C(43')-Ru(2')-N(6')	92.9(3)
C(43')-Ru(2')-N(8')	91.1(4)
C(43')-Ru(2')-N(9')	169.6(4)

C(47')-O(2')-Ru(1')	118.0(8)
C(44')-O(3')-Ru(1')	124.0(7)
C(44')-O(4')-Ru(2')	112.3(7)
C(11')-N(1')-C(1')	117.9(9)
C(15')-N(1')-C(1')	123.2(8)
C(15')-N(1')-C(11')	118.9(8)
C(16')-N(2')-Ru(1')	126.4(9)
C(16')-N(2')-C(20')	118.4(11)
C(20')-N(2')-Ru(1')	114.3(10)
C(21')-N(3')-Ru(1')	117.3(10)
C(25')-N(3')-Ru(1')	117.7(7)
C(25')-N(3')-C(21')	124.8(12)
C(26')-N(4')-Ru(1')	115.0(7)
C(26')-N(4')-C(30')	119.9(12)
C(30')-N(4')-Ru(1')	125.0(11)
C(41')-N(5')-C(31')	119.3(8)
C(46')-N(5')-C(31')	123.5(8)
C(46')-N(5')-C(41')	117.2(8)
C(58')-N(6')-Ru(2')	112.2(7)
C(62')-N(6')-Ru(2')	128.6(6)
C(62')-N(6')-C(58')	119.1(8)
C(53')-N(7')-Ru(2')	120.0(7)
C(57')-N(7')-Ru(2')	118.9(7)
C(57')-N(7')-C(53')	120.3(10)
C(48')-N(8')-Ru(2')	125.3(12)
C(48')-N(8')-C(52')	121.4(13)
C(52')-N(8')-Ru(2')	113.1(7)
C(63')-N(9')-Ru(2')	177.4(9)
N(1')-C(1')-C(2')	108.3(7)
N(1')-C(1')-C(6')	108.4(7)
C(3')-C(1')-N(1')	111.5(8)
C(3')-C(1')-C(2')	109.2(8)
C(3')-C(1')-C(6')	108.8(7)
C(6')-C(1')-C(2')	110.6(9)
C(1')-C(2')-H(2'A)	110.0
C(1')-C(2')-H(2'B)	110.0
H(2'A)-C(2')-H(2'B)	108.3
C(7')-C(2')-C(1')	108.6(8)
C(7')-C(2')-H(2'A)	110.0
C(7')-C(2')-H(2'B)	110.0
C(1')-C(3')-H(3'A)	109.7
C(1')-C(3')-H(3'B)	109.7
C(1')-C(3')-C(4')	109.9(8)
H(3'A)-C(3')-H(3'B)	108.2
C(4')-C(3')-H(3'A)	109.7
C(4')-C(3')-H(3'B)	109.7
C(3')-C(4')-H(4')	109.6
C(3')-C(4')-C(5')	109.1(7)
C(5')-C(4')-H(4')	109.6
C(10')-C(4')-C(3')	109.4(7)
C(10')-C(4')-H(4')	109.6
C(10')-C(4')-C(5')	109.5(9)
C(4')-C(5')-H(5'A)	109.9
C(4')-C(5')-H(5'B)	109.9
H(5'A)-C(5')-H(5'B)	108.3
C(7')-C(5')-C(4')	109.1(8)
C(7')-C(5')-H(5'A)	109.9
C(7')-C(5')-H(5'B)	109.9
C(1')-C(6')-H(6'A)	109.9
C(1')-C(6')-H(6'B)	109.9
C(1')-C(6')-C(9')	109.0(8)
H(6'A)-C(6')-H(6'B)	108.3
C(9')-C(6')-H(6'A)	109.9
C(9')-C(6')-H(6'B)	109.9
C(2')-C(7')-H(7')	109.2
C(5')-C(7')-C(2')	110.7(11)
C(5')-C(7')-H(7')	109.2
C(8')-C(7')-C(2')	108.5(10)
C(8')-C(7')-C(5')	109.9(9)
C(8')-C(7')-H(7')	109.2
C(7')-C(8')-H(8'A)	109.4
C(7')-C(8')-H(8'B)	109.4
C(7')-C(8')-C(9')	111.0(9)
H(8'A)-C(8')-H(8'B)	108.0
C(9')-C(8')-H(8'A)	109.4
C(9')-C(8')-H(8'B)	109.4
C(6')-C(9')-C(8')	109.1(8)
C(6')-C(9')-H(9')	109.9
C(8')-C(9')-H(9')	109.9
C(10')-C(9')-C(6')	108.7(8)
C(10')-C(9')-C(8')	109.2(8)
C(10')-C(9')-H(9')	109.9
C(4')-C(10')-H(10C)	109.7
C(4')-C(10')-H(10D)	109.7
C(9')-C(10')-C(4')	109.9(8)
C(9')-C(10')-H(10C)	109.7
C(9')-C(10')-H(10D)	109.7
H(10C)-C(10')-H(10D)	108.2
N(1')-C(11')-H(11')	119.3
N(1')-C(11')-C(12')	121.4(11)
C(12')-C(11')-H(11')	119.3
C(11')-C(12')-H(12')	119.7
C(11')-C(12')-C(13')	120.5(11)
C(13')-C(12')-H(12')	119.7
C(12')-C(13')-Ru(1')	130.8(8)
C(14')-C(13')-Ru(1')	112.1(9)
C(14')-C(13')-C(12')	116.9(9)
C(13')-C(14')-C(47')	117.6(9)
C(15')-C(14')-C(13')	119.8(11)
C(15')-C(14')-C(47')	122.5(10)
N(1')-C(15')-C(14')	122.4(10)
N(1')-C(15')-H(15')	118.8
C(14')-C(15')-H(15')	118.8
N(2')-C(16')-H(16')	117.3
N(2')-C(16')-C(17')	125.4(18)
C(17')-C(16')-H(16')	117.3
C(16')-C(17')-H(17')	120.9
C(18')-C(17')-C(16')	118.1(18)
C(18')-C(17')-H(17')	120.9
C(17')-C(18')-H(18')	119.9
C(17')-C(18')-C(19')	120.2(14)
C(19')-C(18')-H(18')	119.9
C(18')-C(19')-H(19')	120.8
C(18')-C(19')-C(20')	118.4(13)
C(20')-C(19')-H(19')	120.8
N(2')-C(20')-C(19')	119.2(14)

N(2')-C(20')-C(21')	114.7(10)
C(21')-C(20')-C(19')	125.9(13)
N(3')-C(21')-C(20')	114.2(12)
C(22')-C(21')-N(3')	118.2(15)
C(22')-C(21')-C(20')	127.4(12)
C(21')-C(22')-H(22')	120.4
C(21')-C(22')-C(23')	119.2(13)
C(23')-C(22')-H(22')	120.4
C(22')-C(23')-H(23')	119.2
C(22')-C(23')-C(24')	121.6(14)
C(24')-C(23')-H(23')	119.2
C(23')-C(24')-H(24')	121.3
C(25')-C(24')-C(23')	117.4(15)
C(25')-C(24')-H(24')	121.3
N(3')-C(25')-C(24')	118.7(11)
N(3')-C(25')-C(26')	116.0(12)
C(24')-C(25')-C(26')	125.2(14)
N(4')-C(26')-C(25')	112.6(12)
N(4')-C(26')-C(27')	121.5(11)
C(27')-C(26')-C(25')	125.8(14)
C(26')-C(27')-H(27')	120.7
C(26')-C(27')-C(28')	118.6(15)
C(28')-C(27')-H(27')	120.7
C(27')-C(28')-H(28')	120.0
C(29')-C(28')-C(27')	120.0(14)
C(29')-C(28')-H(28')	120.0
C(28')-C(29')-H(29')	120.1
C(28')-C(29')-C(30')	119.7(11)
C(30')-C(29')-H(29')	120.1
N(4')-C(30')-C(29')	120.3(14)
N(4')-C(30')-H(30')	119.9
C(29')-C(30')-H(30')	119.9
N(5')-C(31')-C(32')	109.4(8)
N(5')-C(31')-C(33')	111.1(8)
N(5')-C(31')-C(40')	107.8(7)
C(32')-C(31')-C(33')	109.4(9)
C(32')-C(31')-C(40')	110.7(8)
C(33')-C(31')-C(40')	108.4(8)
C(31')-C(32')-H(32C)	109.9
C(31')-C(32')-H(32D)	109.9
C(31')-C(32')-C(37')	109.0(9)
H(32C)-C(32')-H(32D)	108.3
C(37')-C(32')-H(32C)	109.9
C(37')-C(32')-H(32D)	109.9
C(31')-C(33')-H(33C)	109.8
C(31')-C(33')-H(33D)	109.8
C(31')-C(33')-C(34')	109.3(9)
H(33C)-C(33')-H(33D)	108.3
C(34')-C(33')-H(33C)	109.8
C(34')-C(33')-H(33D)	109.8
C(33')-C(34')-H(34')	109.4
C(35')-C(34')-C(33')	109.0(10)
C(35')-C(34')-H(34')	109.4
C(35')-C(34')-C(39')	110.7(10)
C(39')-C(34')-C(33')	108.9(9)
C(39')-C(34')-H(34')	109.4
C(34')-C(35')-H(35C)	109.9
C(34')-C(35')-H(35D)	109.9
C(34')-C(35')-C(37')	109.0(9)
H(35C)-C(35')-H(35D)	108.3
C(37')-C(35')-H(35C)	109.9
C(37')-C(35')-H(35D)	109.9
C(38')-C(36')-H(36')	109.4
C(38')-C(36')-C(39')	110.5(9)
C(38')-C(36')-C(40')	109.4(8)
C(39')-C(36')-H(36')	109.4
C(39')-C(36')-C(40')	108.5(8)
C(40')-C(36')-H(36')	109.4
C(32')-C(37')-H(37')	109.2
C(35')-C(37')-C(32')	109.1(10)
C(35')-C(37')-H(37')	109.2
C(38')-C(37')-C(32')	109.3(9)
C(38')-C(37')-C(35')	110.7(10)
C(38')-C(37')-H(37')	109.2
C(36')-C(38')-H(38C)	109.6
C(36')-C(38')-H(38D)	109.6
C(37')-C(38')-C(36')	110.5(9)
C(37')-C(38')-H(38C)	109.6
C(37')-C(38')-H(38D)	109.6
H(38C)-C(38')-H(38D)	108.1
C(34')-C(39')-H(39C)	109.8
C(34')-C(39')-H(39D)	109.8
C(36')-C(39')-C(34')	109.3(9)
C(36')-C(39')-H(39C)	109.8
C(36')-C(39')-H(39D)	109.8
H(39C)-C(39')-H(39D)	108.3
C(31')-C(40')-H(40C)	110.0
C(31')-C(40')-H(40D)	110.0
C(36')-C(40')-C(31')	108.6(7)
C(36')-C(40')-H(40C)	110.0
C(36')-C(40')-H(40D)	110.0
H(40C)-C(40')-H(40D)	108.3
N(5')-C(41')-H(41')	119.2
C(42')-C(41')-N(5')	121.5(10)
C(42')-C(41')-H(41')	119.2
C(41')-C(42')-H(42')	118.7
C(41')-C(42')-C(43')	122.7(9)
C(43')-C(42')-H(42')	118.7
C(42')-C(43')-Ru(2')	133.6(7)
C(45')-C(43')-Ru(2')	113.3(8)
C(45')-C(43')-C(42')	113.1(9)
O(3')-C(44')-O(4')	123.3(11)
O(3')-C(44')-C(45')	119.8(9)
O(4')-C(44')-C(45')	116.9(9)
C(43')-C(45')-C(44')	116.3(9)
C(46')-C(45')-C(43')	123.0(10)
C(46')-C(45')-C(44')	120.8(9)
N(5')-C(46')-C(45')	122.4(9)
N(5')-C(46')-H(46')	118.8
C(45')-C(46')-H(46')	118.8
O(1')-C(47')-O(2')	124.0(11)
O(1')-C(47')-C(14')	125.3(9)
O(2')-C(47')-C(14')	110.7(11)
N(8')-C(48')-H(48')	120.6
N(8')-C(48')-C(49')	118.8(18)
C(49')-C(48')-H(48')	120.6

C(48')-C(49')-H(49')	119.8
C(48')-C(49')-C(50')	120.4(16)
C(50')-C(49')-H(49')	119.8
C(49')-C(50')-H(50')	120.1
C(51')-C(50')-C(49')	119.8(18)
C(51')-C(50')-H(50')	120.1
C(50')-C(51')-H(51')	120.9
C(52')-C(51')-C(50')	118(2)
C(52')-C(51')-H(51')	120.9
N(8')-C(52')-C(51')	121.2(13)
N(8')-C(52')-C(53')	116.1(11)
C(51')-C(52')-C(53')	122.6(17)
N(7')-C(53')-C(52')	110.4(13)
C(54')-C(53')-N(7')	120.8(10)
C(54')-C(53')-C(52')	128.9(13)
C(53')-C(54')-H(54')	121.0
C(55')-C(54')-C(53')	117.9(12)
C(55')-C(54')-H(54')	121.0
C(54')-C(55')-H(55')	118.7
C(56')-C(55')-C(54')	122.6(12)
C(56')-C(55')-H(55')	118.7
C(55')-C(56')-H(56')	120.9
C(55')-C(56')-C(57')	118.3(10)
C(57')-C(56')-H(56')	120.9
N(7')-C(57')-C(56')	120.0(10)
N(7')-C(57')-C(58')	113.0(9)
C(56')-C(57')-C(58')	127.1(8)
N(6')-C(58')-C(57')	114.6(8)
C(59')-C(58')-N(6')	121.0(9)
C(59')-C(58')-C(57')	124.4(9)
C(58')-C(59')-H(59')	120.5
C(58')-C(59')-C(60')	119.0(9)
C(60')-C(59')-H(59')	120.5
C(59')-C(60')-H(60')	119.9
C(59')-C(60')-C(61')	120.1(10)
C(61')-C(60')-H(60')	119.9
C(60')-C(61')-H(61')	120.6
C(62')-C(61')-C(60')	118.8(11)
C(62')-C(61')-H(61')	120.6
N(6')-C(62')-C(61')	121.9(10)
N(6')-C(62')-H(62')	119.0
C(61')-C(62')-H(62')	119.0
N(9')-C(63')-C(64')	178.2(16)
C(63')-C(64')-H(64D)	109.5
C(63')-C(64')-H(64E)	109.5
C(63')-C(64')-H(64F)	109.5
H(64D)-C(64')-H(64E)	109.5
H(64D)-C(64')-H(64F)	109.5
H(64E)-C(64')-H(64F)	109.5
F(25)-P(4)-F(26)	87.6(6)
F(25)-P(4)-F(27)	85.4(5)
F(25)-P(4)-F(28)	172.6(6)
F(25)-P(4)-F(30)	92.3(6)
F(27)-P(4)-F(26)	87.0(5)
F(28)-P(4)-F(26)	87.9(5)
F(28)-P(4)-F(27)	88.5(5)
F(28)-P(4)-F(30)	93.5(5)
F(29)-P(4)-F(25)	93.3(7)
F(29)-P(4)-F(26)	176.8(6)
F(29)-P(4)-F(27)	90.0(5)
F(29)-P(4)-F(28)	90.9(5)
F(29)-P(4)-F(30)	94.9(6)
F(30)-P(4)-F(26)	88.1(5)
F(30)-P(4)-F(27)	174.6(6)
F(13)-P(6)-F(14)	89.7(3)
F(13)-P(6)-F(16)	178.9(4)
F(13)-P(6)-F(18)	89.9(3)
F(15)-P(6)-F(13)	90.4(3)
F(15)-P(6)-F(14)	89.1(3)
F(15)-P(6)-F(16)	89.2(3)
F(15)-P(6)-F(18)	177.5(4)
F(16)-P(6)-F(14)	89.3(3)
F(16)-P(6)-F(18)	90.5(3)
F(17)-P(6)-F(13)	91.1(3)
F(17)-P(6)-F(14)	178.9(4)
F(17)-P(6)-F(15)	91.6(4)
F(17)-P(6)-F(16)	89.9(3)
F(17)-P(6)-F(18)	90.9(4)
F(18)-P(6)-F(14)	88.4(4)
F(20)-P(5)-F(19)	87.0(7)
F(21)-P(5)-F(19)	84.6(6)
F(21)-P(5)-F(20)	89.9(6)
F(21)-P(5)-F(22)	93.6(6)
F(21)-P(5)-F(24)	91.9(6)
F(22)-P(5)-F(19)	177.8(6)
F(22)-P(5)-F(20)	91.7(8)
F(23)-P(5)-F(19)	91.2(7)
F(23)-P(5)-F(20)	88.2(6)
F(23)-P(5)-F(21)	175.4(8)
F(23)-P(5)-F(22)	90.6(7)
F(23)-P(5)-F(24)	89.6(6)
F(24)-P(5)-F(19)	88.1(6)
F(24)-P(5)-F(20)	174.6(8)
F(24)-P(5)-F(22)	93.3(6)
F(1)-P(1)-F(5)	89.2(3)
F(1)-P(1)-F(6)	89.5(3)
F(2)-P(1)-F(1)	91.0(3)
F(2)-P(1)-F(4)	89.3(3)
F(2)-P(1)-F(5)	179.7(4)
F(2)-P(1)-F(6)	89.8(3)
F(3)-P(1)-F(1)	89.6(3)
F(3)-P(1)-F(2)	90.7(3)
F(3)-P(1)-F(4)	90.5(4)
F(3)-P(1)-F(5)	89.5(3)
F(3)-P(1)-F(6)	179.0(4)
F(4)-P(1)-F(1)	179.7(4)
F(4)-P(1)-F(5)	90.5(3)
F(4)-P(1)-F(6)	90.4(4)
F(6)-P(1)-F(5)	90.0(3)
F(7)-P(2)-F(8)	81.5(11)
F(7)-P(2)-F(9)	93.7(11)
F(7)-P(2)-F(10)	167.3(16)
F(7)-P(2)-F(11)	103.3(14)
F(7)-P(2)-F(12)	87.8(11)
F(8)-P(2)-F(9)	75.2(5)
F(8)-P(2)-F(10)	88.3(6)

F(8)-P(2)-F(12)	100.7(11)
F(10)-P(2)-F(9)	90.9(6)
F(11)-P(2)-F(8)	168.5(10)
F(11)-P(2)-F(9)	94.0(10)
F(11)-P(2)-F(10)	88.1(7)
F(11)-P(2)-F(12)	89.9(11)
F(12)-P(2)-F(9)	175.4(13)
F(12)-P(2)-F(10)	86.8(10)
F(31)-P(3)-F(32)	88.3(5)
F(31)-P(3)-F(33)	89.2(5)
F(31)-P(3)-F(34)	174.9(8)
F(31)-P(3)-F(35)	87.8(6)
F(31)-P(3)-F(36)	91.4(4)
F(33)-P(3)-F(32)	90.0(6)
F(33)-P(3)-F(34)	92.0(6)
F(33)-P(3)-F(35)	92.7(7)
F(33)-P(3)-F(36)	179.0(7)
F(34)-P(3)-F(32)	86.8(8)
F(34)-P(3)-F(35)	97.1(8)
F(34)-P(3)-F(36)	87.3(5)
F(35)-P(3)-F(32)	175.2(6)
F(35)-P(3)-F(36)	88.1(6)
F(36)-P(3)-F(32)	89.3(5)
C(66)-O(5)-C(67)	118.1(13)
H(65A)-C(65)-H(65B)	109.5
H(65A)-C(65)-H(65C)	109.5
H(65B)-C(65)-H(65C)	109.5
C(66)-C(65)-H(65A)	109.5
C(66)-C(65)-H(65B)	109.5
C(66)-C(65)-H(65C)	109.5
O(5)-C(66)-C(65)	110.7(16)
O(5)-C(66)-H(66A)	109.5
O(5)-C(66)-H(66B)	109.5
C(65)-C(66)-H(66A)	109.5
C(65)-C(66)-H(66B)	109.5
H(66A)-C(66)-H(66B)	108.1
O(5)-C(67)-H(67A)	108.6
O(5)-C(67)-H(67B)	108.6
O(5)-C(67)-C(68)	114.6(14)
H(67A)-C(67)-H(67B)	107.6
C(68)-C(67)-H(67A)	108.6
C(68)-C(67)-H(67B)	108.6
C(67)-C(68)-H(68A)	109.5
C(67)-C(68)-H(68B)	109.5
C(67)-C(68)-H(68C)	109.5
H(68A)-C(68)-H(68B)	109.5
H(68A)-C(68)-H(68C)	109.5
H(68B)-C(68)-H(68C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (Å2x 103) for grot531_a_sq_sq. The anisotropic displacement factor exponent takes the form: -2□2[h2 a*2U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ru(1)	22(1)	30(1)	28(1)	-4(1)	-12(1)	-6(1)
Ru(2)	26(1)	39(1)	27(1)	2(1)	-13(1)	-13(1)
O(1)	31(3)	47(3)	27(3)	-4(2)	-8(2)	-15(2)
O(2)	27(3)	33(3)	28(3)	-5(2)	-12(2)	-8(2)
O(3)	23(2)	33(3)	32(3)	-8(2)	-13(2)	-6(2)
O(4)	26(3)	35(3)	31(3)	-2(2)	-13(2)	-5(2)
N(1)	26(3)	32(4)	38(4)	-11(3)	-10(3)	-4(3)
N(2)	27(3)	23(3)	37(4)	-1(3)	-16(3)	-6(2)
N(3)	28(3)	37(4)	34(4)	-9(3)	-12(3)	-9(3)
N(4)	25(3)	27(3)	35(4)	-5(3)	-13(3)	-4(3)
N(5)	24(3)	33(4)	28(3)	-4(3)	-9(3)	-7(3)
N(6)	41(4)	45(4)	23(3)	2(3)	-13(3)	-14(3)
N(7)	39(4)	45(4)	23(3)	5(3)	-14(3)	-15(3)
N(8)	28(3)	35(4)	32(4)	5(3)	-15(3)	-11(3)
N(9)	37(4)	50(4)	35(4)	8(3)	-19(3)	-20(3)
C(1)	30(4)	45(5)	42(5)	-17(4)	-12(3)	-8(3)
C(2)	45(5)	46(5)	51(5)	-13(4)	-13(4)	-8(4)
C(3)	46(5)	37(5)	63(6)	-13(4)	-18(5)	0(4)
C(4)	63(6)	43(6)	62(7)	-13(5)	-17(5)	2(5)
C(5)	51(6)	45(6)	77(7)	-25(5)	-11(5)	2(4)
C(6)	39(5)	43(5)	52(5)	-16(4)	-14(4)	-8(4)
C(7)	51(5)	44(5)	53(6)	-22(4)	-9(4)	-6(4)
C(8)	65(6)	48(6)	67(7)	-22(5)	-22(5)	-16(5)
C(9)	37(5)	56(6)	66(6)	-26(5)	-11(4)	-13(4)
C(10)	65(7)	46(6)	72(7)	-23(5)	-3(5)	-17(5)
C(11)	37(4)	38(5)	32(4)	-2(4)	-9(3)	-15(4)

C(12)	33(4)	40(5)	27(4)	-8(3)	-7(3)
	-9(3)				
C(13)	16(3)	34(4)	34(4)	-8(3)	-13(3)
	1(3)				
C(14)	18(3)	39(4)	32(4)	-6(3)	-11(3)
	-6(3)				
C(15)	24(4)	42(5)	30(4)	-5(4)	-10(3)
	-11(3)				
C(16)	35(4)	28(4)	40(5)	3(3)	-21(4)
	-11(3)				
C(17)	34(4)	30(4)	62(6)	8(4)	-31(4)
	-11(3)				
C(18)	25(4)	45(5)	72(7)	2(5)	-18(4)
	-6(4)				
C(19)	24(4)	46(5)	50(5)	-9(4)	-8(4)
	-4(4)				
C(20)	26(4)	41(5)	44(5)	-7(4)	-17(4)
	-5(3)				
C(21)	24(4)	50(5)	44(5)	-8(4)	-10(4)
	-3(4)				
C(22)	37(5)	96(8)	43(5)	-22(5)	-8(4)
	-6(5)				
C(23)	39(5)	117(10)	40(5)	-13(6)	-3(4)
	-6(6)				
C(24)	41(5)	94(8)	31(5)	-1(5)	-19(4)
	-11(5)				
C(25)	28(4)	52(5)	34(4)	-4(4)	-16(3)
	-8(4)				
C(26)	33(4)	44(5)	31(4)	-10(4)	-14(3)
	-6(3)				
C(27)	36(5)	55(6)	37(5)	-2(4)	-19(4)
	-7(4)				
C(28)	30(4)	54(6)	43(5)	0(4)	-20(4)
	-2(4)				
C(29)	25(4)	39(5)	45(5)	-3(4)	-11(3)
	-6(3)				
C(30)	26(4)	33(4)	31(4)	-5(3)	-8(3)
	-4(3)				
C(31)	29(4)	37(4)	27(4)	6(3)	-8(3)
	-15(3)				
C(32)	35(4)	61(6)	34(5)	4(4)	-10(4)
	-21(4)				
C(33)	37(4)	42(5)	32(4)	1(4)	-12(3)
	-16(4)				
C(34)	47(5)	57(6)	36(5)	12(4)	-24(4)
	-20(4)				
C(35)	57(6)	78(7)	30(5)	19(5)	-15(4)
	-33(5)				
C(36)	47(5)	35(5)	56(6)	6(4)	-20(4)
	-16(4)				
C(37)	41(5)	76(7)	34(5)	15(5)	-10(4)
	-30(5)				
C(38)	49(5)	50(6)	61(6)	20(5)	-28(5)
	-26(5)				
C(39)	43(5)	45(5)	65(6)	18(5)	-29(5)
	-16(4)				
C(40)	33(4)	36(5)	43(5)	10(4)	-14(4)
	-14(4)				
C(41)	27(4)	35(4)	36(4)	-3(4)	-7(3)
	-11(3)				
C(42)	31(4)	40(5)	33(4)	-2(4)	-15(3)
	-15(3)				
C(43)	19(3)	33(4)	28(4)	-6(3)	-5(3)
	-5(3)				
C(44)	21(3)	32(4)	30(4)	-6(3)	-9(3)
	-8(3)				
C(45)	21(3)	31(4)	28(4)	-3(3)	-6(3)
	-7(3)				
C(46)	20(3)	33(4)	25(4)	-5(3)	-9(3)
	-4(3)				
C(47)	19(3)	37(4)	36(5)	-8(4)	-13(3)
	-9(3)				
C(48)	28(4)	42(5)	43(5)	-2(4)	-16(4)
	-10(3)				
C(49)	33(4)	48(5)	48(5)	-8(4)	-12(4)
	-9(4)				
C(50)	23(4)	53(5)	45(5)	4(4)	-9(4)
	-14(4)				
C(51)	35(4)	58(6)	42(5)	3(4)	-20(4)
	-19(4)				
C(52)	30(4)	42(5)	31(4)	4(4)	-16(3)
	-17(3)				
C(53)	39(4)	53(5)	26(4)	7(4)	-17(3)
	-23(4)				
C(54)	51(5)	84(7)	38(5)	-9(5)	-14(4)
	-38(5)				
C(55)	69(7)	114(10)	44(6)	-34(6)	-4(5)
	-52(7)				
C(56)	70(7)	101(9)	36(5)	-27(5)	-5(5)
	-39(6)				
C(57)	48(5)	63(6)	24(4)	-4(4)	-9(4)
	-25(4)				
C(58)	50(5)	53(5)	23(4)	-3(4)	-11(4)
	-13(4)				
C(59)	64(6)	55(6)	30(5)	-3(4)	-12(4)
	-16(5)				
C(60)	52(5)	54(6)	28(5)	-2(4)	-1(4)
	-3(4)				
C(61)	33(5)	67(6)	40(5)	-2(5)	-11(4)
	-1(4)				
C(62)	33(4)	53(5)	39(5)	-3(4)	-12(4)
	-10(4)				
C(63)	66(7)	75(7)	56(6)	22(6)	-35(5)
	-43(6)				
C(64)	173(15)	158(15)	103(11)	100(11)	-106(11)
	-105(13)				
Ru(1')	67(1)	153(1)	30(1)	-35(1)	9(1)
	-70(1)				
Ru(2')	90(1)	90(1)	30(1)	10(1)	-25(1)
	-58(1)				
O(1')	63(5)	98(6)	40(4)	-14(4)	-21(3)
	7(4)				
O(2')	53(4)	135(7)	34(4)	-34(4)	1(3)
	-30(4)				
O(3')	111(6)	164(8)	41(4)	-56(5)	19(4)
	-96(6)				

O(4')	95(6)	123(7)	27(3)	-17(4)	0(3)
	-73(5)				
N(1')	48(4)	93(7)	24(4)	-13(4)	0(3)
	-36(4)				
N(2')	54(6)	136(10)	57(6)	-63(6)	19(5)
	-52(6)				
N(3')	80(7)	168(11)	25(4)	-13(5)	-3(4)
	-82(7)				
N(4')	81(7)	182(12)	23(4)	-25(6)	1(4)
	-85(7)				
N(5')	61(5)	68(5)	37(4)	-9(4)	-16(4)
	-31(4)				
N(6')	81(6)	61(5)	27(4)	5(4)	-16(4)
	-44(5)				
N(7')	67(5)	74(6)	46(5)	20(4)	-26(4)
	-44(5)				
N(8')	110(8)	128(10)	46(5)	20(6)	-40(5)
	-73(8)				
N(9')	103(8)	103(8)	34(5)	15(5)	-27(5)
	-70(6)				
C(1')	46(5)	84(7)	26(4)	-12(5)	-1(4)
	-34(5)				
C(2')	80(8)	134(11)	29(5)	-16(6)	2(5)
	-72(8)				
C(3')	42(5)	80(7)	27(4)	-8(4)	-5(4)
	-18(5)				
C(4')	57(6)	62(6)	29(5)	-6(4)	-6(4)
	-25(5)				
C(5')	71(7)	109(9)	25(5)	-7(5)	-6(5)
	-44(6)				
C(6')	68(6)	65(6)	29(5)	-5(4)	-4(4)
	-28(5)				
C(7')	93(9)	117(11)	41(6)	-21(6)	-9(6)
	-62(8)				
C(8')	148(13)	57(7)	35(6)	-14(5)	5(7)
	-48(8)				
C(9')	71(7)	62(7)	38(5)	-4(5)	-1(5)
	-13(5)				
C(10')	52(6)	73(7)	38(5)	-16(5)	1(4)
	-26(5)				
C(11')	68(7)	100(9)	32(5)	-12(5)	-5(5)
	-52(6)				
C(12')	73(7)	129(11)	28(5)	-6(6)	1(5)
	-68(8)				
C(13')	48(6)	107(9)	42(6)	-25(6)	-5(4)
	-39(6)				
C(14')	34(5)	121(10)	33(5)	-15(6)	-7(4)
	-31(5)				
C(15')	36(5)	94(8)	31(5)	-16(5)	-10(4)
	-15(5)				
C(16')	44(7)	157(15)	158(15)	-114(13)	14(8)
	-22(8)				
C(17')	62(8)	117(13)	199(18)	-96(13)	13(10)
	-26(8)				
C(18')	59(8)	125(14)	139(14)	-70(12)	0(9)
	-15(9)				
C(19')	81(8)	123(11)	58(7)	-50(7)	5(6)
	-60(8)				
C(20')	74(8)	151(13)	42(6)	-48(7)	-2(6)
	-57(9)				
C(21')	95(9)	162(13)	20(5)	-13(7)	8(5)
	-88(10)				
C(22')	104(11)	160(14)	70(8)	46(9)	-42(8)
	-87(11)				
C(23')	106(12)	153(15)	133(14)	68(12)	-49(11)
	-89(11)				
C(24')	109(11)	187(17)	80(10)	49(11)	-50(9)
	-89(12)				
C(25')	92(9)	145(13)	34(6)	15(7)	-14(6)
	-71(9)				
C(26')	86(9)	163(14)	33(6)	8(7)	-21(6)
	-77(9)				
C(27')	86(9)	203(17)	40(6)	9(8)	-16(6)
	-87(10)				
C(28')	77(9)	220(19)	39(7)	-2(9)	-16(6)
	-73(11)				
C(29')	88(9)	210(18)	35(6)	-20(9)	-2(6)
	-104(11)				
C(30')	72(7)	183(14)	30(5)	-31(7)	5(5)
	-82(9)				
C(31')	55(6)	63(6)	50(6)	-10(5)	-12(5)
	-28(5)				
C(32')	67(7)	72(7)	73(7)	5(6)	-38(6)
	-27(6)				
C(33')	82(8)	99(9)	58(7)	-26(6)	-12(6)
	-52(7)				
C(34')	78(8)	94(9)	67(7)	-26(7)	-7(6)
	-56(7)				
C(35')	75(9)	149(14)	88(9)	-16(9)	-35(7)
	-55(9)				
C(36')	65(6)	49(6)	48(6)	-10(5)	-11(5)
	-17(5)				
C(37')	56(6)	74(8)	87(8)	-15(6)	-30(6)
	-14(6)				
C(38')	59(6)	69(7)	70(7)	-14(6)	-22(6)
	-12(5)				
C(39')	65(7)	58(6)	68(7)	-21(5)	-4(5)
	-26(5)				
C(40')	55(5)	46(5)	47(5)	-11(4)	-24(4)
	-7(4)				
C(41')	66(6)	50(6)	53(6)	-8(5)	-29(5)
	-18(5)				
C(42')	65(6)	62(6)	55(6)	2(5)	-28(5)
	-33(5)				
C(43')	74(7)	72(7)	35(5)	2(5)	-24(5)
	-40(6)				
C(44')	95(9)	119(10)	34(5)	-16(6)	-6(5)
	-73(8)				
C(45')	84(7)	93(8)	28(5)	-10(5)	-7(5)
	-60(7)				
C(46')	89(8)	98(9)	34(5)	-7(5)	-19(5)
	-61(7)				
C(47')	35(5)	107(10)	52(6)	-44(7)	-16(5)
	-5(5)				
C(48')	152(14)	177(15)	47(7)	40(8)	-63(8)
	-97(12)				

C(49')	230(20)	230(20)	86(12)	68(15)	-110(14)	F(18)	37(3)	151(6)	46(3)	-8(4)	-12(2)
	-140(20)						-20(3)				
C(50')	200(20)	210(20)	131(17)	104(18)	-126(17)	P(5)	67(2)	146(4)	88(3)	32(3)	-26(2)
	-110(20)						-47(2)				
C(51')	141(14)	136(14)	103(11)	59(10)	-82(11)	F(19)	205(11)	137(8)	146(9)	-2(7)	-74(8)
	-65(11)						-83(8)				
C(52')	95(9)	124(12)	69(8)	43(8)	-52(7)	F(20)	105(7)	132(8)	228(12)	76(8)	64(7)
	-65(9)						14(6)				
C(53')	75(8)	84(9)	62(7)	25(7)	-35(6)	F(21)	68(5)	207(11)	158(9)	-72(8)	-38(5)
	-43(7)						12(6)				
C(54')	74(8)	73(8)	82(9)	15(7)	-31(7)	F(22)	145(9)	188(10)	107(7)	-49(7)	-50(6)
	-26(6)						40(7)				
C(55')	72(7)	65(7)	73(8)	2(6)	-26(6)	F(23)	147(9)	149(9)	267(14)	70(9)	-142(10)
	-20(6)						-71(7)				
C(56')	68(6)	56(6)	52(6)	7(5)	-27(5)	F(24)	177(9)	162(9)	100(6)	-23(6)	22(6)
	-29(5)						-121(8)				
C(57')	63(6)	66(7)	39(5)	11(5)	-23(5)	P(1)	29(1)	55(2)	50(1)	-17(1)	-3(1)
	-40(5)						-11(1)				
C(58')	65(6)	47(5)	37(5)	7(4)	-19(4)	F(1)	64(3)	53(3)	51(3)	-13(3)	-24(3)
	-32(5)						9(3)				
C(59')	67(6)	46(6)	38(5)	-1(4)	-18(4)	F(2)	28(2)	61(3)	47(3)	-9(2)	-8(2)
	-22(5)						-13(2)				
C(60')	68(7)	70(7)	41(5)	-3(5)	-16(5)	F(3)	57(3)	63(4)	54(3)	3(3)	-31(3)
	-27(6)						-4(3)				
C(61')	101(9)	51(6)	35(5)	-2(5)	-1(5)	F(4)	30(3)	84(4)	147(6)	-68(4)	-12(3)
	-16(6)						0(3)				
C(62')	103(9)	49(6)	33(5)	0(5)	-17(5)	F(5)	44(3)	86(4)	103(5)	-46(4)	-6(3)
	-29(6)						-28(3)				
C(63')	97(9)	104(10)	41(6)	33(6)	-32(6)	F(6)	105(5)	95(5)	47(3)	-26(3)	16(3)
	-54(8)						-66(4)				
C(64')	87(9)	163(15)	73(9)	45(9)	-29(7)	P(2)	122(4)	183(6)	237(7)	-152(6)	83(4)
	-62(10)						-93(4)				
P(4)	47(2)	221(6)	76(2)	-59(3)	-12(2)	F(7)	310(20)	117(11)	670(40)	-76(17)	290(30)
	-13(3)						-116(13)				
F(25)	114(7)	223(12)	86(6)	-46(7)	-4(5)	F(8)	319	361	340	0	0
	-12(7)						87				
F(26)	73(5)	208(10)	98(6)	-13(6)	-28(4)	F(9)	147(10)	173(11)	172(10)	-32(8)	-39(8)
	-45(6)						-29(8)				
F(27)	97(6)	224(10)	58(4)	-19(5)	-23(4)	F(10)	132(8)	203(11)	76(6)	-5(6)	11(5)
	-50(6)						-1(8)				
F(28)	75(4)	154(7)	45(4)	-5(4)	-2(3)	F(11)	530(30)	136(9)	73(6)	-44(6)	-88(11)
	-21(4)						30(13)				
F(29)	188(10)	105(7)	76(5)	3(5)	16(6)	F(12)	82(8)	320(20)	550(40)	-140(20)	51(14)
	-16(7)						-65(11)				
F(30)	132(7)	165(8)	88(5)	-1(5)	-72(5)	P(3)	67(2)	137(4)	79(2)	28(2)	-21(2)
	-28(6)						-35(2)				
P(6)	32(1)	60(2)	31(1)	-7(1)	-9(1)	F(31)	54(4)	101(5)	66(4)	5(4)	-8(3)
	-10(1)						-12(3)				
F(13)	33(2)	55(3)	38(3)	-5(2)	-5(2)	F(32)	187(10)	170(9)	68(5)	-38(6)	-40(6)
	-14(2)						16(8)				
F(14)	94(4)	72(4)	44(3)	-12(3)	9(3)	F(33)	194(10)	193(10)	130(7)	104(7)	-96(7)
	-42(3)						-157(9)				
F(15)	45(3)	96(4)	48(3)	-17(3)	-21(2)	F(34)	84(6)	216(12)	245(14)	130(11)	-8(7)
	0(3)						-45(7)				
F(16)	48(3)	101(5)	32(3)	-11(3)	-1(2)	F(35)	315(16)	178(10)	166(10)	31(8)	-151(11)
	-11(3)						-162(11)				
F(17)	93(5)	57(4)	63(4)	-14(3)	5(3)	F(36)	87(5)	112(6)	78(5)	7(4)	-20(4)
	-8(3)						-5(4)				

O(5)	93(6)	52(4)	73(5)	-7(4)	-12(5)
	-18(4)				
C(65)	109(13)	44(8)	280(30)	-28(12)	-14(15)
	-2(8)				
C(66)	116(14)	240(20)	93(12)	-35(14)	-35(11)
	-52(15)				
C(67)	129(14)	198(19)	56(8)	18(10)	-24(9)
	-73(14)				
C(68)	84(9)	93(9)	69(8)	-39(7)	-9(7)
	-23(7)				

Table 5. Hydrogen coordinates (x 104) and isotropic displacement parameters (Å2x 10 3) for grot531_a_sq_sq.

	x	y	z	U(eq)
H(2A)	2786	1692	8929	55
H(2B)	1897	1977	8757	55
H(3A)	1954	822	10517	58
H(3B)	2821	979	10008	58
H(4)	2503	-57	10048	68
H(5A)	2650	73	8969	69
H(5B)	3237	521	9069	69
H(6A)	509	1743	9561	51
H(6B)	517	1296	10237	51
H(7)	2469	1090	8299	57
H(8A)	944	1298	8613	67
H(8B)	1203	565	8670	67
H(9)	198	706	9596	60
H(10A)	984	141	10365	73
H(10B)	1239	-169	9781	73
H(11)	1245	1648	10860	42
H(12)	1224	2484	11280	40
H(15)	2262	2638	9142	37
H(16)	417	4197	9867	40
H(17)	-1046	4525	10033	49
H(18)	-1826	4662	11018	59
H(19)	-1155	4366	11861	49
H(22)	-356	4030	12633	70
H(23)	579	3625	13302	81
H(24)	2002	3291	12890	66
H(27)	3402	2982	12345	51
H(28)	4755	2797	11707	51
H(29)	4933	3015	10612	44
H(30)	3770	3459	10174	36
H(32A)	3510	7722	9200	53
H(32B)	3549	7222	8807	53
H(33A)	1393	6793	9442	44
H(33B)	2265	6654	8958	44
H(34)	1277	7334	8396	56
H(35A)	2211	8123	7789	69
H(35B)	2763	7465	7949	69
H(36)	1116	8642	9418	56
H(37)	3380	8265	8168	64
H(38A)	2116	8935	8424	66
H(38B)	2605	8776	8972	66
H(39A)	495	7846	9201	63
H(39B)	802	8359	8568	63
H(40A)	1281	7612	10065	47
H(40B)	2084	7973	9979	47
H(41)	3343	7324	10224	39
H(42)	3650	6654	11116	40
H(46)	2098	6046	9977	31
H(48)	4326	4434	10911	44
H(49)	5733	4349	10350	51
H(50)	6716	4931	10498	51
H(51)	6247	5566	11216	53
H(54)	5635	6174	11978	65
H(55)	4875	6689	12750	84
H(56)	3428	6590	13184	78
H(59)	1991	6329	13581	60
H(60)	542	6171	13791	58
H(61)	121	5631	13182	59
H(62)	1138	5263	12398	51
H(64A)	4065	3313	13583	218
H(64B)	3074	3373	13901	218
H(64C)	3670	3835	13964	218
H(2'A)	3142	-41	12392	92
H(2'B)	2722	625	12072	92
H(3'A)	4363	1553	12031	60
H(3'B)	3481	1599	11844	60
H(4')	4633	1641	10927	58
H(5'A)	3414	1164	10940	81
H(5'B)	4252	830	10566	81
H(6'A)	4579	-106	12698	65
H(6'B)	5041	515	12538	65
H(7')	3400	54	11288	94
H(8'A)	4881	-228	11098	96
H(8'B)	4448	-547	11805	96
H(9')	5703	-91	11768	73
H(10C)	5662	748	10865	65
H(10D)	5708	1025	11428	65
H(11')	3281	-140	13370	76
H(12')	2647	-83	14395	90
H(15')	3256	1718	12818	62
H(16')	432	1850	14581	133
H(17')	-1016	1815	14797	145
H(18')	-1587	893	15388	125
H(19')	-726	77	15898	96
H(22')	392	-705	16223	136
H(23')	1532	-1341	16571	166
H(24')	2878	-954	16349	153
H(27')	4125	-434	16066	130
H(28')	5226	221	15809	132
H(29')	5069	1228	15211	126
H(30')	3791	1610	14891	107
H(32C)	-1812	2598	17306	82
H(32D)	-1635	2733	17909	82
H(33C)	-810	1010	17482	89
H(33D)	-1302	1544	17041	89
H(34')	-2272	789	17699	89

H(35C)	-3395	1510	18098	118
H(35D)	-2879	1853	17422	118
H(36')	-1827	1122	19278	64
H(37')	-3089	2507	18140	84
H(38C)	-3102	1719	19072	78
H(38D)	-2413	2183	18986	78
H(39C)	-2594	639	18811	75
H(39D)	-1599	463	18562	75
H(40C)	-535	1193	18448	56
H(40D)	-829	1854	18625	56
H(41')	-267	2750	17885	63
H(42')	1016	3144	17361	70
H(46')	141	1570	16773	82
H(48')	1782	3082	14928	146
H(49')	1121	3953	14308	206
H(50')	911	4946	14541	218
H(51')	1251	5043	15454	153
H(54')	1628	5029	16397	94
H(55')	2089	4851	17316	85
H(56')	2739	3882	17746	69
H(59')	3572	2894	17968	58
H(60')	4378	1914	18095	70
H(61')	4420	1257	17433	79
H(62')	3666	1599	16651	73
H(64D)	5264	3502	14407	172
H(64E)	5306	2787	14394	172
H(64F)	5674	2966	14895	172
H(65A)	-261	389	11567	228
H(65B)	433	102	11965	228
H(65C)	-225	679	12121	228
H(66A)	-591	-590	12380	173
H(66B)	-768	-175	12877	173
H(67A)	-2266	-435	13168	157
H(67B)	-2098	-787	12623	157
H(68A)	-3057	-21	12181	117
H(68B)	-3285	226	12802	117
H(68C)	-3466	-464	12835	117

1.6.5.2. Ru_2(OCCO) dimer

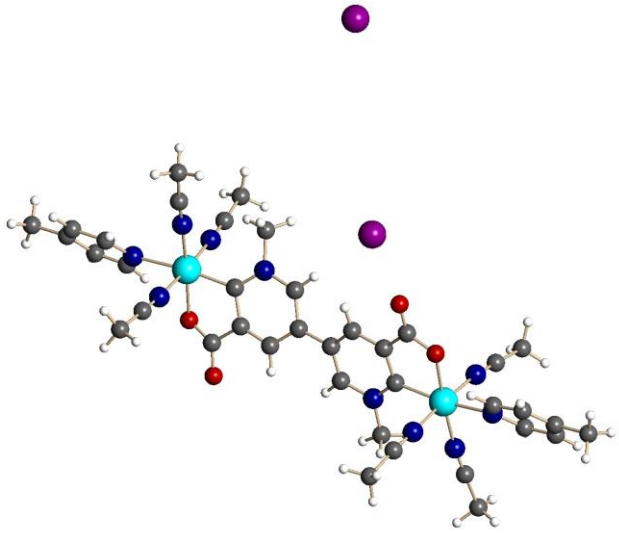


Table 1. Crystal data and structure refinement for grot479.

Identification code	grot479	
Empirical formula	C38 H42 I2 N10 O4 Ru2	
Formula weight	1158.75	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 10.9702(18) Å	α= 90.815(7)°.
	b = 13.864(3) Å	β= 93.826(5)°.
	c = 16.190(3) Å	γ = 113.291(4)°.
Volume	2254.5(8) $Å^3$	
Z	2	
Density (calculated)	1.707 Mg/m^3	
Absorption coefficient	2.087 mm^{-1}	
F(000)	1132	
Crystal size	0.200 x 0.150 x 0.080 mm^3	
Theta range for data collection	1.262 to 25.375°.	
Index ranges	-13<=h<=11, -16<=k<=16, -19<=l<=19	
Reflections collected	24827	
Independent reflections	8169 [R(int) = 0.0808]	
Completeness to theta = 25.000°	98.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8169 / 9 / 515	
Goodness-of-fit on F^2	1.024	
Final R indices [I>2sigma(I)]	R1 = 0.0989, wR2 = 0.2322	
R indices (all data)	R1 = 0.1748, wR2 = 0.2730	
Extinction coefficient	n/a	
Largest diff. peak and hole	3.177 and -2.188 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3)
for grot479. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	9790(1)	7781(1)	6665(1)	38(1)
I(2)	3280(1)	6355(1)	5368(1)	68(1)
Ru(2)	-88(1)	2019(1)	8221(1)	46(1)
I(1)	4303(2)	6944(2)	10625(2)	117(1)
O(3)	1570(11)	1957(9)	6056(9)	55(3)
O(2)	9682(10)	8192(8)	7885(7)	44(3)
O(4)	191(11)	1551(8)	7050(7)	50(3)
N(5)	6893(12)	6234(10)	6289(8)	40(3)
N(9)	-1017(13)	2920(10)	7741(8)	44(3)
N(2)	11821(11)	8937(10)	6658(9)	43(3)
N(1)	10526(12)	6760(10)	7120(8)	42(3)
N(10)	-1988(13)	687(11)	8161(9)	50(4)
N(4)	9179(12)	8842(10)	6168(8)	44(3)
C(26)	10994(14)	6198(11)	7346(10)	39(4)
C(25)	1295(14)	2123(11)	6736(12)	42(4)
N(6)	2599(14)	3900(11)	8601(10)	53(4)
C(38)	7962(15)	6808(11)	6826(11)	43(4)
N(3)	9935(12)	7240(10)	5546(9)	43(3)
N(8)	-504(14)	2375(12)	9326(11)	58(4)
C(23)	7678(15)	6698(13)	7673(10)	43(4)
C(20)	5703(16)	5505(12)	6556(12)	47(4)
C(18)	3844(15)	4602(13)	8372(12)	50(4)
C(16)	3408(15)	3714(12)	7059(11)	46(4)
C(21)	5486(15)	5336(12)	7393(11)	44(4)
N(7)	772(15)	1145(12)	8768(11)	68(5)
C(28)	10022(15)	6836(14)	4948(11)	45(4)
C(14)	1754(15)	3133(13)	8068(11)	47(4)
C(15)	2192(14)	3019(12)	7280(12)	47(4)
C(5)	-3098(16)	755(14)	8457(12)	56(5)
C(30)	8822(17)	9437(12)	5837(11)	49(4)
C(22)	6540(15)	5991(14)	7935(12)	52(5)
C(19)	6934(15)	6390(13)	5411(11)	47(4)
O(1)	8652(14)	7526(17)	8987(10)	118(7)
C(36)	12157(16)	9879(11)	7033(12)	54(5)
C(32)	12757(16)	8749(14)	6294(11)	55(5)
C(17)	4229(14)	4539(13)	7593(11)	46(4)
C(24)	8763(17)	7520(16)	8240(12)	58(5)
C(6)	-4307(18)	-127(16)	8410(14)	71(6)
C(35)	13375(18)	10643(14)	6964(12)	60(5)
C(2)	-4404(17)	-1087(14)	8007(11)	50(4)
C(34)	14342(17)	10490(15)	6576(14)	66(6)
C(27)	11631(17)	5560(13)	7666(12)	58(5)
C(33)	14041(17)	9504(15)	6224(13)	64(5)
C(29)	10020(20)	6268(17)	4186(12)	70(5)
C(9)	-1612(16)	3390(12)	7544(12)	52(5)
C(4)	-2134(17)	-209(13)	7810(13)	61(5)
C(31)	8420(20)	10157(16)	5406(13)	71(6)
C(3)	-3277(19)	-1091(13)	7718(15)	75(7)
C(10)	-2393(19)	4012(14)	7303(14)	70(6)
C(13)	2280(20)	4006(16)	9430(13)	71(6)
C(1)	-5720(20)	-2024(15)	7980(14)	76(6)
C(7)	-874(18)	2520(20)	9932(13)	74(7)
C(37)	15700(20)	11343(17)	6544(18)	112(11)
C(11)	1360(30)	770(30)	9140(20)	139(15)
C(8)	-1350(30)	2740(30)	10702(16)	134(13)
C(12)	2030(30)	230(40)	9650(30)	290(40)

Table 3. Bond lengths [Å] and angles [°] for grot479.

Ru(1)-C(38)	1.962(16)
Ru(1)-N(3)	1.991(14)
Ru(1)-N(4)	2.002(14)
Ru(1)-N(1)	2.012(13)
Ru(1)-O(2)	2.072(11)
Ru(1)-N(2)	2.171(12)
Ru(2)-N(8)	1.979(19)
Ru(2)-N(7)	1.991(16)
Ru(2)-N(9)	2.032(14)
Ru(2)-C(14)	2.034(15)
Ru(2)-O(4)	2.075(12)
Ru(2)-N(10)	2.165(15)
O(3)-C(25)	1.204(19)
O(2)-C(24)	1.25(2)
O(4)-C(25)	1.298(18)
N(5)-C(38)	1.368(19)
N(5)-C(20)	1.399(19)
N(5)-C(19)	1.44(2)
N(9)-C(9)	1.126(19)
N(2)-C(32)	1.33(2)
N(2)-C(36)	1.33(2)
N(1)-C(26)	1.143(18)
N(10)-C(4)	1.31(2)
N(10)-C(5)	1.37(2)
N(4)-C(30)	1.167(19)
C(26)-C(27)	1.41(2)
C(25)-C(15)	1.47(2)
N(6)-C(14)	1.35(2)
N(6)-C(18)	1.41(2)
N(6)-C(13)	1.43(2)
C(38)-C(23)	1.42(2)
N(3)-C(28)	1.14(2)
N(8)-C(7)	1.13(2)
C(23)-C(22)	1.35(2)
C(23)-C(24)	1.52(2)
C(20)-C(21)	1.40(2)
C(20)-H(20)	0.9500
C(18)-C(17)	1.37(2)
C(18)-H(18)	0.9500
C(16)-C(15)	1.38(2)
C(16)-C(17)	1.39(2)
C(16)-H(16)	0.9500
C(21)-C(22)	1.39(2)
C(21)-C(17)	1.45(2)
N(7)-C(11)	1.13(2)
C(28)-C(29)	1.45(2)
C(14)-C(15)	1.42(2)
C(5)-C(6)	1.40(2)
C(5)-H(5)	0.9500
C(30)-C(31)	1.42(2)
C(22)-H(22)	0.9500
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
O(1)-C(24)	1.22(2)
C(36)-C(35)	1.35(2)
C(36)-H(36)	0.9500
C(32)-C(33)	1.40(2)
C(32)-H(32)	0.9500
C(6)-C(2)	1.44(3)
C(6)-H(6)	0.9500
C(35)-C(34)	1.35(3)
C(35)-H(35)	0.9500
C(2)-C(3)	1.35(2)
C(2)-C(1)	1.51(2)
C(34)-C(33)	1.38(3)
C(34)-C(37)	1.49(2)
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(33)-H(33)	0.9500
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(9)-C(10)	1.48(2)
C(4)-C(3)	1.36(2)
C(4)-H(4)	0.9500
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(3)-H(3)	0.9500
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(7)-C(8)	1.46(3)
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(11)-C(12)	1.47(3)
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(12)-H(12A)	1.0291
C(12)-H(12B)	1.0250
C(12)-H(12C)	1.0261
C(38)-Ru(1)-N(3)	98.4(6)
C(38)-Ru(1)-N(4)	92.3(5)
N(3)-Ru(1)-N(4)	91.2(5)
C(38)-Ru(1)-N(1)	91.6(5)
N(3)-Ru(1)-N(1)	86.5(5)
N(4)-Ru(1)-N(1)	175.8(5)
C(38)-Ru(1)-O(2)	80.5(6)
N(3)-Ru(1)-O(2)	173.1(5)
N(4)-Ru(1)-O(2)	95.6(5)
N(1)-Ru(1)-O(2)	86.8(5)
C(38)-Ru(1)-N(2)	172.2(6)
N(3)-Ru(1)-N(2)	89.4(5)

N(4)-Ru(1)-N(2)	88.1(5)
N(1)-Ru(1)-N(2)	88.3(5)
O(2)-Ru(1)-N(2)	91.8(5)
N(8)-Ru(2)-N(7)	88.7(6)
N(8)-Ru(2)-N(9)	87.3(6)
N(7)-Ru(2)-N(9)	175.9(6)
N(8)-Ru(2)-C(14)	104.5(7)
N(7)-Ru(2)-C(14)	88.9(6)
N(9)-Ru(2)-C(14)	92.8(6)
N(8)-Ru(2)-O(4)	175.3(5)
N(7)-Ru(2)-O(4)	91.9(6)
N(9)-Ru(2)-O(4)	92.0(5)
C(14)-Ru(2)-O(4)	80.2(6)
N(8)-Ru(2)-N(10)	86.9(5)
N(7)-Ru(2)-N(10)	89.6(6)
N(9)-Ru(2)-N(10)	89.4(5)
C(14)-Ru(2)-N(10)	168.5(7)
O(4)-Ru(2)-N(10)	88.5(5)
C(24)-O(2)-Ru(1)	114.3(12)
C(25)-O(4)-Ru(2)	116.8(11)
C(38)-N(5)-C(20)	122.5(15)
C(38)-N(5)-C(19)	120.7(13)
C(20)-N(5)-C(19)	116.8(14)
C(9)-N(9)-Ru(2)	172.8(14)
C(32)-N(2)-C(36)	117.8(14)
C(32)-N(2)-Ru(1)	122.8(11)
C(36)-N(2)-Ru(1)	119.4(11)
C(26)-N(1)-Ru(1)	176.2(13)
C(4)-N(10)-C(5)	117.1(15)
C(4)-N(10)-Ru(2)	120.8(11)
C(5)-N(10)-Ru(2)	122.1(12)
C(30)-N(4)-Ru(1)	176.3(14)
N(1)-C(26)-C(27)	175.9(17)
O(3)-C(25)-O(4)	123.8(16)
O(3)-C(25)-C(15)	122.0(14)
O(4)-C(25)-C(15)	114.3(16)
C(14)-N(6)-C(18)	121.4(16)
C(14)-N(6)-C(13)	121.2(15)
C(18)-N(6)-C(13)	117.4(16)
N(5)-C(38)-C(23)	113.4(14)
N(5)-C(38)-Ru(1)	133.0(13)
C(23)-C(38)-Ru(1)	113.6(11)
C(28)-N(3)-Ru(1)	172.5(14)
C(7)-N(8)-Ru(2)	173.0(16)
C(22)-C(23)-C(38)	123.8(16)
C(22)-C(23)-C(24)	123.9(17)
C(38)-C(23)-C(24)	112.2(14)
C(21)-C(20)-N(5)	122.9(16)
C(21)-C(20)-H(20)	118.5
N(5)-C(20)-H(20)	118.5
C(17)-C(18)-N(6)	120.8(16)
C(17)-C(18)-H(18)	119.6
N(6)-C(18)-H(18)	119.6
C(15)-C(16)-C(17)	121.2(17)
C(15)-C(16)-H(16)	119.4
C(17)-C(16)-H(16)	119.4
C(22)-C(21)-C(20)	113.8(15)
C(22)-C(21)-C(17)	128.3(16)
C(20)-C(21)-C(17)	117.9(15)
C(11)-N(7)-Ru(2)	171(3)
N(3)-C(28)-C(29)	175.4(18)
N(6)-C(14)-C(15)	117.8(14)
N(6)-C(14)-Ru(2)	130.1(13)
C(15)-C(14)-Ru(2)	112.0(12)
C(16)-C(15)-C(14)	120.3(16)
C(16)-C(15)-C(25)	123.0(17)
C(14)-C(15)-C(25)	116.7(14)
N(10)-C(5)-C(6)	120.3(17)
N(10)-C(5)-H(5)	119.8
C(6)-C(5)-H(5)	119.9
N(4)-C(30)-C(31)	178(2)
C(23)-C(22)-C(21)	122.9(17)
C(23)-C(22)-H(22)	118.6
C(21)-C(22)-H(22)	118.6
N(5)-C(19)-H(19A)	109.5
N(5)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
N(5)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
N(2)-C(36)-C(35)	120.2(17)
N(2)-C(36)-H(36)	119.9
C(35)-C(36)-H(36)	119.9
N(2)-C(32)-C(33)	123.9(18)
N(2)-C(32)-H(32)	118.0
C(33)-C(32)-H(32)	118.1
C(18)-C(17)-C(16)	118.2(15)
C(18)-C(17)-C(21)	117.1(16)
C(16)-C(17)-C(21)	124.7(17)
O(1)-C(24)-O(2)	124.7(19)
O(1)-C(24)-C(23)	119.5(17)
O(2)-C(24)-C(23)	115.6(17)
C(5)-C(6)-C(2)	119.7(17)
C(5)-C(6)-H(6)	120.2
C(2)-C(6)-H(6)	120.1
C(36)-C(35)-C(34)	123.3(17)
C(36)-C(35)-H(35)	118.3
C(34)-C(35)-H(35)	118.3
C(3)-C(2)-C(6)	116.7(17)
C(3)-C(2)-C(1)	125.1(18)
C(6)-C(2)-C(1)	118.1(17)
C(35)-C(34)-C(33)	117.4(17)
C(35)-C(34)-C(37)	122(2)
C(33)-C(34)-C(37)	121(2)
C(26)-C(27)-H(27A)	109.4
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(34)-C(33)-C(32)	117.1(19)
C(34)-C(33)-H(33)	121.5
C(32)-C(33)-H(33)	121.5
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.4
H(29A)-C(29)-H(29B)	109.5

C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
N(9)-C(9)-C(10)	179(2)
N(10)-C(4)-C(3)	126.2(17)
N(10)-C(4)-H(4)	116.9
C(3)-C(4)-H(4)	116.9
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(2)-C(3)-C(4)	119.8(18)
C(2)-C(3)-H(3)	120.1
C(4)-C(3)-H(3)	120.1
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
N(6)-C(13)-H(13A)	109.5
N(6)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
N(6)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.4
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
N(8)-C(7)-C(8)	178(3)
C(34)-C(37)-H(37A)	109.5
C(34)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(34)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
N(7)-C(11)-C(12)	175(3)
C(7)-C(8)-H(8A)	109.4
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(11)-C(12)-H(12A)	114.9
C(11)-C(12)-H(12B)	113.9
H(12A)-C(12)-H(12B)	104.4
C(11)-C(12)-H(12C)	114.2
H(12A)-C(12)-H(12C)	104.0
H(12B)-C(12)-H(12C)	104.3

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for grot479. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	30(1)	29(1)	56(1)	5(1)	2(1)	13(1)
I(2)	58(1)	59(1)	99(1)	4(1)	1(1)	37(1)
Ru(2)	37(1)	43(1)	64(1)	17(1)	13(1)	20(1)
I(1)	80(1)	106(1)	184(2)	38(1)	3(1)	56(1)
O(3)	41(6)	41(7)	81(10)	11(6)	20(6)	12(5)
O(2)	31(6)	42(6)	54(7)	0(5)	-7(5)	11(5)
O(4)	53(7)	29(6)	72(8)	16(5)	17(6)	19(5)
N(5)	36(7)	38(7)	55(9)	11(6)	12(6)	24(6)
N(9)	43(8)	41(8)	45(9)	13(6)	7(6)	11(6)
N(2)	20(6)	38(8)	64(9)	9(7)	-1(6)	4(5)
N(1)	39(7)	36(7)	54(9)	4(6)	7(6)	18(6)
N(10)	56(9)	59(9)	54(9)	3(7)	20(7)	41(8)
N(4)	29(7)	44(8)	50(9)	0(7)	2(6)	6(6)
C(26)	35(8)	23(7)	55(11)	1(7)	-2(7)	8(7)
C(25)	30(8)	30(8)	70(13)	10(8)	18(8)	14(7)
N(6)	49(9)	50(9)	70(11)	24(8)	18(8)	28(7)
C(38)	39(9)	24(8)	72(13)	-4(8)	-5(8)	23(7)
N(3)	33(7)	47(8)	52(7)	13(5)	7(6)	17(6)
N(8)	44(8)	57(9)	73(12)	28(8)	5(8)	16(7)
C(23)	40(9)	53(10)	47(11)	12(8)	2(8)	30(8)
C(20)	43(9)	33(9)	79(14)	16(8)	7(9)	29(7)
C(18)	33(9)	52(10)	65(13)	10(9)	-9(8)	20(8)
C(16)	39(9)	41(9)	61(11)	15(8)	5(8)	21(8)

C(21)	35(9) 21(7)	44(9)	57(12)	22(8)	5(8)
N(7)	58(10) 28(8)	51(9)	106(14)	34(9)	39(9)
C(28)	30(8) 24(7)	59(9)	53(7)	8(6)	2(6)
C(14)	28(8) 1(7)	45(10)	58(12)	23(9)	6(8)
C(15)	28(8) 13(7)	38(9)	77(13)	19(9)	2(8)
C(5)	36(9) 22(8)	53(11)	84(14)	14(10)	15(9)
C(30)	52(10) 14(8)	26(8)	67(12)	3(8)	-5(9)
C(22)	35(9) 31(9)	73(12)	60(12)	35(10)	11(8)
C(19)	33(8) 20(7)	47(10)	65(12)	5(8)	4(8)
O(1)	45(8) 10(10)	220(20)	54(10)	7(11)	5(7)
C(36)	44(10) 11(7)	17(8)	98(15)	-15(9)	-1(9)
C(32)	42(10) 12(8)	51(11)	67(13)	21(9)	1(9)
C(17)	27(8) 13(7)	48(10)	64(12)	18(9)	10(8)
C(24)	37(10) 15(9)	80(14)	51(13)	16(10)	2(9)
C(6)	44(11) 40(10)	76(14)	109(17)	33(13)	13(10)
C(35)	59(12) 26(9)	39(10)	86(15)	-5(9)	-20(10)
C(2)	52(10) 23(9)	50(11)	51(11)	11(8)	0(8)
C(34)	38(10) 17(9)	52(12)	106(17)	13(11)	-2(10)
C(27)	53(10) 22(8)	36(9)	85(14)	-5(9)	-20(10)
C(33)	36(9) 5(8)	54(12)	89(15)	8(11)	-10(9)
C(29)	81(14) 48(11)	85(13)	59(8)	0(8)	3(8)
C(9)	37(9) 9(7)	22(8)	92(14)	5(8)	-5(9)
C(4)	44(10) 28(8)	39(10)	115(17)	22(10)	18(10)
C(31)	70(13) 43(11)	67(13)	90(16)	25(11)	4(11)
C(3)	66(13) 27(9)	27(9)	140(20)	24(11)	39(13)
C(10)	59(12) 32(9)	48(11)	115(18)	20(11)	8(11)
C(13)	67(13) 16(10)	60(13)	79(16)	5(11)	21(11)
C(1)	73(14) 12(10)	50(12)	94(17)	24(11)	5(12)
C(7)	39(10) 40(12)	140(20)	49(13)	15(13)	10(9)
C(37)	53(13) -15(10)	56(13)	190(30)	49(16)	-27(15)
C(11)	89(18) 110(20)	180(30)	220(30)	140(30)	80(20)
C(8)	95(19) 120(30)	270(40)	90(20)	10(20)	19(15)
C(12)	120(30) 150(40)	390(70)	430(70)	360(60)	90(40)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for grot479.

	x	y	z	U(eq)
H(20)	5012	5107	6151	57
H(18)	4425	5128	8763	59
H(16)	3689	3627	6531	55
H(5)	-3045	1402	8695	67
H(22)	6451	5937	8514	63
H(19A)	7686	7046	5313	70
H(19B)	6102	6432	5192	70
H(19C)	7041	5800	5132	70
H(36)	11537	10013	7349	65
H(32)	12542	8060	6068	67
H(6)	-5060	-90	8644	85
H(35)	13562	11322	7201	72
H(27A)	12185	5455	7252	87
H(27B)	10959	4877	7799	87
H(27C)	12193	5904	8169	87
H(33)	14678	9344	5945	77
H(29A)	10088	6721	3716	105
H(29B)	9193	5637	4106	105
H(29C)	10782	6064	4221	105
H(4)	-1367	-249	7598	74
H(31A)	8287	9970	4811	106
H(31B)	9104	10869	5505	106
H(31C)	7579	10129	5605	106
H(3)	-3285	-1709	7452	90
H(10A)	-2505	4014	6698	106
H(10B)	-1925	4736	7529	106
H(10C)	-3270	3701	7524	106
H(13A)	2202	3377	9729	107
H(13B)	1431	4090	9418	107
H(13C)	2984	4626	9713	107
H(1A)	-5736	-2440	8467	114
H(1B)	-5830	-2460	7476	114
H(1C)	-6446	-1782	7980	114
H(37A)	15696	11780	6074	168
H(37B)	16346	11030	6479	168
H(37C)	15935	11778	7060	168
H(8A)	-1702	3288	10615	201
H(8B)	-614	2992	11134	201
H(8C)	-2058	2102	10873	201
H(12A)	1524	-528	9583	438
H(12B)	2094	459	10232	438
H(12C)	2932	409	9472	438

Part 2. Origin of High (E)-selectivity in Alkene Isomerization by a CpRu(PN) Catalyst[57]

Thomas Chi Cao, Arnold L. Rheingold, and Douglas B. Grotjahn

2.1. Introduction

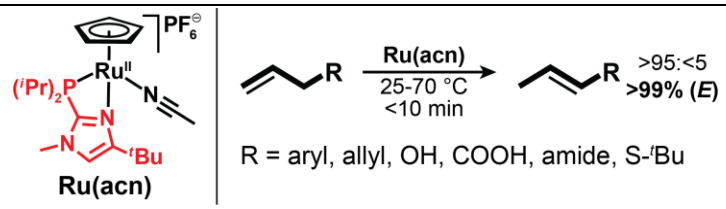


Figure 36. Structure of **Ru(acn)** and its typical reactivity profile

Many transition metal complexes are known to catalyze alkene isomerization, which can be viewed as a [3,1]-hydrogen shift in the double bond of an alkene.[58] This isomerization offers a potentially useful methodology in the synthesis of alkenes, since no reagents are needed other than a suitable catalyst and an isomer to start with. However, many alkene isomerization catalysts operate under thermodynamic control, which leads to mixtures of positional or geometric isomers in proportions determined by thermodynamic stability of the products.[58,59] Such reaction outcomes hinder the adoption of alkene isomerization as a practical methodology in the synthetic organic chemists' toolbox.[60]

In 2007, the Grotjahn lab reported a CpRu complex **Ru(acn)** ($Ru^{II}(\eta^5\text{-}C_5H_5)(\kappa^2\text{-PN})(L)]^+[PF_6]^-$; PN = (1-methyl-4-*tert*-butylimidazol-2-yl)-di-*iso*-propylphosphine, acn = acetonitrile, **Figure 36**) capable of isomerizing terminal alkenes into their internal isomers under mild conditions and low catalyst loadings. Unusually for an alkene isomerization catalyst, **Ru(acn)** was kinetically selective for (*E*) geometric isomers; under typical catalytic conditions for many olefin substrates, (*Z*)-isomers are not detected. For but-1-ene, the model substrate studied in this work, an equilibrium ratio of 95:5 (*E*)-but-2-ene:but-1-ene is reached within 10 minutes at 30°C, using a catalyst loading of just 0.05 mol%.

Despite the unique reactivity of **Ru(acn)**, the mechanistic details have insofar been unclear. A computational study modelling the isomerization of pent-1-ene to (*E*)-pent-2-ene has been conducted by Tao et al.,[61] but the authors' work was largely theoretical in nature, and did not provide a rationale for the unusual (*E*)-selectivity of **Ru(acn)**. We were thus inspired to rectify gap in our understanding of the mechanism for **Ru(acn)**-

mediated alkene isomerization by undertaking a new comprehensive computational study while simultaneously obtaining experimental parameters to validate our theoretical models.

2.2. Concentration profiles and reaction intermediates

Ru(acn) rapidly isomerizes model substrate **1** at ambient temperature to a thermodynamic mixture of 96:4 **2E**:**1**, although as discovered in this study, the ratio increases further with decreasing temperature. To quantify the activation parameters for this reaction, time-dependent concentration changes of **1** and **2E** in the presence of **Ru(acn)** were monitored in-situ via ^{1}H NMR spectroscopy at temperatures spanning 253K-283K. Concentrations under the experimental conditions were 0.19-0.24 M for **1**, and 0.31-0.46 mM for **Ru** (0.02 mol % catalyst loading) as measured by peak integrals relative to a $C(SiMe_3)_4$ internal standard. The cryogenic temperatures and low catalyst loadings were necessary because the onset of catalysis was too rapid at ambient temperatures to achieve the desired resolution of the kinetics data.

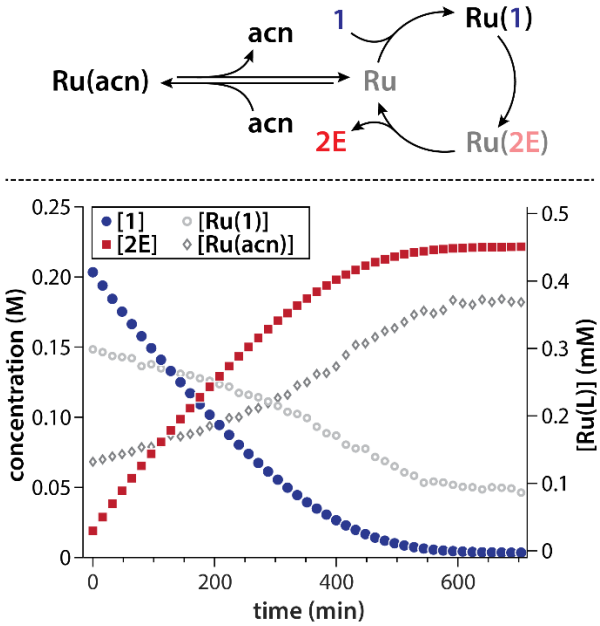


Figure 37. *Top:* kinetics model for the isomerization of 1 to 2E by Ru(acn). Species that could not be conclusively identified are shown in faded text. Bottom: selected concentration profiles of free alkene and observed catalyst complexes. Conditions for the experiment were 253 K with a catalyst loading of 0.2 mol%. Note that concentrations of Ru(acn) and Ru(1) are between 0.1 and 0.4 mM.

The concentration profiles of **1** and **2E** followed a Michaelis-Menten mechanism, with an effectively zeroth-order (linear) decrease in [**1**] at early times, when the reaction rate is limited by catalyst availability, and a first-order (exponential) decrease of [**1**] to the equilibrium concentration at later times. The change in order occurs

gradually as [**1**] drops from roughly 50 times to 20 times the catalyst concentration, meaning after 90-95% of **1** was consumed. Corresponding changes were seen for **2E**. A more detailed kinetics analysis will be discussed later in the text.

Despite the low catalyst loadings used during the kinetics experiments, it was also possible to observe the concentration profiles of **Ru(acn)** and a reaction intermediate tentatively identified as **Ru(1)**. To our knowledge, this is the first report of a reaction intermediate using this catalytic system.

At early time points where [**1**] is much greater than [**2E**], the N-CH_3 signal of **Ru(acn)** at δ 3.82 is accompanied by fluxional signals appearing at ca. δ 3.843 and 3.866 that coalesce to a single peak at δ 3.84 above 290 K. This signal suggests a dissociative mechanism for **Ru(acn)** resulting in the formation of coordinatively unsaturated **Ru** followed by coordination of **1** (Figure 37, top). The temperature dependence of the peaks can be rationalized since complexation of prochiral **1** to the prochiral fragment **Ru** could result in the formation of two diastereomers of **Ru(1)**. The asymmetry of **Ru(acn)** is clear from its ^{1}H NMR spectrum, showing four different signals for the diastereotopic isopropyl methyls, but in the planar, symmetrical 16e⁻ Cp* analogue only two are seen.[62]

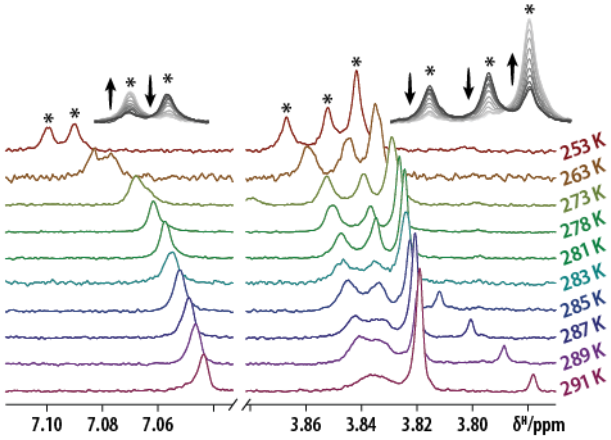


Figure 38. Black traces at top: Time-dependence of assigned Ru(acn) and Ru(1) NMR signals (*). colored traces: Temperature dependence of N-CH_3 and ligand aromatic C-H signals (*) at early reaction times when amount of 1 is maximal.

The intensities of the minor and major N-CH_3 singlets exhibit changes over time consistent with **Ru(1)** and **Ru(acn)**, respectively (**Figure 38**, grey entries). The signal for **Ru(acn)** rises gradually over time, while the signal for **Ru(1)** decreases. We conclude that **Ru(acn)** exchanges with **1** to generate some **Ru(1)** prior to the first

experimental measurement. As **1** is depleted by the isomerization to **2E**, the concentration of **Ru(1)** drops, roughly in proportion. On the timescale of the experiment, therefore, **1** and **Ru(1)** are nearly in fast equilibrium.

After the equilibrium between **1** and **2E** is established (e.g., **Figure 37** after 600 min), even though [**2E**] is 10^3 greater than $[\mathbf{Ru(acn)}]_0$, signals belonging to a tentative **Ru(2E)** complex cannot be reliably identified and integrated under our conditions. Thus, it appears that **2E** rapidly dissociates from the catalyst and is replaced by **acn**. Our failure to observe the product-catalyst complex **Ru(2E)** suggests that equilibrium favors ligand dissociation of **Ru(2E)** much more than the equilibria for both **Ru(1)** and **Ru(acn)**, which may partly explain why **Ru(acn)** isomerizes terminal alkenes faster than internal alkenes.[62,63] At higher catalyst loadings, only **Ru(acn)** signals could be easily identified, consistent with competition between alkene and higher relative concentrations of **acn** outcompeting **1**/**2E**/**2Z** for coordination to **Ru**.

2.3. Isomerization of but-1-ene.

Using the time-dependent concentration data available for **1**, ***2E***, **Ru(acn)** and **Ru(1)**, rate constants were least squares fit to the time-dependent NMR spectroscopic data using a FORTRAN program *rate.f* developed and used by the Cooksy group. For any reaction mechanism entered by the user, the rate laws are numerically integrated at each time step to provide a simulated concentration profile. The program employs a 4th order Runge-Kutta integration scheme to model the kinetics and Press' numerical recipes for least squares fitting and uncertainty analysis (for details, please see the SI in the published version of this work).

In these fits, we modeled the reaction step to form the complex **Ru(1)** and the step to convert **Ru(1)** to **2E** (Eqn. 1). The forward steps are resolved by the independent measurements of the **Ru(1)** concentration. If we fit both forward reaction rates, a reverse reaction rate must also be fit to account for the non-zero equilibrium concentrations of **Ru(1)** and free **1**. It is possible to fit the data well by including a single rate constant for the overall reverse reaction **2E** →**1**. However, because the equilibrium concentration of **Ru(1)** then depends on forward reaction 1, this fit overestimates the value of k_1. Therefore, we instead fit two reverse rate constants k_{-1} and k_{-2}:

$$\mathbf{Ru(acn)} + \mathbf{1} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \mathbf{Ru(1)} + \mathbf{acn} \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} \mathbf{Ru(acn)} + \mathbf{2E} \qquad \textbf{Eqn. 1}$$

The temperature-dependent rate constants in **Table 4** were then fit to an Arrhenius rate constant expression $k = A\, e^{-E_a/RT}$, obtaining the values listed in **Table 5**. The activation energies for the forward reaction steps are relatively insensitive to the specific mechanism used to fit the rate constants, and so we have higher confidence in the E_a values in **Table 5** than in the individual rate constants in **Table 4**.

Table 4. Fitted values of 1→2E rate constants. Uncertainties given are 1σ.

T K	k_1 L·mol^{-1}·min^{-1}	k_{-1} min^{-1}	k_2 min^{-1}	k_{-2} L·mol^{-1}·min^{-1}
253	37 ± 12	1.76 ± 0.14	0.5 ± 1.2	1.3 ± 2.8
263	140 ± 12	5.51 ± 0.17	1.6 ± 0.9	8.2 ± 3.8
273	373 ± 23	17.5 ± 0.6	5.3 ± 2.9	25 ± 12
283	710 ± 140	48.6 ± 7.1	9 ± 11	77 ± 92

Table 5. Derived 1→2E pre-exponential factors (A) and activation energies (E_a). Uncertainties given are 1σ.

step	units	ln[A/units]	E_a (kcal·mol^{-1})
1	L·mol^{-1}·min^{-1}	31.7 ± 2.2	14.0 ± 1.2
-1	min^{-1}	31.96 ± 0.34	15.79 ± 0.18
2	min^{-1}	28.1 ± 2.6	14.5 ± 1.4
-2	L·mol^{-1}·min^{-1}	38.3 ± 2.6	19.0 ± 1.4

Table 6. Thermodynamic data for the 1→2E reaction.

T (K)	$\mathbf{K_{eq}} = [\mathbf{2E}]_{eq} / [\mathbf{1}]_{eq}$	**ΔG°** (kcal·mol^{-1})
253.1	61.2	-2.070
263.2	52.1	-2.068
273.1	42.3	-2.032
283.1	35.5	-2.008
	ΔH° (kcal·mol^{-1})	**ΔS°** (cal·K^{-1}·mol^{-1})
This work	-2.63 ± 0.13	-2.17 ± 0.48
Gas-phase[64]	-2.99	-3.6

The rate constants for the reverse reactions in this study are determined by the approach to equilibrium concentrations among the reaction components at long times. In the **1→2E** reaction, equilibrium between reactant and product was sufficiently established to allow us to measure the temperature dependence of the equilibrium constant, and extract ΔH° and ΔS° values for that isomerization in acetone solvent, as given in **Table 6**.

The loss in entropy from **1** to **2E** is expected given the relative rigidity of the carbon chain when the double bond moves to the interior. Similarly, it was possible to fit enthalpy and entropy changes for the formation of the **Ru(1)** complex and **acn** from **1** + **Ru(acn)**, although the relatively low concentration of catalyst makes these values more uncertain. We determine $\Delta H° = -1.11 \pm 0.38$ kcal·mol^{-1} and $\Delta S° = +4.1 \pm 1.4$ cal·K^{-1}·mol^{-1} this complexation, indicating that the but-1-ene forms a slightly stronger bond to the ruthenium than the acetonitrile does.

The increase in entropy when the but-1-ene binds suggests that librational motions of the free acetonitrile in solution contribute more to the entropy of the system than the torsions of the butene, which are dampened upon complexation. Our calculations predict $\Delta H° = -1.23$ kcal·mol^{-1} in excellent agreement with experiment, but the calculated $\Delta S° = -2.5$ cal·K^{-1}·mol^{-1} indicating that our encounter complex does not adequately model the librational dynamics of the free acetonitrile and butene in solution.

2.4. Isomerization of (Z)-but-2-ene

As previously mentioned, isomerization of **1**→**2Z** was too slow to be kinetically resolved since lower product equilibrium concentration of **2Z** relative to that of **2E**. For this reason, the reverse reaction in which **2Z** was converted equilibrium mixture of **1**, **2E**, and **2Z**. Still, this required significantly higher catalyst concentrations of 5-10 mM, as well as higher temperatures ranging 50-70°C.

The isomerization of **2*Z*** to **2*E*** could proceed through at least three pathways: (1) catalysis of **2*Z*** to free **1**, then 1 to 2E; (2) catalysis of **2*Z*** to **2*E*** via Ru(1) without formation of free **1**; (3) direct catalysis of **2*Z*** to **2*E*** without **1** as an intermediate. For pathways (2) and (3), free **1** only appears as an isomerization from **2*E***. However, in the experiments at 319 K and 323 K, **2*E*** rapidly approaches a relative concentration of about 30 times the 1 concentration (**Figure 39**), suggesting a rapid equilibrium between those two species on the comparatively long timescale of the consumption of **2*Z***. Furthermore, the earliest time steps in each reaction show the rise of [**2*E***] as slightly lagging the rise of [**1**], which is inconsistent with **2*E*** being formed prior to **1**. Therefore, for the purpose of determining rate constants, this reaction mechanism was modeled as:

$$\mathbf{Ru(acn) + 2Z} \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} \mathbf{Ru(acn) + 1} \overset{k_1}{\rightarrow} \mathbf{Ru(1) + acn} \overset{k_2}{\rightarrow} \mathbf{Ru(acn) + 2E};\ \mathbf{1} \underset{k_{-4}}{\overset{}{\leftarrow}} \mathbf{2E} \qquad \textbf{Eqn. 2}$$

In the **2*Z*** isomerization experiments at 319 K and 323 K, **2*E*** rapidly approaches a relative concentration of about 30 times the **1** concentration (**Figure 39**), suggesting a rapid equilibrium between those two species on the comparatively long timescale of the reaction. The rapid equilibrium between **1** and **2*E*** is consistent with a slow isomerization of the **2*Z*** to **1**, acting as an intermediate which then quickly leads to formation of **2*E***, rather than catalysis of **2*Z*** directly to **2*E***.

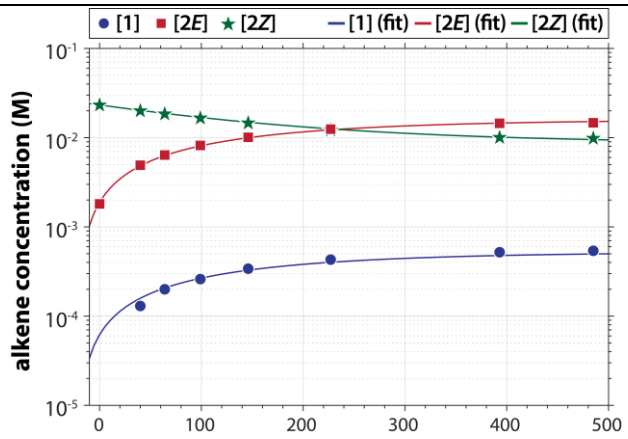


Figure 39. Observed and fitted concentrations for 2Z→ 2E reaction at 343 K. Note log scale of vertical axis to better capture changes in but-1-ene concentration.

The rate constants were fitted to the data available at each of four temperatures. Because conditions had been adjusted to bring the reaction close to completion in reasonable times, the equilibrium between **2*E*** and **1** was reached too quickly for the rate constants associated with that step to be well-resolved, so the values of k_1 and k_2 in **Eq. 2** were fixed in these fits at the values predicted by the Arrhenius parameters in Table 2. These assumptions were adequate to model the formation rate of **2*E*** but led to erroneous concentration ratios at long times. The high uncertainty in the pre-exponential factor *A* for k_{-2} and the neglect of any temperature dependence in *A* is sufficient to account for the discrepancy. Therefore, rather than fixing the reverse rate constants k_{-1} and k_{-2} in the same way, we fitted a new combined reverse rate constant k_{-4} for the conversion of **2*E*** back into **1**. The values of the rate constants and the derived Arrhenius parameters appear in **Table 7** and **Table 8**. Unfortunately, even long experiment times, the slow **2*Z*** → **2*E*** reaction did not come close enough to equilibrium to allow a precise analysis of the thermodynamics of that reaction.

Table 7. Fitted values of 2Z→2E rate constants. Uncertainties given are 1σ.

T (K)	k_3 (L·mol^{-1}·min^{-1})	k_{-3} (min^{-1})	k_{-4} (min^{-1})
323.6	0.1470 ± 0.0016	2.58 ± 0.24	(9.9 ± 1.0) × 10^2
333.2	0.467 ± 0.018	6.7 ± 2.0	(2.67 ± 0.79) × 10^3
338.4	0.610 ± 0.027	10.5 ± 3.8	(3.4 ± 1.1) × 10^3
343.2	0.782 ± 0.015	12.9 ± 1.7	(5.21 ± 0.66) × 10^3

Table 8. Derived 2Z→2E pre-exponential factors (A) and activation energies (E_a). Uncertainties given are 1σ.

step	units	ln[A/units]	E_a (kcal·mol^{-1})
3	L·mol^{-1}·min^{-1}	27.7 ± 4.1	19.0 ± 2.8
-3	L·mol^{-1}·min^{-1}	30.0 ± 2.5	18.6 ± 1.7
-4	min^{-1}	35.4 ± 2.4	18.3 ± 1.6

2.5. DFT results

Theoretical reaction coordinates for **Ru(acn)**-mediated alkene isomerization were constructed from the optimized geometries of key transition states and intermediates (see computational methods for details). A summary of the pathways characterized by the computational effort is given in the flowchart in **Figure 40**. Each pathway consisted of multiple steps for hydrogen transfer and intramolecular conformational changes to allow them to occur. Full details for each pathway can be found in Appendix 2.9.4, however, a summary of the relative free energies are presented in **Table 9**.

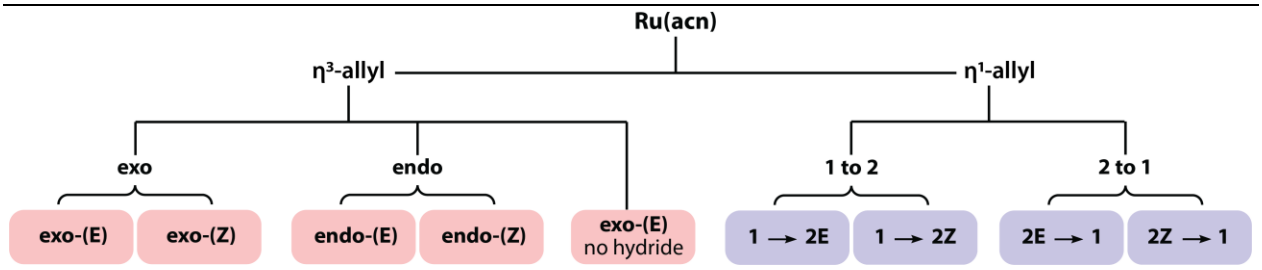


Figure 40. Flowchart of the named pathways found as part of this work.

Table 9. Summary of relative free energies for isomerization pathways in kcal/mol. The free energies in this table were obtained from data obtained at the B3LYP/cc-pVDz level.

	η³-allyl					η¹-allyl			
	exo-(E)	exo-(Z)	endo-(E)	endo-(Z)	no hydride	1 -2E	2E-1	1-2Z	2Z-1
average, IM	7.0	12.0	10.5	9.1	5.6	15.4	8.9	12.3	10.7
barrier, forward	15.7	13.2	19.6	19.5	22.4	26.4	36.8	21.0	26.9
barrier, reverse	16.8	21.3	18.0	21.6	21.8	17.8	25.1	21.1	24.5

Several mechanistic scenarios were considered for catalyst-substrate interactions of but-1-ene with **Ru(acn)**. An initial consideration is the hapticity of the allyl ligand; deprotonation of the π-coordinated but-1-ene

can yield either an η^1- or η^3-allyl depending on whether **acn** remains within the inner coordination sphere to block the allyl ligand from coordinating in an η^3 fashion. The η^1-allyl pathways (**Figure 41**) were ruled out since experimental data discussed later in this work suggests that **Ru(acn)** undergoes a dissociative mechanism during isomerization of but-1-ene. Moreover, the barriers obtained from the calculations of the η^1-allyl pathways were significantly higher than the lower energy pathways present in the η^3-allyl pathways.

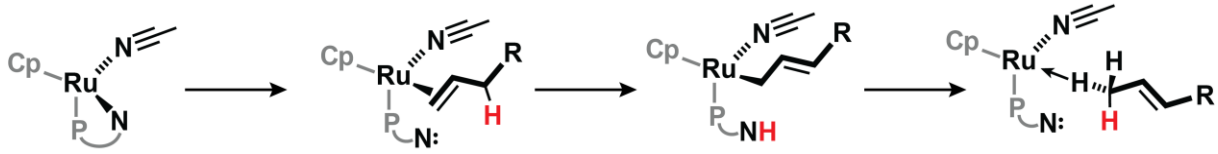


Figure 41. Schematic of steps in η^1-allyl mechanism.

For the lower energy pathways proceeding via an η^3-allyl intermediate, four pathways characterized by the formation of a Ru(H)(η^3-allyl) intermediate were located. These pathways shared a similar series of steps during the catalytic cycle (**Figure 42**) and varied only on the geometry of the allyl ligand as well as *exo*-/*endo*-coordination (Chart 1). This allowed for direct comparisons of the energetics of (*E*)- and (*Z*)-forming steps. An additional (*E*)-η^3-allyl pathway was found that precluded formation of a hydride intermediate (i.e., direct deprotonation), but was higher in energy and mechanistically unfeasible since the geometries needed for an analogous process to form a (*Z*)-η^3-allyl would require an inordinate number of conformational changes to link together relevant transition states along a continuous reaction coordinate.

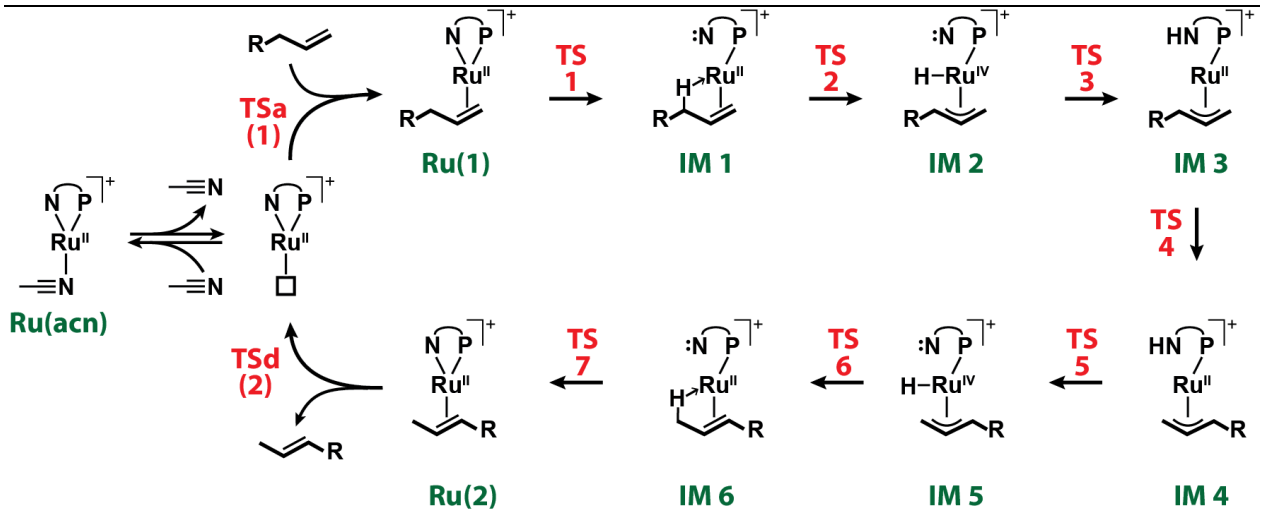


Figure 42. Schematic of steps in η^3-allyl mechanism.

An energy diagram for comparing Ru(H)(η^3-allyl) pathways are shown. Note that the energies in the energy diagram correspond to higher level single point energies calculated using the B3LYP/cc-PVDz optimized structures used for the values in **Table 9**.

The Ru(H)(η^3-allyl) pathway starts **Ru(acn)** dissociating **acn** to yield five-coordinate intermediate **Ru**. The resulting vacancy is filled during the formation of the metal-alkene π-bond in **Ru(1)**. The approach of but-1-ene (**1**) to 16e$^-$ intermediate **Ru** was modeled by scanning the distance coordinate between the Ru atom of **Ru** and the terminal sp^2 carbon on **1**. In this way, C1-H complex **Ru•1** was found, along with the transition state $\mathbf{TS_{Ru•1\text{-}Ru(1)}}$ leading to the more stable π-complex **Ru(1)**. In C-H complex $\mathbf{Ru•1^{exoE}}$, the coordinated C1-H distance is computed to be 1.128 Å, whereas the uncoordinated C1-H on the same terminal alkene carbon is 1.088 Å. As seen below, a more robust agostic interaction is computed to lengthen a C-H bond by more than 0.1 Å, whereas here the difference is only 0.04 Å. We therefore make use of the weakly coordinated C-H complexes **3** and **10** as proxies for free alkene plus catalytic intermediate **Ru** in order to model the dissociation of the bound alkene from the catalyst for the forward and reverse reaction along each of the four pathways. These structures have weak alkene-metal C-H bonding, but retain a unity of molecular structure that reduces the impact of basis set superposition error and cavity-separation in the solvation model.

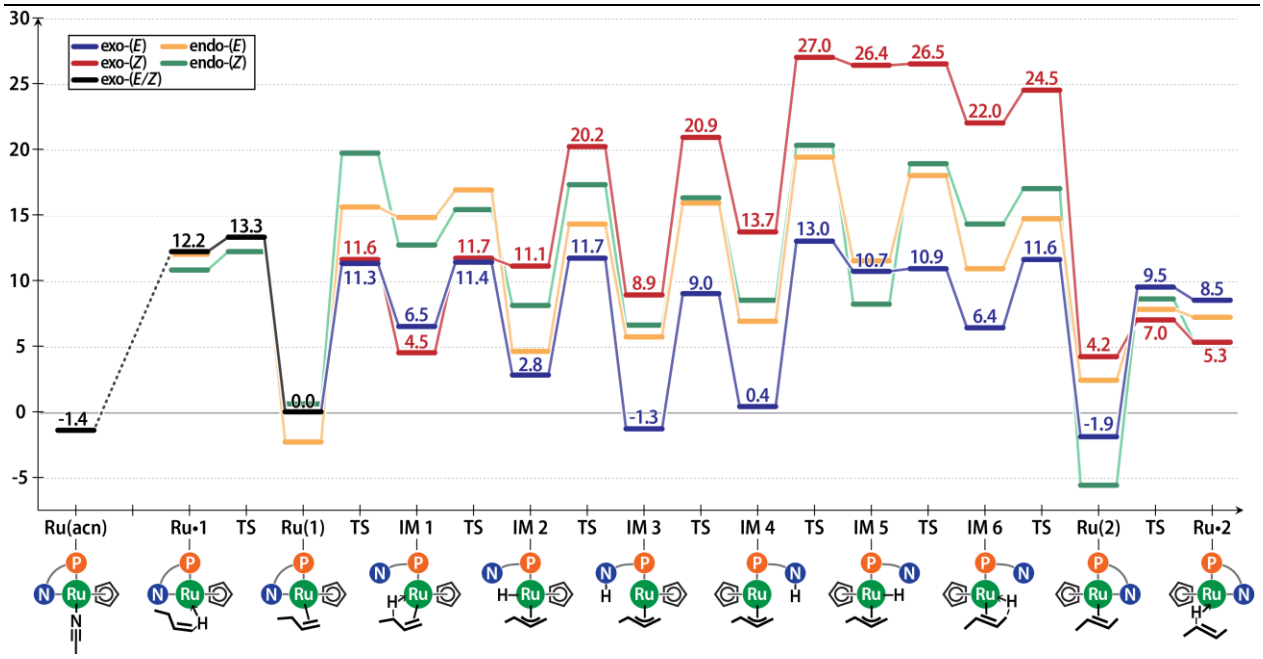


Figure 43. MN15/cc-pVTZ/COSMO//B3LYP/cc-pVDZ relative free energies (kcal mol-1) of stationary points along the four pathways. Free energy values for the exo-(E) and exo-(Z) pathways are given. Some minor conformational isomerizations are omitted; figure and table with all stationary points are given in the SI.

Complex **Ru(1)** is coordinatively saturated, meaning that oxidative addition cannot occur due to lack of a vacant site to accommodate a new hydride ligand. Furthermore, the κ^2-PN ligand cannot act as a base when the lone pair of N is involved in bonding. Dissociation of the Ru-N bond generates a $2e^-$ vacancy and allows the N atom to function as a base. In $\mathbf{TS_{Ru(1)\text{-}IM1}}$, the coordinative unsaturation from N dissociation is intercepted by an allylic C3-H, forming agostic complex **IM 1**. In **IM 1**^{exoE}, the agostic C3-H bond distance is computed to be 1.222 Å, whereas the uncoordinated C3-H on the same carbon is 1.095 Å. Moreover the distances between Ru and alkene sp^2 carbons are distorted: C1-Ru is 2.227 Å, whereas C2-Ru is shortened to 2.110 Å to accommodate the neighboring agostic interaction at C3. Next, oxidative addition of the agostic C3-H bond to **Ru** gives hydride intermediate **5**, and subsequently the κ^1-P ligand then reductively deprotonates the hydride to give the η^3-allyl complex **6**. Comparing allyl complexes **IM 2**^{exoE} and **IM 3**^{exoE}, reductive deprotonation is calculated to change the C3-Ru distance the most of all, likely because the hydride ligand in **IM 2**^{exoE} is closest to C3: changes the C1-Ru, C2-Ru, and C3-Ru distances are -0.004, -0.030 and -0.037 Å, respectively.

Conformational change of **IM 3** is needed, since the road to **Ru(2*E*)** requires the NH hydrogen on the PN ligand, which originated from C3 of **1**, to reach C1 Torsion of the Cp-Ru-allyl moiety along the Ru-P bond axis,

where the allyl ligand migrates to a sterically similar environment on the opposing enantioface of **Ru**, resulting in **IM 4**. Although the step from **IM 3** to **IM 4** is only a conformational change, for three of the four pathways shown in Figure 5 this step is associated with an increase in free energy of 7-8 kcal mol^{-1}, which apparently arises from an increasing number of H-H steric interactions. For example, **IM 3**$^{exo\boldsymbol{E}}$ has 12 such interactions involving H-H distances <2.3 Å while **IM 4**$^{exo\boldsymbol{E}}$ has 16.

Oxidative protonation of Ru by the N-H bond in $\mathbf{TS}_{\mathbf{IM4\text{-}IM5}}$ yields Ru^{IV} hydride intermediate **IM 5**. Reductive elimination of Ru(H) in $\mathbf{TS}_{\mathbf{IM5\text{-}IM6}}$ to the allyl forms agostic complex **IM 6**. Complex **IM 6**$^{exo\boldsymbol{E}}$ is computed to have structural features similar to those of **IM 1**$^{exo\boldsymbol{E}}$: the agostic C1-H bond distance is computed to be 1.210 Å, whereas the two uncoordinated C1-H distances are 1.097 and 1.098 Å. Moreover the distances between Ru and alkene sp^2 carbons are distorted: C3-Ru is 2.268 Å, whereas C2-Ru is shortened to 2.122 Å to accommodate the neighboring agostic interaction at C1. The Ru-alkene and Ru-CH distances in **Ru•2*E***$^{exo\boldsymbol{E}}$ are all larger by 0.02-0.04 Å than for **IM 1**$^{exo\boldsymbol{E}}$, consistent with the greater steric demands of ***2E*** compared with those of **1**. Dissociation of the agostic CH in $\mathbf{TS}_{\mathbf{IM6\text{-}Ru(2E)}}$ gives π-complex **Ru(2*E*)**. The Ru-alkene distances in **Ru(2*E*)**$^{exo\boldsymbol{E}}$ are 2.233 and 2.252 Å, greater than **Ru(1)**$^{exo\boldsymbol{E}}$ (2.209 and 2.228 Å), consistent with greater steric demand in the ***2E*** complex. In $\mathbf{TS}_{\mathbf{Ru(2E)\text{-}Ru\bullet 2E}}$, the ***2E*** ligand migrates to yield unstable C-H complex **Ru•2*E***. Once again, the greater steric demands around the coordinated internal alkene C-H in **Ru•2*E***$^{exo\boldsymbol{E}}$ lead to longer metal-ligand distances: Ru-C 2.689 vs 2.461 Å in **Ru•1**$^{exo\boldsymbol{E}}$, and Ru-H 2.001 vs. 1.969 Å in **Ru•1**$^{exo\boldsymbol{E}}$.

Tao et al. described the *exo*-(*E*) pathway for transformation of 1-pentene to (*E*)-2-pentene.[4] We examine four competing pathways for butene. Our *exo*-(*E*) calculations generally reproduce theirs, but with additional smaller conformational changes with low barriers. In general, their computed bond distances for various metal-alkene interactions tend to be greater than ours, but by less than 0.08 Å, which is not chemically significant and expected given the differences in basis set and treatment of dispersion.

2.6. Origin of (E)-selectivity

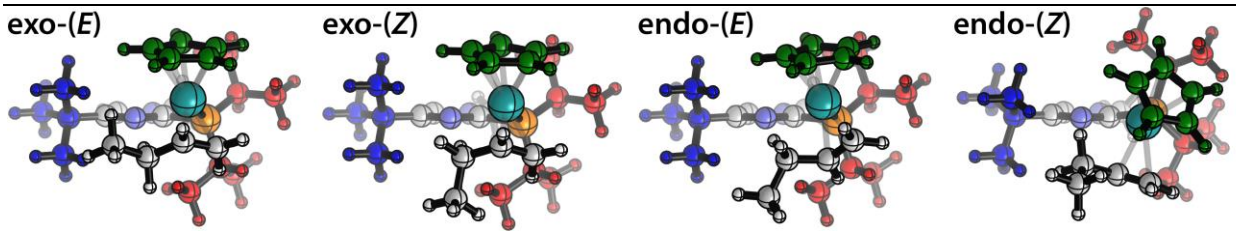


Figure 44. B3LYP-D2/cc-pVDZ optimized geometries of alkene in relation to metal center for $\mathbf{TS_{Ru(1)\text{-}IM\ 1}}$

Four pathways were characterized for intermediates that differ in terms of relative stereochemistry between prochiral alkene and prochiral metal fragment Ru (**Figure 44**). Ultimately, we conclude that the lowest energy pathway is *exo*-(*E*), but first let us look at the others. Both *endo* pathways start with the *endo*-coordinated diastereomer of Ru(1) and are clearly less favorable for formation of but-2-ene than the corresponding *exo* pathways, given the significantly higher barriers encountered at $\mathbf{TS_{Ru(1)\text{-}IM\ 1}}$. **Figure 44** shows the greater interaction between alkene and catalyst alkyl groups in $\mathbf{TS_{Ru(1)\text{-}IM\ 1}^{endoE}}$ that accounts for the 5-6 kcal mol^{-1} higher activation energy at this early stage of the *endo* pathway. The reaction diagrams in **Figure 43** are similar for the *endo*-(*E*) and *endo*-(*Z*) pathways, both in terms of individual barriers and the free energies of the intermediates.

In contrast, from *exo*-coordinated **1**, the *exo*-(*Z*)-pathway begins to rise in energy ~10 kcal mol^{-1} above the *exo*-(*E*) pathway at **IM 2** and $\mathbf{TS_{IM\ 2\text{-}IM\ 3}}$, and remains so over several steps, rising further to ~15 kcal mol^{-1} between $\mathbf{TS_{IM\ 4\text{-}IM\ 5}}$ and $\mathbf{TS_{IM\ 6\text{-}Ru(2x)}}$ (x = *E* or *Z*). The individual barriers for the *exo*-(*Z*) pathway are not vastly greater than for *exo*-(*E*), but the free energies of the (*E*)- and (*Z*)-intermediates and TS remain separated by ~10-15 kcal/mol from **IM 2** all the way to $\mathbf{TS_{IM\ 6\text{-}Ru(2x)}}$. A likely explanation is restriction of conformational freedom about the Ru center, due to inner-sphere crowding resultant from the oxidation of Ru^{II} to Ru^{IV} as well as the need to accommodate an additional hydride ligand. These changes force the substrate to interact more strongly with steric bulk of the PN ligand, illustrated for **IM 3** in **Figure 45**. More specifically, the energy increase along the (*Z*) pathway can be rationalized by the axial interaction between the isopropyl groups of the PN ligand and the methyl substituent on the allyl ligand.

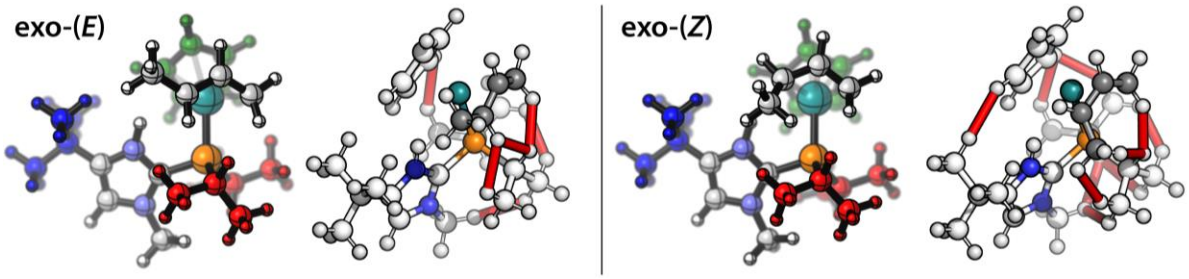


Figure 45. B3LYP-D2/cc-pVDZ optimized geometries of (a) **6**^{exoE} and (b) **6**^{exoZ}, showing the interaction with *i*-Pr with the methyl group of the allyl ligand.

Selection of either (*E*)- or (*Z*)-pathways occurs at $\mathbf{TS_{Ru(1)\text{-}IM\ 1}}$. Dissociation of the ligand nitrogen forms a 16e$^-$ Ru center and allows an agostic interaction with either of two diastereotopic C3-H of coordinated **1**. The choice of which C3-H agostic interaction conformationally locks the bound alkene **1** to convert adopt either pro-(*E*)- or pro-(*Z*)- geometries. Although individual forward reaction steps for the *exo*-(*Z*) pathway appear surmountable, the *exo*-(*E*) pathway is uniformly more favorable. Correspondingly low barriers for the reverse reaction steps of the *exo*-(*Z*) pathway also contribute to strong kinetic bias towards the **1**→**2E** over the **1**→**2Z** reaction. Therefore, the computational model reproduces the experimentally observed (*E*)-selectivity.

2.7. Rate-determining steps.

A key finding is that the steepest free energy activation barriers G_a in the calculated *exo*-(*E*) reaction diagram occur at the first H-abstraction step ($\mathbf{TS_{Ru(1)\text{-}IM\ 1}}$ G_a=11.3 kcal mol^{-1}), at the Ru-P torsion ($\mathbf{TS_{IM\ 3\text{-}IM\ 4}}$, 10.3 kcal mol^{-1}), and at the but-2-ene dissociation ($\mathbf{TS_{Ru(2E)\text{-}Ru\bullet 2E}}$, 11.4 kcal mol^{-1}), making these the likeliest candidates for the rate-determining step (RDS) of the **1**→**2E** reaction. The experimental data unambiguously indicate that the RDS occurs at some point after formation of **Ru(1)** and *before* formation of **Ru(2*E*)**, because no other catalyst-derived complex (catalyst-alkene or catalyst-allyl) builds up a comparable concentration to that of **Ru(1)**. The absence of other identifiable species rules out **Ru(2*E*)** → **Ru•2*E*** as the RDS. As shown in **Figure 37**, at any given time during the reaction, the sum [**Ru(acn)**]+[**Ru(1)**] is roughly constant and accounts for nearly all the catalyst present. The calculations indicate that the correct RDS occurs at **Ru(1)** → **IM 1**, although **IM 3** → **IM 4** remains a viable candidate. The assignment of the RDS to the first H-transfer step is consistent with the findings of Tao et al., who found a free energy barrier of 11 kcal mol^{-1} for the same step in the pentene reaction.[61]

The calculated G_a values combine both the Arrhenius activation energy E_a and the entropic contribution to the Arrhenius pre-exponential factor, and therefore should be good indicators of the RDS, the step with the slowest reaction rate. However, only the activation energy E_a (not G_a) carries the temperature dependence on which the experimental activation barriers in **Table 5** and **Table 8** are based. For example, we should compare the E_a value in **Table 5** derived from k_2 (14.5 kcal/mol) to the calculated E_a at $\mathbf{TS_{Ru(1)\text{-}4}}$ of 14.0 kcal/mol, which falls well within the expected error for DFT calculations on systems of this type.[65]

The energetic span of the reaction offers a more accurate relationship between the calculated mechanism and the relative efficiencies of competing catalytic pathways.[66,67] The free energies in **Figure 43** and **Eqn. 2** in Kozuch[67] predict turnover frequencies of 7.75 min^{-1} for the exo-(E) pathway and less than 10^{-3} min^{-1} for the other three pathways, indicating that the exo-(E) pathway is indeed the most effective by 3-4 orders of magnitude.

Although the exo-(E) pathway appears most favorable for the **1**→**2E** reaction, the **2Z**→**1** reaction, which was also carried out in this work, appears to have similarly favorable free energy profiles following either the endo-(Z) or exo-(Z) pathways (**Figure 43**). The RDS for both pathways appears at $\mathbf{TS_{IM\ 6\text{-}Ru(2x)}}$ (x = E or Z), which presents energy barriers G_a and E_a of 20-22 kcal mol^{-1}, comparable to the value of 19 kcal mol^{-1} for the forward energy barrier in **Table 8**.

2.8. Conclusion & Future Work

This detailed experimental and computational study of the catalysis of **1** to **2*E*** and **2*Z*** by catalyst **Ru(acn)** finds that the observed high (***E***)-selectivity likely arises from increased steric interaction of the **(*Z*)**-alkene with one of the isopropyl groups on the **PN** ligand. Experimental observation of the **Ru(1)** complex establishes that the rate-determining step occurs prior to formation of the alk-2-ene on the catalyst, and computations suggest that the RDS is the initial H-abstraction by the metal. Temperature-dependent measurements have determined activation barriers in good agreement with calculations.

This work was originally inspired by a desire to investigate unpublished results indicating that changing the identity of the bulky substituents on the **PN** ligand to *tert*-butyl groups results not only in a reduction in activity, but also a loss of (*E*)-selectivity.[68] The *tert*-butyl analog of **Ru(acn)** is intriguing because the increased steric

demands of a *tert*-butyl versus an isopropyl group could ostensibly hinder a mechanism proceeding by Ru-P torsion of an η^3-allyl intermediate as discussed in this work. This could force isomerization via the *tert*-butyl catalyst to occur via a higher energy pathway consistent with the experimentally observed need for increased temperatures and longer reaction times,[68] a possibility that has been established by the present work in the form of the η^1-allyl pathways characterized, but not examined in detail here. Future work in this area could lead to additional structure-activity insight that can potentially be used as a tool to shape the outcome of other CpRu-catalyzed transformations.

2.9. Appendix 2

2.9.1. Methods

2.9.1.1. General

Synthesis of **Ru(acn)** was undertaken as described in the literature.[69] Reagents were purchased from Sigma-Aldrich or Acros and used as is without further purification. NMR solvents were purchased from Cambridge Isotopes and deoxygenated by bubbling nitrogen through them. Butenes were obtained from Synquest or Phillips and used without further purification. A Varian INOVA 500 MHz spectrometer was used.

2.9.1.2. General procedure; reaction monitoring for but-1-ene.

But-1-ene stock solutions were made in a glovebox. One representative procedure is described. A Chemglass heavy-walled tube with resealable Teflon valve on the balance was charged with $C(SiMe_3)_4$ (28.4 mg, 0.0964 mmol). Any solid sticking to upper walls was rinsed down using portions of acetone-d_6 (total: 10.0 mL). But-1-ene was withdrawn by plastic syringe from a Schlenk flask that had been purged with the gas, and the gas portion was slowly (over 2-3 min) injected below the surface of the acetone-d_6. An aliquot (900 μL) was withdrawn by syringe and added to a J. Young resealable NMR tube for analysis by ^{1}H NMR spectroscopy, using 10^o pulses and 10 sec delay between pulses. If the amount of but-1-ene was insufficient, back in the glovebox the contents of the J. Young were poured back into the heavy-walled tube and more but-1-ene was added. The last aliquot tested gave the following integrations, in arbitrary units: $C(SiMe_3)_4$ set to 100.00 and but-1-ene (CH signals 98.93, 99.30, 98.60; CH_3 signal 298.17). We calculate 0.258 mmol in the 900 μL sample.

Catalyst stock solutions were created by charging a vial with **Ru(acn)** (6.2 mg, 0.0102 mmol) and adding acetone-d_6 (2.05 mL) for [**Ru(acn)**]$_0$ = 5.1 mM.

Each kinetics run involved adding 100 μL catalyst stock solution to 900 μL of but-1-ene stock solution. Two different kinds of NMR tubes were used: either J. Young resealable tubes, to which catalyst had to be added in the glovebox, or screw-cap NMR tubes, to which catalyst could be added at the spectrometer by injecting catalyst solution through a septum in the cap. No matter what kind of tube was used, the catalyzed reactions were so fast that only temperatures between 253 and 283 K were practical. For the J. Young experiments, the tube was

placed in a stainless-steel insulated container and aluminum foil was used to cover the top of NMR tube and container. The resulting assembly was precooled in the glovebox -30 °C freezer for at least an hour. Catalyst solution was injected quickly, and the foil-covered assembly carried to the spectrometer; typically the time between catalyst injection and placing in the probe was 3 min, and launching of the kinetics run occurred within another 2-6 min.

A second variant of the general procedure used a stock solution of but-1-ene without the internal standard. In this variant, a J. Young NMR tube on the balance was charged with an amount of $C(SiMe_3)_4$ (3-10 mg). An initial ^1H NMR spectrum was acquired, which was analyzed to give the but-1-ene concentration. The tube was then chilled in the glovebox freezer for at least 1 h and the rest of the experiment was the same as described above.

2.9.1.3. General procedure; reaction monitoring for (*Z*)-but-2-ene.

Catalyst stock solutions were prepared by weighing **Ru(acn)** (~12 mg) and $C(SiMe_3)_4$ (~1 mg) internal standard into a conical vial. Acetone-d_6 was added to the 2.0 mL graduation mark on the vial. Samples for NMR were prepared using 1.0 mL and 0.50 mL aliquots of catalyst stock solution. In a vial, (*Z*)-but-2-ene was injected into catalyst stock solution. For the 0.50 mL aliquots, fresh acetone-d_6 (0.50 mL) was added to ensure adequate sample volume for NMR. Sample solution (about 0.80 mL) was added to a J. Young NMR tube with Teflon seal.

Samples were heated in a temperature-controlled oven (Robbins Scientific Flex Chem model 404) with rotating NMR tube holders. The oven was preheated to stable temperature prior to adding the NMR tube. For data acquisition, the NMR tube was removed from the oven and immediately immersed in room temperature DI water (800 mL) to cool the tube and halt reaction progress. Single ^1H NMR spectra acquired using a Varian 500 MHz spectrometer (8 scans, pulse angle = 30°) at 23.5 °C with a pre-acquisition delay of 60 seconds to ensure thermal equilibrium.

Initially, the kinetics experiment for **2Z** was performed in a more standard fashion, using NMR tubes immersed in a heated oil bath. Unfortunately, the concentration of total alkenes (as measured by integration of the sp^2 proton peaks relative to $C(SiMe_3)_4$ internal standard) appeared to drop over the course of the experiment.

The total alkene concentration returned to initially measured values when the NMR tube was manipulated to allow mixing of the contents at the end of a run. The calculated *k* values using this set of data gave unusually low activation barriers, which we attributed to the volatilization of **2Z** into the headspace of the NMR tube. This would result in lower observed concentrations of **2Z** relative to **2E**, leading to faster apparent reaction rates. Hence, the rotating oven heating technique is needed.

2.9.1.4. Computations

Geometries for all stationary points were optimized using the B3LYP DFT method[54,70] and a basis set combining Dunning's cc-pVDZ basis set for the main group atoms and Peterson's aug-cc-pVDZ-pp basis for the metal.[52,53] Grimme's D2 empirical dispersion correction was incorporated in view of possible interactions involving the aromatic Cp and imidazole moieties. This B3LYP-D2 methodology has been benchmarked against similar systems in previous work.[71,72] However, given the sensitivity of the conclusions to energy differences of 2—3 kcal/mol, single-point energy calculations were then carried out at the B3LYP-optimized geometry of each stationary point using the MN15 DFT method[73] and a relatively large cc-pVTZ basis set[52,53] (1432 contracted functions). Transition states were confirmed in all cases using vibrational analysis followed by intrinsic reaction coordinate (IRC) scans to the neighboring minimum energy structures. Natural bond order (NBO) analysis was used to model and visualize the molecular orbitals.[74] Additional details of the computational methods, as well as optimized geometries and absolute energies, are provided in the SI. All calculations were carried out using the Gaussian 09 and Gaussian 16 suite of programs[75] running on an Intel Linux cluster.

2.9.2. Experimental for the Isomerization of 1bu to ^{E}2bu

2.9.2.1. Summary

run no.	temp. K	$[cat]_0$ M	$[1]_0$ M	TMS_4C mg	$[cat]_f$ M	conversion $2E_f$	conversion $2E_0$
e5	263	3.38E-04	0.237	6.30	2.81E-04	97.5%	44.8%
e6	263	3.60E-04	0.237	8.40	3.66E-04	97.6%	14.8%
e7	263	3.14E-04	0.185	3.70	2.98E-04	98.1%	16.1%
e8	273	3.67E-04	0.203	6.50	3.84E-04	97.7%	24.4%
e9	273	4.14E-04	0.198	9.10	4.25E-04	97.6%	19.7%
d3	263	4.38E-04	0.240	2.13	4.44E-04	98.2%	11.8%
d4	253	4.54E-04	0.241	2.13	4.38E-04	97.3%	5.4%
d5	273	4.09E-04	0.237	2.13	4.31E-04	97.8%	17.2%
d6	273	3.99E-04	0.235	2.13	4.03E-04	97.8%	26.6%
d7	273	4.48E-04	0.206	2.13	4.48E-04	97.8%	13.4%
d8	283	4.57E-04	0.209	2.13	4.58E-04	97.3%	21.9%
d9	283	4.43E-04	0.195	2.13	4.48E-04	97.3%	19.9%
d10	253	4.31E-04	0.222	2.13	4.55E-04	98.5%	8.5%

Erik Paulson assisted with running these experiments. The values for $[cat]_0$, $[bu]_0$, and $[cat]_f$ was calculated from NMR integrations. The columns titled **conversion** is a qualitative indicator of the kinetic resolution of the dataset. The entries under $2E_0$ is the ratio of 2E:1 at the first data point. Likewise, the entries under $2E_f$ is the ratio of 2E:1 at the last data point for a kinetics run.

Due to fast catalysis and time needed to insert the sample, it was not possible for us to start data collection before isomerization had reached about 8.5% conversion. Lower concentrations of catalyst would lower the intensity ^{1}H signal of the $(^i$Pr$)_2$**PN** ligand below our detection threshold. The entries under $2E_f$ shows that each run had reached thermodynamic equilibrium of 2E:1 (97-98%).

e5

time (min)	[1bu]	[E2bu]	[Ru(acn)]	[Ru(1bu)]
0	0.1308	0.1061	1.101E-04	2.279E-04
5	0.1239	0.1121	1.113E-04	2.216E-04
10	0.1179	0.1184	1.213E-04	2.335E-04
15	0.1120	0.1244	1.269E-04	2.360E-04
20	0.1063	0.1304	1.301E-04	2.118E-04
25	0.1007	0.1363	1.347E-04	2.144E-04
30	0.0951	0.1422	1.453E-04	2.241E-04
35	0.0898	0.1478	1.472E-04	2.289E-04
40	0.0844	0.1532	1.570E-04	2.124E-04
45	0.0793	0.1586	1.380E-04	2.028E-04
50	0.0744	0.1638	1.407E-04	2.090E-04
55	0.0697	0.1687	1.559E-04	2.053E-04
60	0.0651	0.1737	1.677E-04	2.169E-04
65	0.0606	0.1783	1.538E-04	1.939E-04
70	0.0563	0.1828	1.541E-04	1.833E-04
75	0.0522	0.1871	1.730E-04	1.709E-04
80	0.0483	0.1911	1.616E-04	1.806E-04
85	0.0445	0.1950	1.747E-04	1.825E-04
90	0.0414	0.1987	1.871E-04	1.671E-04
95	0.0379	0.2024	1.841E-04	1.715E-04
100	0.0348	0.2054	1.967E-04	1.576E-04
105	0.0320	0.2085	1.928E-04	1.615E-04
110	0.0293	0.2114	1.880E-04	1.576E-04
115	0.0268	0.2140	1.835E-04	1.522E-04
120	0.0245	0.2165	1.989E-04	1.463E-04
125	0.0226	0.2188	2.036E-04	1.514E-04
130	0.0207	0.2209	1.956E-04	1.529E-04
135	0.0190	0.2229	2.123E-04	1.319E-04
140	0.0173	0.2245	2.058E-04	1.362E-04
145	0.0158	0.2262	2.110E-04	1.388E-04
150	0.0145	0.2275	2.089E-04	1.111E-04
155	0.0133	0.2288	2.016E-04	1.456E-04
160	0.0124	0.2300	2.153E-04	1.129E-04
165	0.0114	0.2309	2.207E-04	1.125E-04
170	0.0106	0.2317	2.201E-04	9.197E-05
175	0.0099	0.2326	2.180E-04	9.671E-05
180	0.0092	0.2331	2.247E-04	1.077E-04
185	0.0087	0.2338	2.168E-04	1.251E-04
190	0.0083	0.2344	2.155E-04	1.149E-04
195	0.0078	0.2348	2.054E-04	1.026E-04
200	0.0073	0.2353	2.135E-04	8.264E-05
205	0.0071	0.2356	2.223E-04	8.954E-05
210	0.0069	0.2360	2.099E-04	9.353E-05
215	0.0064	0.2361	1.981E-04	8.197E-05
220	0.0062	0.2365	1.994E-04	1.069E-04
225	0.0062	0.2366	1.993E-04	1.024E-04
230	0.0059	0.2366	2.094E-04	8.812E-05
235	0.0060	0.2369	1.983E-04	8.281E-05

e6

time (min)	[1bu]	[E2bu]	[Ru(acn)]	[Ru(1bu)]
0	0.2016	0.0350	1.019E-04	2.576E-04
6	0.1921	0.0436	9.972E-05	2.522E-04
12	0.1841	0.0525	9.710E-05	2.396E-04
18	0.1762	0.0612	9.685E-05	2.626E-04
24	0.1686	0.0697	1.097E-04	2.463E-04
30	0.1609	0.0781	1.141E-04	2.473E-04
36	0.1535	0.0864	1.101E-04	2.304E-04
42	0.1461	0.0946	1.155E-04	2.471E-04
48	0.1389	0.1023	1.348E-04	2.476E-04
54	0.1318	0.1100	1.141E-04	2.207E-04
60	0.1249	0.1177	1.342E-04	2.270E-04
66	0.1182	0.1250	1.326E-04	2.438E-04
72	0.1114	0.1321	1.387E-04	2.530E-04
78	0.1052	0.1391	1.403E-04	2.298E-04
84	0.0988	0.1459	1.481E-04	2.159E-04
90	0.0928	0.1525	1.557E-04	2.121E-04
96	0.0868	0.1591	1.328E-04	2.238E-04
102	0.0810	0.1654	1.497E-04	2.193E-04
108	0.0755	0.1715	1.523E-04	2.108E-04
114	0.0700	0.1775	1.539E-04	2.109E-04
120	0.0650	0.1832	1.683E-04	2.014E-04
126	0.0601	0.1887	1.590E-04	1.807E-04
132	0.0553	0.1941	1.787E-04	1.767E-04
138	0.0508	0.1990	1.542E-04	2.005E-04
144	0.0465	0.2038	1.680E-04	1.834E-04
150	0.0426	0.2085	1.877E-04	1.806E-04
156	0.0386	0.2127	1.849E-04	1.751E-04
162	0.0350	0.2168	1.845E-04	1.845E-04
168	0.0317	0.2207	1.947E-04	1.827E-04
174	0.0290	0.2245	2.009E-04	1.688E-04
180	0.0258	0.2275	2.011E-04	1.451E-04
186	0.0233	0.2306	2.136E-04	1.696E-04
192	0.0209	0.2335	2.097E-04	1.400E-04
198	0.0190	0.2362	2.225E-04	1.452E-04
204	0.0170	0.2383	2.266E-04	1.314E-04
210	0.0153	0.2405	2.245E-04	1.649E-04
216	0.0138	0.2425	2.262E-04	1.359E-04
222	0.0125	0.2444	2.168E-04	1.561E-04
228	0.0114	0.2459	2.537E-04	1.496E-04
234	0.0104	0.2474	2.345E-04	1.216E-04
240	0.0097	0.2487	2.488E-04	1.271E-04
246	0.0088	0.2497	2.423E-04	1.494E-04
252	0.0082	0.2507	2.431E-04	1.473E-04
258	0.0076	0.2517	2.431E-04	1.176E-04
264	0.0072	0.2525	2.384E-04	1.159E-04
270	0.0069	0.2533	2.509E-04	1.341E-04
276	0.0066	0.2541	2.447E-04	1.114E-04
282	0.0065	0.2548	2.467E-04	1.208E-04
288	0.0063	0.2555	2.613E-04	1.050E-04
294	0.0062	0.2561	2.592E-04	1.073E-04

e7

time (min)	[1bu]	[E2bu]	[Ru(acn)]	[Ru(1bu)]
0	0.1556	0.0298	8.459E-05	2.293E-04
6	0.1473	0.0374	8.844E-05	2.264E-04
12	0.1400	0.0450	9.261E-05	2.051E-04
18	0.1326	0.0524	8.503E-05	2.072E-04
24	0.1258	0.0598	1.001E-04	1.965E-04
30	0.1189	0.0670	1.019E-04	2.135E-04
36	0.1123	0.0739	1.058E-04	2.050E-04
42	0.1057	0.0807	1.091E-04	2.081E-04
48	0.0993	0.0875	1.172E-04	1.872E-04
54	0.0931	0.0938	1.141E-04	1.931E-04
60	0.0868	0.1001	1.193E-04	1.869E-04
66	0.0809	0.1060	1.107E-04	1.831E-04
72	0.0752	0.1119	1.277E-04	1.709E-04
78	0.0697	0.1174	1.283E-04	1.677E-04
84	0.0643	0.1228	1.233E-04	1.723E-04
90	0.0590	0.1281	1.338E-04	1.645E-04
96	0.0542	0.1330	1.366E-04	1.459E-04
102	0.0496	0.1377	1.409E-04	1.603E-04
108	0.0449	0.1423	1.488E-04	1.580E-04
114	0.0407	0.1467	1.416E-04	1.433E-04
120	0.0367	0.1507	1.529E-04	1.308E-04
126	0.0328	0.1547	1.593E-04	1.459E-04
132	0.0293	0.1582	1.700E-04	1.369E-04
138	0.0260	0.1615	1.601E-04	1.372E-04
144	0.0232	0.1643	1.856E-04	1.224E-04
150	0.0204	0.1673	1.916E-04	1.230E-04
156	0.0180	0.1698	1.850E-04	1.198E-04
162	0.0157	0.1720	1.918E-04	1.100E-04
168	0.0139	0.1740	2.150E-04	1.156E-04
174	0.0122	0.1757	2.023E-04	1.013E-04
180	0.0107	0.1773	2.011E-04	9.894E-05
186	0.0093	0.1785	2.006E-04	1.115E-04
192	0.0083	0.1798	2.101E-04	8.763E-05
198	0.0074	0.1805	2.163E-04	7.490E-05
204	0.0067	0.1812	2.283E-04	8.659E-05
210	0.0060	0.1819	2.217E-04	7.546E-05
216	0.0055	0.1824	2.268E-04	8.080E-05
222	0.0051	0.1828	2.158E-04	7.394E-05
228	0.0048	0.1832	2.333E-04	6.608E-05
234	0.0046	0.1834	2.246E-04	7.324E-05
240	0.0043	0.1836	2.367E-04	8.053E-05
246	0.0041	0.1837	2.317E-04	6.759E-05
252	0.0039	0.1839	2.301E-04	8.108E-05
258	0.0040	0.1840	2.361E-04	6.121E-05
264	0.0038	0.1841	2.439E-04	7.320E-05
270	0.0039	0.1842	2.270E-04	6.188E-05
276	0.0038	0.1841	2.295E-04	7.057E-05
282	0.0038	0.1842	2.321E-04	6.816E-05
288	0.0037	0.1842	2.380E-04	6.899E-05
294	0.0036	0.1842	2.295E-04	6.813E-05

e8

time (min)	[1bu]	[E2bu]	[Ru(acn)]	[Ru(1bu)]
0	0.1531	0.0495	1.142E-04	2.531E-04
2	0.1430	0.0584	1.112E-04	2.407E-04
4	0.1342	0.0665	1.121E-04	2.576E-04
6	0.1261	0.0747	1.067E-04	2.344E-04
8	0.1182	0.0826	1.118E-04	2.352E-04
10	0.1106	0.0901	1.222E-04	2.248E-04
12	0.1032	0.0974	1.269E-04	2.205E-04
14	0.0959	0.1044	1.147E-04	2.110E-04
16	0.0888	0.1112	1.243E-04	2.179E-04
18	0.0824	0.1179	1.346E-04	2.184E-04
20	0.0761	0.1242	1.352E-04	2.125E-04
22	0.0699	0.1302	1.400E-04	2.055E-04
24	0.0640	0.1361	1.519E-04	2.106E-04
26	0.0587	0.1417	1.690E-04	2.009E-04
28	0.0532	0.1470	1.609E-04	1.738E-04
30	0.0482	0.1522	1.552E-04	1.815E-04
32	0.0436	0.1568	1.673E-04	1.803E-04
34	0.0391	0.1612	1.801E-04	1.950E-04
36	0.0349	0.1653	1.650E-04	1.809E-04
38	0.0311	0.1692	1.969E-04	1.838E-04
40	0.0277	0.1726	1.860E-04	1.617E-04
42	0.0249	0.1758	1.886E-04	1.430E-04
44	0.0217	0.1787	1.883E-04	1.675E-04
46	0.0191	0.1812	1.990E-04	1.327E-04
48	0.0169	0.1837	2.238E-04	1.410E-04
50	0.0150	0.1856	2.237E-04	1.228E-04
52	0.0133	0.1876	2.229E-04	1.336E-04
54	0.0118	0.1890	2.324E-04	1.389E-04
56	0.0105	0.1904	2.414E-04	1.464E-04
58	0.0093	0.1915	2.265E-04	1.141E-04
60	0.0086	0.1923	2.319E-04	1.236E-04
62	0.0078	0.1932	2.551E-04	1.152E-04
64	0.0071	0.1937	2.315E-04	1.201E-04
66	0.0066	0.1943	2.291E-04	1.096E-04
68	0.0063	0.1946	2.335E-04	1.144E-04
70	0.0061	0.1951	2.454E-04	1.142E-04
72	0.0057	0.1954	2.292E-04	1.046E-04
74	0.0055	0.1956	2.576E-04	9.806E-05
76	0.0054	0.1959	2.438E-04	9.507E-05
78	0.0052	0.1959	2.540E-04	1.091E-04
80	0.0051	0.1960	2.428E-04	1.146E-04
82	0.0050	0.1962	2.302E-04	8.304E-05
84	0.0051	0.1964	2.529E-04	9.527E-05
86	0.0050	0.1963	2.462E-04	9.683E-05
88	0.0049	0.1964	2.515E-04	7.505E-05
90	0.0048	0.1965	2.437E-04	8.544E-05
92	0.0047	0.1964	2.564E-04	1.274E-04

e9

time (min)	[1bu]	[E2bu]	[Ru(acn)]	[Ru(1bu)]
0	0.1591	0.0391	1.380E-04	2.756E-04
2	0.1487	0.0489	1.206E-04	2.707E-04
4	0.1390	0.0581	1.317E-04	2.675E-04
6	0.1301	0.0673	1.469E-04	2.888E-04
8	0.1213	0.0759	1.332E-04	2.501E-04
10	0.1128	0.0842	1.433E-04	2.619E-04
12	0.1047	0.0924	1.454E-04	2.718E-04
14	0.0970	0.1001	1.407E-04	2.523E-04
16	0.0895	0.1075	1.629E-04	2.252E-04
18	0.0823	0.1148	1.784E-04	2.319E-04
20	0.0755	0.1216	1.795E-04	2.378E-04
22	0.0690	0.1281	1.652E-04	2.053E-04
24	0.0627	0.1344	2.054E-04	2.339E-04
26	0.0566	0.1402	1.896E-04	2.251E-04
28	0.0513	0.1459	1.976E-04	2.130E-04
30	0.0460	0.1509	2.037E-04	2.023E-04
32	0.0413	0.1559	1.855E-04	2.134E-04
34	0.0369	0.1603	2.191E-04	1.932E-04
36	0.0325	0.1643	2.132E-04	1.874E-04
38	0.0289	0.1682	2.201E-04	1.793E-04
40	0.0253	0.1716	2.282E-04	1.885E-04
42	0.0223	0.1748	2.220E-04	1.394E-04
44	0.0196	0.1775	2.545E-04	1.607E-04
46	0.0173	0.1799	2.378E-04	1.466E-04
48	0.0150	0.1819	2.602E-04	1.635E-04
50	0.0132	0.1838	2.405E-04	1.601E-04
52	0.0117	0.1853	2.443E-04	1.254E-04
54	0.0104	0.1867	2.743E-04	1.353E-04
56	0.0092	0.1876	2.689E-04	1.146E-04
58	0.0083	0.1885	2.658E-04	1.283E-04
60	0.0078	0.1894	2.947E-04	1.375E-04
62	0.0069	0.1899	2.805E-04	1.180E-04
64	0.0068	0.1904	2.692E-04	1.346E-04
66	0.0063	0.1908	2.705E-04	1.212E-04
68	0.0060	0.1911	2.735E-04	1.181E-04
70	0.0057	0.1914	2.932E-04	1.255E-04
72	0.0053	0.1915	3.033E-04	1.118E-04
74	0.0053	0.1915	2.785E-04	1.162E-04
76	0.0052	0.1917	2.651E-04	1.263E-04
78	0.0051	0.1919	2.729E-04	1.233E-04
80	0.0053	0.1921	2.948E-04	1.175E-04
82	0.0049	0.1919	2.903E-04	1.083E-04
84	0.0048	0.1921	2.866E-04	9.200E-05
86	0.0048	0.1920	2.854E-04	1.222E-04
88	0.0048	0.1921	2.932E-04	9.840E-05
90	0.0048	0.1923	2.889E-04	9.622E-05
92	0.0048	0.1922	3.052E-04	1.200E-04

d3

time (min)	[1bu]	[E2bu]	[Ru(acn)]	[Ru(1bu)]
0	0.2116	0.0284	1.334E-04	3.042E-04
8	0.1944	0.0433	1.426E-04	3.032E-04
16	0.1799	0.0577	1.437E-04	2.915E-04
24	0.1660	0.0718	1.514E-04	2.908E-04
32	0.1521	0.0854	1.430E-04	2.811E-04
40	0.1389	0.0988	1.636E-04	2.815E-04
48	0.1262	0.1117	1.709E-04	2.716E-04
56	0.1137	0.1241	1.717E-04	2.511E-04
64	0.1020	0.1361	1.868E-04	2.636E-04
72	0.0905	0.1474	1.983E-04	2.444E-04
80	0.0797	0.1584	2.012E-04	2.323E-04
88	0.0697	0.1685	2.135E-04	2.252E-04
96	0.0600	0.1784	2.230E-04	2.251E-04
104	0.0511	0.1873	2.300E-04	2.149E-04
112	0.0431	0.1954	2.403E-04	1.957E-04
120	0.0357	0.2028	2.581E-04	1.905E-04
128	0.0293	0.2093	2.613E-04	1.780E-04
136	0.0236	0.2151	2.800E-04	1.694E-04
144	0.0189	0.2201	2.894E-04	1.575E-04
152	0.0149	0.2240	3.104E-04	1.405E-04
160	0.0117	0.2272	3.100E-04	1.158E-04
168	0.0094	0.2297	3.261E-04	1.365E-04
176	0.0078	0.2315	3.358E-04	1.178E-04
184	0.0066	0.2326	3.271E-04	1.071E-04
192	0.0057	0.2335	3.472E-04	1.041E-04
200	0.0052	0.2340	3.528E-04	1.105E-04
208	0.0048	0.2344	3.470E-04	9.847E-05
216	0.0046	0.2346	3.536E-04	9.821E-05
224	0.0045	0.2347	3.504E-04	9.202E-05
232	0.0045	0.2350	3.510E-04	9.700E-05
240	0.0043	0.2349	3.589E-04	9.609E-05
248	0.0043	0.2350	3.532E-04	9.330E-05
256	0.0042	0.2350	3.494E-04	1.064E-04
264	0.0044	0.2353	3.450E-04	1.016E-04
272	0.0043	0.2352	3.517E-04	9.635E-05
280	0.0043	0.2352	3.474E-04	9.565E-05
288	0.0043	0.2353	3.517E-04	9.297E-05
296	0.0043	0.2352	3.602E-04	8.511E-05
304	0.0042	0.2352	3.566E-04	1.011E-04
312	0.0043	0.2353	3.449E-04	9.915E-05

d4

time (min)	[1bu]	[E2bu]	[Ru(acn)]	[Ru(1bu)]
0	0.2284	0.0129	1.428E-04	3.108E-04
16	0.2191	0.0222	1.282E-04	2.896E-04
32	0.2101	0.0314	1.245E-04	3.028E-04
48	0.2015	0.0404	1.305E-04	2.893E-04
64	0.1930	0.0492	1.535E-04	2.857E-04
80	0.1846	0.0578	1.447E-04	2.744E-04
96	0.1762	0.0661	1.526E-04	2.774E-04
112	0.1681	0.0745	1.531E-04	2.742E-04
128	0.1599	0.0827	1.487E-04	2.769E-04
144	0.1518	0.0907	1.595E-04	2.659E-04
160	0.1442	0.0988	1.539E-04	2.656E-04
176	0.1364	0.1064	1.614E-04	2.676E-04
192	0.1288	0.1142	1.518E-04	2.639E-04
208	0.1214	0.1217	1.638E-04	2.674E-04
224	0.1142	0.1294	1.781E-04	2.512E-04
240	0.1069	0.1367	1.855E-04	2.507E-04
256	0.0998	0.1437	1.768E-04	2.451E-04
272	0.0931	0.1509	1.986E-04	2.455E-04
288	0.0865	0.1577	1.885E-04	2.457E-04
304	0.0800	0.1642	1.903E-04	2.268E-04
320	0.0738	0.1705	2.084E-04	2.256E-04
336	0.0677	0.1768	2.101E-04	2.203E-04
352	0.0619	0.1827	2.123E-04	2.221E-04
368	0.0563	0.1885	2.183E-04	2.188E-04
384	0.0510	0.1939	2.341E-04	2.034E-04
400	0.0458	0.1992	2.349E-04	2.055E-04
416	0.0409	0.2042	2.393E-04	1.895E-04
432	0.0366	0.2087	2.578E-04	1.848E-04
448	0.0323	0.2132	2.544E-04	1.810E-04
464	0.0283	0.2173	2.644E-04	1.758E-04
480	0.0248	0.2209	2.774E-04	1.607E-04
496	0.0215	0.2243	2.793E-04	1.654E-04
512	0.0185	0.2273	2.954E-04	1.537E-04
528	0.0160	0.2300	3.031E-04	1.379E-04
544	0.0135	0.2327	3.118E-04	1.484E-04
560	0.0115	0.2346	3.189E-04	1.300E-04
576	0.0100	0.2363	3.208E-04	1.238E-04
592	0.0086	0.2378	3.314E-04	1.158E-04
608	0.0074	0.2392	3.344E-04	1.175E-04
624	0.0066	0.2399	3.326E-04	1.054E-04

d5

time (min)	[1bu]	[E2bu]	[Ru(acn)]	[Ru(1bu)]
0	0.1965	0.0408	1.192E-04	2.902E-04
4	0.1746	0.0634	1.324E-04	2.797E-04
8	0.1531	0.0849	1.425E-04	2.784E-04
12	0.1327	0.1052	1.534E-04	2.572E-04
16	0.1134	0.1244	1.679E-04	2.580E-04
20	0.0954	0.1425	1.832E-04	2.360E-04
24	0.0788	0.1591	1.930E-04	2.311E-04
28	0.0637	0.1744	2.118E-04	2.296E-04
32	0.0502	0.1880	2.233E-04	1.985E-04
36	0.0386	0.1997	2.592E-04	1.915E-04
40	0.0287	0.2096	2.631E-04	1.693E-04
44	0.0210	0.2174	2.883E-04	1.487E-04
48	0.0153	0.2232	3.073E-04	1.376E-04
52	0.0113	0.2273	3.230E-04	1.277E-04
56	0.0087	0.2299	3.280E-04	1.159E-04
60	0.0072	0.2315	3.381E-04	9.642E-05
64	0.0063	0.2324	3.408E-04	9.486E-05
68	0.0059	0.2329	3.254E-04	9.653E-05
72	0.0057	0.2331	3.354E-04	9.375E-05
76	0.0054	0.2333	3.453E-04	9.020E-05
80	0.0053	0.2334	3.478E-04	9.230E-05
84	0.0054	0.2335	3.468E-04	1.019E-04
88	0.0054	0.2335	3.483E-04	9.500E-05
92	0.0053	0.2335	3.480E-04	8.022E-05
96	0.0053	0.2335	3.369E-04	8.381E-05
100	0.0053	0.2335	3.369E-04	9.033E-05
104	0.0054	0.2337	3.378E-04	9.257E-05
108	0.0053	0.2336	3.516E-04	9.714E-05
112	0.0053	0.2336	3.327E-04	7.825E-05
116	0.0054	0.2336	3.381E-04	9.537E-05
120	0.0053	0.2336	3.466E-04	8.899E-05
124	0.0053	0.2337	3.334E-04	9.872E-05
128	0.0053	0.2337	3.380E-04	8.970E-05
132	0.0053	0.2336	3.363E-04	9.137E-05
136	0.0053	0.2336	3.296E-04	1.014E-04

d6

time (min)	[1bu]	[E2bu]	[Ru(acn)]	[Ru(1bu)]
0	0.1729	0.0626	1.318E-04	2.673E-04
4	0.1524	0.0835	1.272E-04	2.684E-04
8	0.1324	0.1032	1.532E-04	2.448E-04
12	0.1136	0.1220	1.553E-04	2.303E-04
16	0.0960	0.1396	1.648E-04	2.278E-04
20	0.0796	0.1561	1.870E-04	2.225E-04
24	0.0647	0.1710	1.895E-04	1.965E-04
28	0.0514	0.1844	2.165E-04	1.848E-04
32	0.0397	0.1961	2.297E-04	1.792E-04
36	0.0299	0.2059	2.460E-04	1.560E-04
40	0.0221	0.2138	2.756E-04	1.497E-04
44	0.0160	0.2199	2.881E-04	1.254E-04
48	0.0117	0.2242	2.923E-04	1.182E-04
52	0.0091	0.2269	3.102E-04	1.023E-04
56	0.0074	0.2286	3.180E-04	9.552E-05
60	0.0064	0.2297	3.115E-04	8.910E-05
64	0.0058	0.2303	3.278E-04	7.888E-05
68	0.0055	0.2305	3.233E-04	7.916E-05
72	0.0054	0.2308	3.366E-04	8.546E-05
76	0.0053	0.2308	3.196E-04	8.637E-05
80	0.0052	0.2309	3.229E-04	9.051E-05
84	0.0053	0.2309	3.363E-04	9.467E-05
88	0.0052	0.2309	3.299E-04	7.555E-05
92	0.0052	0.2309	3.262E-04	7.704E-05

d7

time (min)	[1bu]	[E2bu]	[Ru(acn)]	[Ru(1bu)]
0	0.1785	0.0275	1.477E-04	3.002E-04
4	0.1549	0.0468	1.607E-04	2.878E-04
8	0.1364	0.0655	1.817E-04	2.801E-04
12	0.1190	0.0834	1.924E-04	2.691E-04
16	0.1024	0.1003	2.070E-04	2.569E-04
20	0.0869	0.1163	2.196E-04	2.471E-04
24	0.0725	0.1312	2.198E-04	2.417E-04
28	0.0592	0.1448	2.296E-04	2.301E-04
32	0.0472	0.1571	2.418E-04	2.204E-04
36	0.0367	0.1680	2.546E-04	2.011E-04
40	0.0277	0.1772	2.695E-04	1.883E-04
44	0.0204	0.1846	2.856E-04	1.636E-04
48	0.0148	0.1903	3.029E-04	1.500E-04
52	0.0108	0.1945	3.191E-04	1.332E-04
56	0.0082	0.1971	3.290E-04	1.244E-04
60	0.0066	0.1987	3.294E-04	1.137E-04
64	0.0057	0.1997	3.435E-04	1.071E-04
68	0.0052	0.2002	3.469E-04	1.064E-04
72	0.0049	0.2004	3.481E-04	1.047E-04
76	0.0047	0.2006	3.434E-04	1.044E-04
80	0.0047	0.2007	3.455E-04	1.077E-04
84	0.0046	0.2007	3.432E-04	1.030E-04
88	0.0047	0.2007	3.484E-04	9.873E-05
92	0.0046	0.2008	3.467E-04	1.014E-04

d8

time (min)	[1bu]	[E2bu]	[Ru(acn)]	[Ru(1bu)]
0	0.1633	0.0457	1.595E-04	2.976E-04
1	0.1559	0.0604	1.572E-04	2.818E-04
2	0.1453	0.0743	1.727E-04	2.842E-04
3	0.1333	0.0880	1.639E-04	2.834E-04
4	0.1209	0.1012	1.694E-04	2.661E-04
5	0.1088	0.1137	1.924E-04	2.647E-04
6	0.0971	0.1253	1.916E-04	2.507E-04
7	0.0862	0.1365	2.141E-04	2.500E-04
8	0.0754	0.1470	2.264E-04	2.295E-04
9	0.0657	0.1568	1.932E-04	2.352E-04
10	0.0566	0.1657	2.294E-04	2.055E-04
11	0.0481	0.1742	2.450E-04	2.134E-04
12	0.0404	0.1817	2.603E-04	2.076E-04
13	0.0336	0.1884	2.563E-04	2.157E-04
14	0.0277	0.1944	2.658E-04	1.863E-04
15	0.0229	0.1994	2.794E-04	1.571E-04
16	0.0188	0.2034	2.882E-04	1.367E-04
17	0.0155	0.2069	2.942E-04	1.477E-04
18	0.0128	0.2094	3.100E-04	1.198E-04
19	0.0109	0.2115	3.184E-04	1.316E-04
20	0.0093	0.2127	3.216E-04	1.220E-04
21	0.0083	0.2142	3.243E-04	1.303E-04
22	0.0077	0.2148	3.554E-04	1.380E-04
23	0.0071	0.2150	3.492E-04	1.267E-04
24	0.0068	0.2155	3.400E-04	1.366E-04
25	0.0066	0.2159	3.238E-04	1.386E-04
26	0.0063	0.2158	3.492E-04	1.229E-04
27	0.0063	0.2161	3.611E-04	1.364E-04
28	0.0063	0.2159	3.437E-04	9.905E-05
29	0.0062	0.2161	3.358E-04	1.106E-04
30	0.0059	0.2161	3.436E-04	9.817E-05
31	0.0061	0.2160	3.404E-04	1.210E-04
32	0.0060	0.2161	3.290E-04	1.022E-04
33	0.0061	0.2162	3.388E-04	1.094E-04
34	0.0061	0.2160	3.455E-04	1.125E-04

d9

time (min)	[1bu]	[E2bu]	[Ru(acn)]	[Ru(1bu)]
0	0.1565	0.0390	1.720E-04	2.708E-04
1	0.1407	0.0503	1.921E-04	2.695E-04
2	0.1284	0.0618	1.871E-04	2.604E-04
3	0.1169	0.0729	1.994E-04	2.588E-04
4	0.1061	0.0838	2.086E-04	2.524E-04
5	0.0960	0.0945	2.234E-04	2.549E-04
6	0.0860	0.1047	2.399E-04	2.413E-04
7	0.0766	0.1142	2.392E-04	2.366E-04

8	0.0676	0.1231	2.304E-04	2.286E-04
9	0.0593	0.1318	2.432E-04	2.268E-04
10	0.0515	0.1397	2.524E-04	2.070E-04
11	0.0443	0.1470	2.563E-04	2.091E-04
12	0.0377	0.1536	2.519E-04	1.966E-04
13	0.0318	0.1596	2.643E-04	1.920E-04
14	0.0267	0.1648	2.793E-04	1.788E-04
15	0.0220	0.1695	2.886E-04	1.695E-04
16	0.0181	0.1733	2.993E-04	1.635E-04
17	0.0150	0.1765	3.014E-04	1.544E-04
18	0.0124	0.1791	3.028E-04	1.410E-04
19	0.0104	0.1811	3.194E-04	1.310E-04
20	0.0089	0.1825	3.287E-04	1.318E-04
21	0.0078	0.1836	3.291E-04	1.187E-04
22	0.0070	0.1845	3.160E-04	1.205E-04
23	0.0064	0.1850	3.308E-04	1.143E-04
24	0.0060	0.1854	3.381E-04	1.121E-04
25	0.0057	0.1856	3.346E-04	9.578E-05
26	0.0055	0.1857	3.449E-04	9.943E-05
27	0.0054	0.1859	3.393E-04	1.060E-04
28	0.0054	0.1860	3.388E-04	1.005E-04
29	0.0053	0.1860	3.347E-04	1.024E-04
30	0.0052	0.1859	3.431E-04	9.670E-05
31	0.0052	0.1860	3.432E-04	9.630E-05
32	0.0052	0.1860	3.239E-04	9.445E-05
33	0.0053	0.1860	3.357E-04	1.012E-04
34	0.0052	0.1861	3.507E-04	9.608E-05
35	0.0052	0.1860	3.461E-04	9.723E-05
36	0.0052	0.1859	3.458E-04	9.694E-05
37	0.0053	0.1861	3.343E-04	9.781E-05
38	0.0053	0.1860	3.440E-04	9.723E-05
39	0.0052	0.1860	3.460E-04	1.024E-04

d10

time (min)	[1bu]	[E2bu]	[Ru(acn)]	[Ru(1bu)]
0	0.2034	0.0190	1.320E-04	2.987E-04
16	0.1939	0.0288	1.355E-04	2.946E-04
32	0.1844	0.0384	1.399E-04	2.888E-04
48	0.1753	0.0476	1.433E-04	2.872E-04
64	0.1664	0.0566	1.470E-04	2.856E-04
80	0.1578	0.0654	1.536E-04	2.738E-04
96	0.1493	0.0740	1.542E-04	2.766E-04
112	0.1410	0.0824	1.609E-04	2.706E-04
128	0.1330	0.0906	1.711E-04	2.678E-04
144	0.1250	0.0986	1.695E-04	2.625E-04
160	0.1171	0.1065	1.731E-04	2.604E-04
176	0.1093	0.1142	1.775E-04	2.557E-04
192	0.1018	0.1218	1.851E-04	2.520E-04
208	0.0945	0.1292	1.848E-04	2.471E-04
224	0.0874	0.1364	1.969E-04	2.434E-04
240	0.0804	0.1434	1.982E-04	2.341E-04
256	0.0739	0.1501	2.078E-04	2.313E-04
272	0.0674	0.1566	2.117E-04	2.277E-04
288	0.0613	0.1628	2.187E-04	2.214E-04
304	0.0555	0.1688	2.267E-04	2.148E-04
320	0.0498	0.1743	2.313E-04	2.060E-04
336	0.0445	0.1797	2.451E-04	2.029E-04
352	0.0394	0.1847	2.500E-04	1.969E-04
368	0.0349	0.1895	2.621E-04	1.840E-04
384	0.0306	0.1940	2.636E-04	1.743E-04
400	0.0266	0.1980	2.735E-04	1.709E-04
416	0.0229	0.2017	2.904E-04	1.574E-04
432	0.0197	0.2050	3.053E-04	1.518E-04
448	0.0167	0.2080	3.075E-04	1.514E-04
464	0.0142	0.2105	3.169E-04	1.391E-04
480	0.0120	0.2127	3.258E-04	1.330E-04
496	0.0102	0.2146	3.302E-04	1.252E-04
512	0.0086	0.2162	3.393E-04	1.163E-04
528	0.0074	0.2175	3.500E-04	1.113E-04
544	0.0064	0.2184	3.560E-04	1.010E-04
560	0.0056	0.2193	3.520E-04	1.028E-04
576	0.0050	0.2198	3.570E-04	1.014E-04
592	0.0046	0.2204	3.716E-04	9.779E-05
608	0.0043	0.2207	3.669E-04	9.485E-05
624	0.0040	0.2210	3.650E-04	9.423E-05
640	0.0038	0.2212	3.725E-04	9.109E-05
656	0.0037	0.2213	3.688E-04	9.418E-05
672	0.0036	0.2213	3.733E-04	9.349E-05
688	0.0035	0.2215	3.692E-04	9.256E-05
704	0.0035	0.2216	3.686E-04	8.634E-05

2.9.3. Isomerization of 2Z

2.9.3.1. Summary

Summary of initial conditions

run no.	[cat] stock M	$[cat]_0$ mM	$[Z2bu]_0^{21°C}$ mM	cat. loading mol%	T_{avg} °C	T_{avg} K
M46	0.0199	5.0	12.8	39%	60.0	333.15
M47	0.0099	9.9	25.3	39%	70.0	343.15
M48	0.0099	4.9	25.3	20%	70.0	343.15
M49	0.0103	10.3	25.3	41%	50.4	323.50
M50	0.0101	10.1	25.3	40%	65.2	338.35
M51	0.0101	5.0	25.3	20%	65.2	338.35

M46

M46	normalized integrations		
hours	E (6H)	Z (6H)	1 (Σ 5H)
0.00	1.0682	13.4118	0.00000
0.75	1.9884	12.4231	0.02879
1.50	2.9749	11.5199	0.07148
5.53	6.9135	7.4444	0.22834
20.27	9.0030	4.6679	0.33884

M47

M47	normalized integrations		
hours	E (6H)	Z (6H)	1 (Σ 5H)
0.000	0.6216	6.9773	0.00000
0.383	1.4580	6.0876	0.01954
0.717	2.0798	5.3899	0.04109
1.617	3.3873	4.0856	0.10517
2.400	3.9568	3.2931	0.12572
3.750	4.6481	2.7502	0.14423
6.517	4.6219	2.5353	0.15241

M48

M48	normalized integrations		
hours	E (6H)	Z (6H)	1 (Σ 5H)
0.000	1.5311	19.8558	0.00000
0.667	4.1535	17.0819	0.10737
1.067	5.4015	15.7564	0.16480
1.650	6.9354	14.1904	0.21843
2.433	8.5913	12.5644	0.28511
3.783	10.3675	10.2344	0.35368
6.550	12.2187	8.5669	0.44096
8.083	12.1267	8.2024	0.44398

M49

M49	normalized integrations		
hours	E (6H)	Z (6H)	1 (Σ 5H)
0.000	0.2935	3.5727	0.00000
0.783	0.4978	3.3645	0.00946
1.650	0.7083	3.1431	0.00998
3.133	1.0348	2.8131	0.02182
4.033	1.1996	2.6268	0.03037
4.900	1.3476	2.4802	0.03406
6.333	1.5429	2.2414	0.04144
8.983	1.8928	1.9134	0.05450
11.317	2.0833	1.6932	0.05963
24.233	2.3761	1.2463	0.07468
28.817	2.4758	1.2549	0.07176

M50

M50	normalized integrations		
hours	E (6H)	Z (6H)	1 (Σ 5H)
0.000	0.7917	10.2310	0.00000
0.517	1.8940	8.8802	0.01196
1.267	3.3168	7.5141	0.08595
2.017	4.5571	6.5621	0.09310
2.567	5.0185	5.9141	0.13540
2.950	5.4748	5.6319	0.13354
3.433	5.7888	5.1494	0.17734
4.417	6.3487	4.5397	0.18133
5.400	6.6963	4.2199	0.20032
6.200	6.8812	4.0659	0.18109
7.750	6.9752	3.9252	0.19505

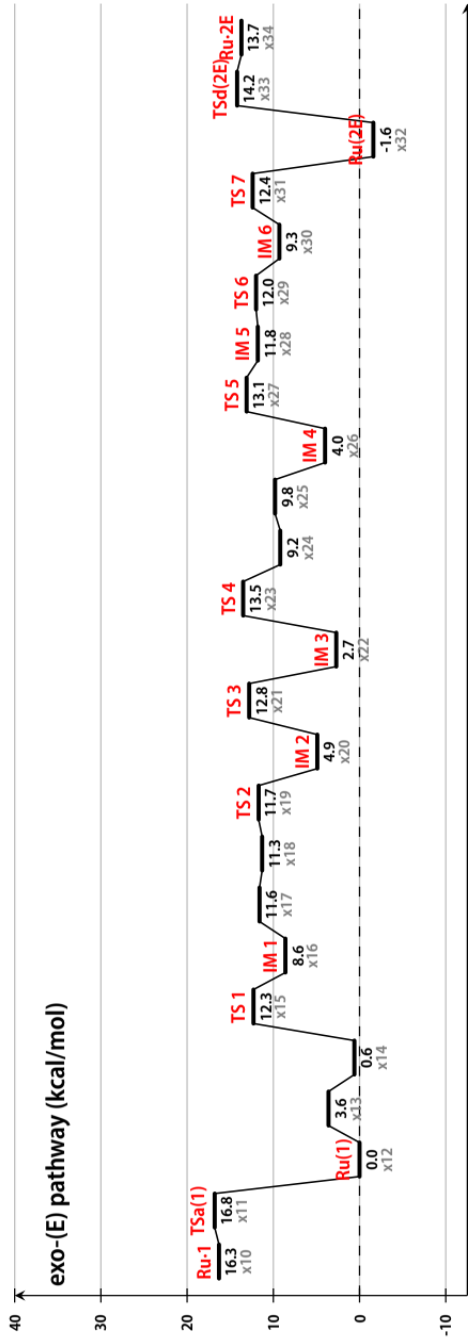
M51

M51		normalized integrations	
hours	E (6H)	Z (6H)	1 (Σ 5H)
0.000	1.7211	20.5052	0.00000
0.517	3.5201	18.8026	0.06229
1.267	5.8018	16.1247	0.16357
2.017	7.9339	14.5669	0.24950
2.567	9.1751	13.4935	0.30991
3.650	10.9865	11.4769	0.36914
4.633	12.2131	9.8799	0.39166
5.617	12.9592	9.2163	0.42992
6.417	13.5746	8.6312	0.47045
7.967	14.0769	7.9629	0.49612

2.9.4. DFT data

All structures in η^3-allyl pathways are referenced to **Ru(1)** (index x12). Values in tables are in kcal/mol.

2.9.4.1. Ru(η^3-allyl), exo-(E/Z) pathway



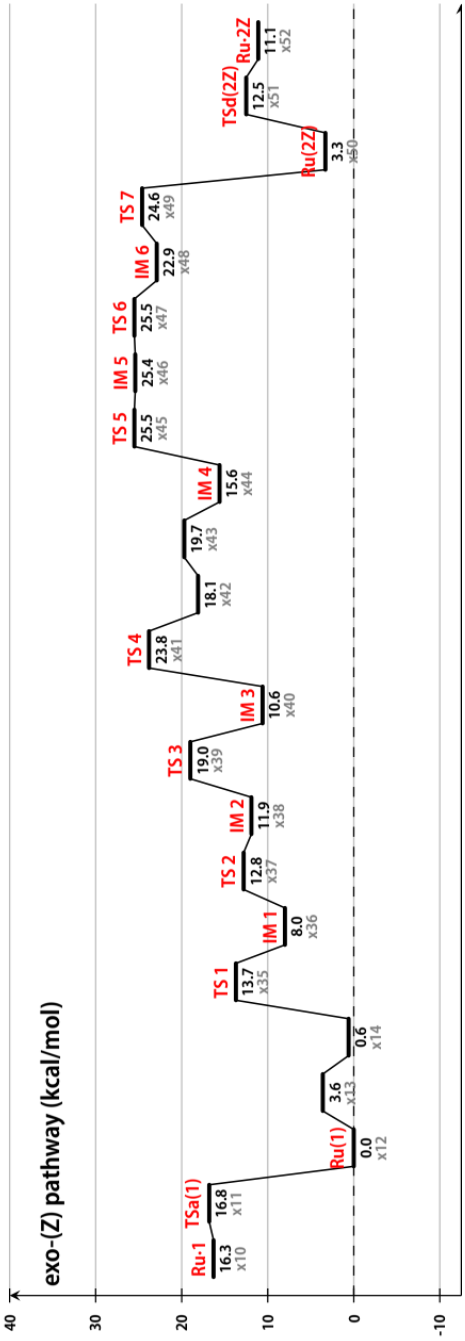


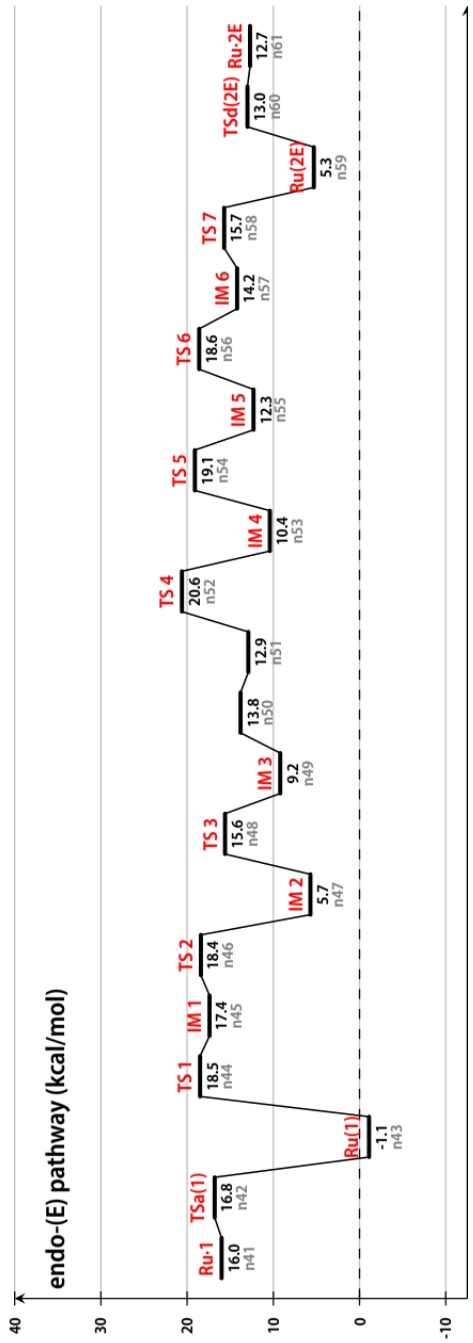
Table 10. Thermodynamic data for exo-(*E*) pathway

filename	index	ZPE	TE	TH	TG	G_solv	label
hu110a-huf15b	x10	17.31	17.96	17.96	16.03	16.33	Ru·1
hu110t-huf15	x11	17.55	17.89	17.89	16.46	16.78	TSa(1)
hu111a-huf51a	x12	0.00	0.00	0.00	0.00	0.00	Ru(1)
hu111t-huf51	x13	3.05	2.63	2.63	3.51	3.56	
hu210a-huf17a	x14	0.91	1.03	1.03	0.73	0.63	
hu210t-huf17	x15	12.30	12.15	12.15	11.89	12.29	TS 1
hu210z-huf17b	x16	8.73	8.58	8.58	8.30	8.58	IM 1
hu220t-huf19	x17	10.83	10.34	10.34	11.27	11.57	
hu220z-huf19b	x18	11.23	11.01	11.01	11.07	11.30	
hu221t-huf45	x19	11.09	10.44	10.44	11.62	11.66	TS 2
hu230a-huf55a	x20	5.76	5.85	5.85	4.96	4.86	IM 2
hu230t-huf55	x21	12.46	12.27	12.27	12.51	12.80	TS 3
hu310a-huf57a	x22	5.14	5.17	5.17	4.63	2.73	IM 3
hu310t-huf57	x23	14.51	13.86	13.86	15.56	13.53	TS 4
hu320a-huf59a	x24	11.05	10.96	10.96	11.01	9.23	
hu320t-huf59	x25	11.20	10.76	10.76	11.36	9.79	
hu410a-huf61b	x26	6.45	6.57	6.57	5.53	4.00	IM 4
hu410t-huf61	x27	13.13	13.07	13.07	12.59	13.10	TS 5
hu420a-huf63a	x28	12.79	12.84	12.84	11.86	11.77	IM 5
hu420t-huf63	x29	12.76	12.64	12.64	11.99	11.95	TS 6
hu430a-huf65a	x30	10.58	10.77	10.77	9.36	9.27	IM 6
hu430t-huf65	x31	13.59	13.91	13.91	12.09	12.42	TS 7
hu510a-huf67a	x32	-1.80	-1.67	-1.67	-1.72	-1.56	Ru(2E)
hu510t-huf67	x33	15.90	16.53	16.53	13.70	14.18	TSd(2E)
hu510z-huf67b	x34	15.64	16.60	16.60	13.32	13.69	Ru·2E

Table 11. Thermodynamic data for exo-(*Z*) pathway

filename	index	ZPE	TE	TH	TG	G_solv	label
hu110a-huf15b	x10	17.31	17.96	17.96	16.03	16.33	Ru·1
hu110t-huf15	x11	17.55	17.89	17.89	16.46	16.78	TSa(1)
hu111a-huf51a	x12	0.00	0.00	0.00	0.00	0.00	Ru(1)
hu111t-huf51	x13	3.05	2.63	2.63	3.51	3.56	
hu210a-huf17a	x14	0.91	1.03	1.03	0.73	0.63	
gu210t-guf15	x35	13.84	13.65	13.65	13.17	13.69	TS 1
gu220a-guf13a	x36	9.66	9.78	9.78	8.17	7.98	IM 1
gu220t-guf13	x37	13.02	12.71	12.71	13.10	12.82	TS 2
gu220z-guf13b	x38	12.13	12.03	12.03	12.13	11.91	IM 2
gu230t-guf11	x39	18.49	18.13	18.13	18.67	18.99	TS 3
gu230z-guf11b	x40	12.60	12.34	12.34	12.48	10.63	IM 3
gu310t-guf23	x41	23.74	22.87	22.87	25.37	23.80	TS 4
gu320a-guf25a	x42	19.46	19.24	19.24	19.75	18.06	
gu320t-guf25	x43	20.58	19.98	19.98	21.26	19.66	
gu410a-guf27b	x44	17.39	17.20	17.20	17.29	15.63	IM 4
gu410t-guf27	x45	24.71	24.28	24.28	24.99	25.52	TS 5
gu420a-guf35a	x46	25.60	25.49	25.49	24.97	25.40	IM 5
gu420t-guf35	x47	25.34	24.98	24.98	25.16	25.53	TS 6
gu420z-guf35b	x48	23.17	23.07	23.07	22.69	22.92	IM 6
gu430t-guf37	x49	24.86	24.75	24.75	24.16	24.64	TS 7
gu430z-guf37b	x50	2.29	2.31	2.31	2.95	3.30	Ru(2Z)
gu510t-guf39	x51	14.46	15.25	15.25	12.10	12.49	TSd(2Z)
gu510z-guf39b	x52	13.18	14.31	14.31	10.63	11.10	Ru·2Z

2.9.4.2. Ru(η³-allyl), endo-(E/Z) pathway



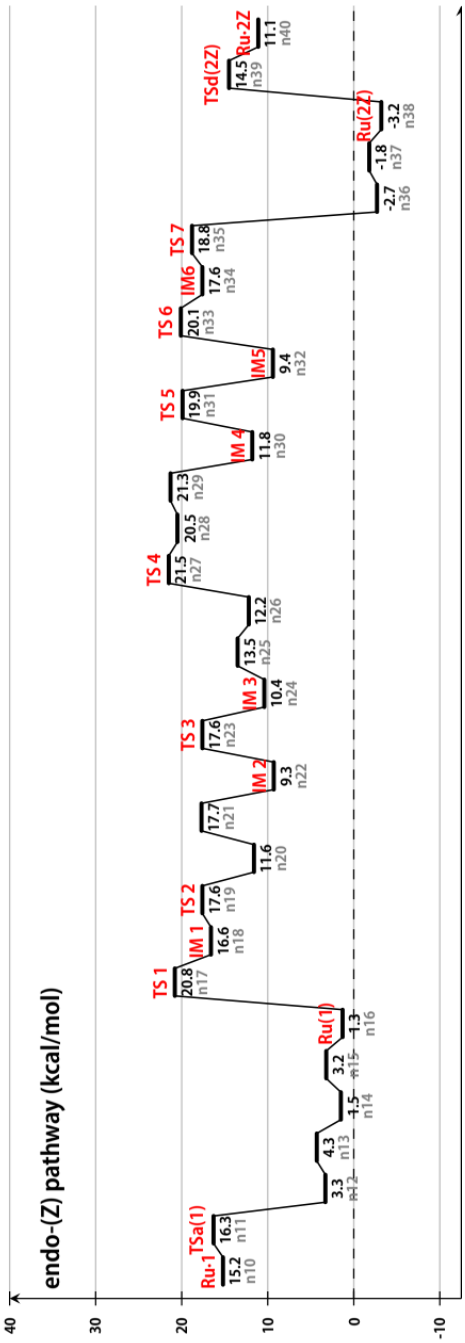


Table 12. Thermodynamic data for endo-(*E*) pathway.

filename	index	ZPE	TE	TH	TG	G_solv	label
ju110a-juf51b	n41	17.08	17.74	17.74	15.67	15.96	Ru·1
ju110t-juf51	n42	17.19	17.42	17.42	16.53	16.84	TSa(1)
ju110z-juf51a	n43	-0.68	-0.49	-0.49	-1.30	-1.13	Ru(1)
ju210t-juf11	n44	18.79	18.69	18.69	18.07	18.49	TS 1
ju220a-juf13b	n45	17.86	17.90	17.90	17.29	17.45	IM 1
ju220t-juf13	n46	18.63	18.38	18.38	18.45	18.42	TS 2
ju220z-juf13a	n47	6.07	5.70	5.70	6.07	5.73	IM 2
ju230t-jug21	n48	15.66	15.53	15.53	15.31	15.56	TS 3
ju230z-jug21a	n49	10.86	10.76	10.76	10.88	9.22	IM 3
ju250t	n50	15.12	14.53	14.53	15.67	13.78	
ju310a-juf25b	n51	14.74	14.58	14.58	14.73	12.92	
ju310t-juf25	n52	21.27	20.80	20.80	22.16	20.58	TS 4
ju410a-juf35a	n53	12.75	12.96	12.97	11.72	10.39	IM 4
ju410t-juf35	n54	19.16	19.08	19.08	18.65	19.13	TS 5
ju420a-juf37a	n55	12.89	12.80	12.80	12.61	12.32	IM 5
ju420t-juf37	n56	19.13	18.95	18.95	18.57	18.59	TS 6
ju420z-juf37b	n57	14.88	15.03	15.03	14.09	14.20	IM 6
ju430t-juf39	n58	16.34	16.48	16.48	15.33	15.72	TS 7
ju510a-jug43b	n59	5.13	5.36	5.36	4.86	5.33	Ru(2E)
ju510t-jug43	n60	14.38	15.05	15.05	12.74	12.96	TSd(2E)
ju510z-jug43a	n61	14.35	15.31	15.31	12.44	12.72	Ru·2E

Table 13. Thermodynamic data for endo-(*Z*) pathway.

filename	index	ZPE	TE	TH	TG	G_solv	label
iu110a-iuf19b	n10	16.28	16.94	16.94	14.71	15.22	Ru·1
iu110t-iuf19	n11	16.58	16.76	16.76	15.81	16.29	TSa(1)
iu110z-iuf19a	n12	2.68	2.49	2.49	3.12	3.34	
iu111t-iuf71	n13	3.05	2.48	2.48	3.97	4.27	
iu112a-iuf73a	n14	1.65	1.77	1.77	1.15	1.46	
iu112t-iuf73	n15	2.36	1.99	1.99	2.93	3.15	
iu210a-iuf21a	n16	0.87	0.88	0.88	0.96	1.29	Ru(1)
iu210t-iuf21	n17	21.37	21.12	21.12	21.32	20.79	TS 1
iu220a-iuf23a	n18	16.93	16.80	16.80	16.56	16.57	IM 1
iu220t-iuf23	n19	17.38	17.00	17.00	17.58	17.57	TS 2
iu221a-iuf25b	n20	12.16	11.93	11.93	11.76	11.57	
iu221t-iuf25	n21	17.18	16.40	16.40	17.75	17.70	
iu230a-iug21b	n22	10.15	9.98	9.98	9.35	9.27	IM 2
iu230t-iug21	n23	17.47	17.25	17.25	17.22	17.58	TS 3
iu230z-iug21a	n24	12.33	12.22	12.22	12.14	10.40	IM 3
iu310t-iuf29	n25	14.51	13.72	13.72	15.45	13.48	
iu310z-iuf29b	n26	14.34	14.08	14.08	14.35	12.20	
iu330t-iuf33	n27	22.45	21.83	21.83	23.28	21.54	TS 4
iu330z-iuf33a	n28	22.32	22.13	22.13	22.20	20.51	
iu340t-iuf35	n29	22.84	22.29	22.29	23.24	21.28	
iu410a-iuf37a	n30	14.16	14.21	14.21	13.47	11.83	IM 4
iu410t-iuf37	n31	19.68	19.48	19.48	19.45	19.89	TS 5
iu410z-iuf37b	n32	9.58	9.25	9.25	9.18	9.38	IM5
iu420t-iuf39	n33	21.08	20.93	20.93	20.05	20.12	TS 6
iu430a-iuf41a	n34	18.38	18.60	18.60	17.20	17.59	IM6
iu430t-iuf41	n35	19.42	19.64	19.64	18.18	18.81	TS 7
iu430z-iuf41b	n36	-1.75	-1.26	-1.26	-2.97	-2.74	
iu431t-iuf81	n37	-1.70	-1.76	-1.76	-2.01	-1.78	
iu431z-iuf81a	n38	-2.97	-2.83	-2.83	-3.33	-3.18	Ru(2Z)
iu510t-iuf43	n39	17.32	18.53	18.53	13.82	14.49	TSd(2Z)
iu510z-iuf43b	n40	13.19	14.33	14.33	10.65	11.13	Ru·2Z

2.9.4.3. Ru(η³-allyl) without hydride intermediate

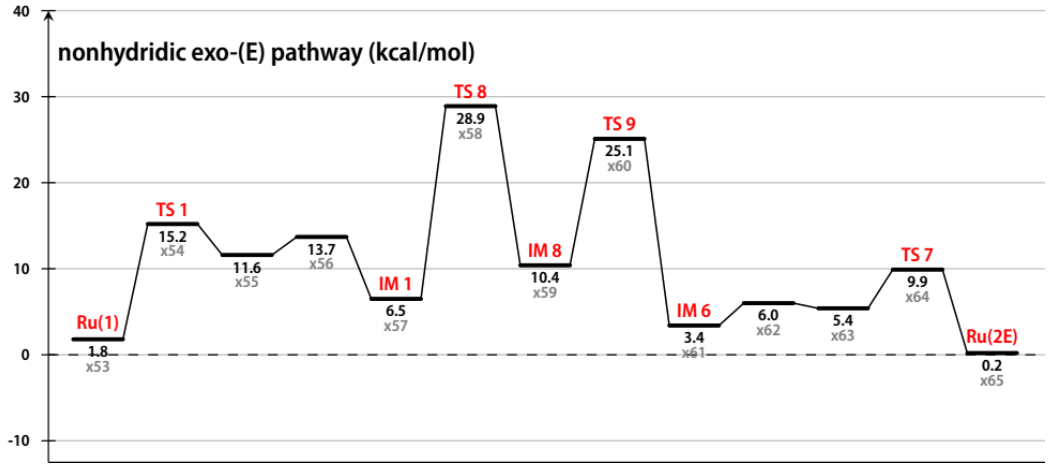


Figure 46. Energy diagram for η³-allyl mechanism without a hydride intermediate

Table 14. Thermodynamic data for η³-allyl mechanism without a hydride intermediate

filename	index	ZPE	TE	TH	TG	G_solv	label
au210a-auf73a	x53	1.90	1.96	1.96	1.80	1.84	Ru(1)
au210t-auf73	x54	16.08	15.93	15.93	15.42	15.15	TS 1
au210z-auf73b	x55	11.63	11.45	11.45	11.60	11.64	
au211t-aug51	x56	12.66	11.96	11.96	13.63	13.71	
au211z-aug51b	x57	8.00	8.10	8.10	6.39	6.45	IM 1
au220t-auf69	x58	29.17	29.02	29.02	28.72	28.87	TS 8
au410a-auf67a	x59	12.58	12.54	12.54	11.69	10.44	IM 8
au410t-auf67	x60	25.04	24.69	24.69	24.89	25.13	TS 9
au411a-aug61a	x61	3.93	3.94	3.94	3.35	3.35	IM 6
au411t-aug61	x62	5.68	5.00	5.00	6.15	6.02	
au420a-auf65a	x63	6.06	5.81	5.81	5.53	5.37	
au420t-auf65	x64	12.00	11.99	11.99	10.74	9.89	TS 7
au420z-auf65b	x65	0.26	0.39	0.39	0.08	0.18	Ru(2E)

2.9.4.4. Dissociation of acetonitrile

Table 15. Thermodynamic data for dissociation of acetonitrile

	ZPE	TE	TH	TG	G_{solv}	G_{solv}	label
exn15a	-1421.08	-1421.05	-1421.05	-1421.14	-1421.65	0.0	Ru·acn
exn15	-1421.05	-1421.01	-1421.01	-1421.12	-1421.62	16.4	TS
exn15b	-1421.05	-1421.01	-1421.01	-1421.12	-1421.62	15.5	Ru(acn)

2.9.4.5. η^1-allyl pathways

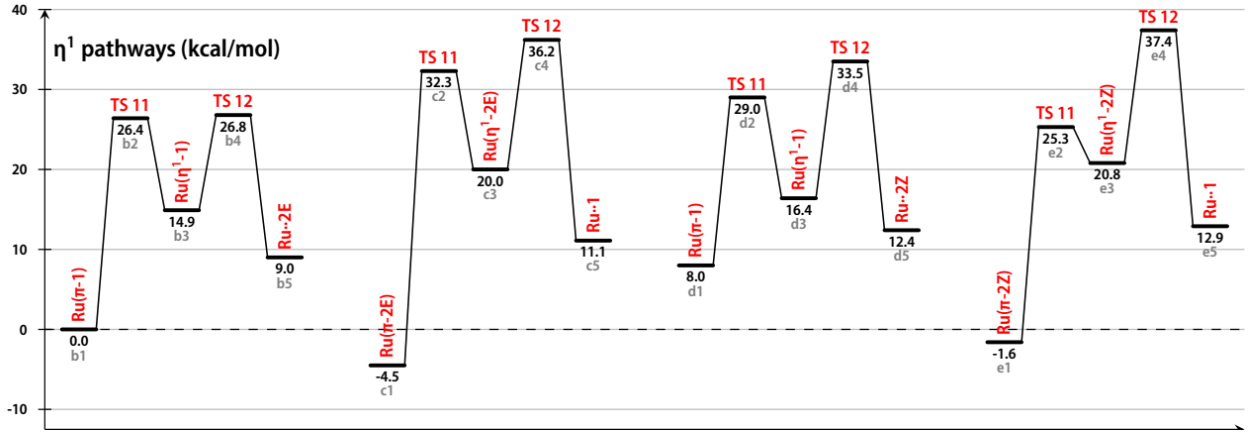


Figure 47. Energy diagram, η^1-allyl pathways.

Table 16. Thermodynamic data for η^1-allyl pathways.

filename	index	ZPE	TE	TH	TG	G_solv	role
η^1-allyl, 1 to 2E							
b1-buf51b	b1	0.00	0.00	0.00	0.00	0.00	Ru(π-1)
b2-buf51	b2	26.77	26.72	26.72	26.97	26.40	TS 11
b3-buf51a	b3	19.36	19.92	19.92	18.00	14.91	Ru(η1-1)
b4-buf53	b4	28.66	29.12	29.12	27.78	26.80	TS 12
b5-buf53a	b5	11.89	12.98	12.98	9.02	9.04	Ru··2E
η^1-allyl, 2E to 1							
c1-cuf61b	c1	-4.32	-4.18	-4.18	-4.44	-4.50	Ru(π-2E)
c2-cuf61	c2	33.09	32.89	32.89	33.38	32.31	TS 11
c3-cuf63b	c3	24.39	24.84	24.84	23.65	20.02	Ru(η1-2E)
c4-cuf63	c4	38.27	38.67	38.67	37.25	36.24	TS 12
c5-cuf63a	c5	13.84	14.94	14.94	10.83	11.15	Ru··1
η^1-allyl, to 2Z							
d1-duf71b	d1	6.90	6.57	6.57	7.72	7.98	Ru(π-1)
d2-duf71	d2	28.42	28.11	28.11	29.30	28.99	TS 11
d3-duf71a	d3	18.74	18.79	18.79	18.84	16.42	Ru(η1-1)
d4-duf73	d4	34.75	34.97	34.97	34.18	33.47	TS 12
d5-duf73a	d5	13.37	14.01	14.01	12.27	12.36	Ru··2Z
η^1-allyl, 2Z to 1							
e1-euf81b	e1	-1.98	-1.99	-1.99	-1.57	-1.58	Ru(π-2Z)
e2-euf81	e2	25.73	25.54	25.54	26.36	25.31	TS 11
e3-euf81a	e3	23.67	23.79	23.79	23.75	20.80	Ru(η1-2Z)
e4-eug81	e4	40.02	40.29	40.29	39.37	37.39	TS 12
e5-eug81a	e5	15.78	16.73	16.73	13.47	12.87	Ru··1

2.9.5. Coordinates of Optimized Geometries

All structures used in this work were fully optimized in the gas phase at the B3LYP[54]/cc-PVDz level with Grimme D2 dispersion.[51] The formatted checkpoint files obtained using Gaussian 09 Rev. D.01[55] for the gas phase optimized geometries of the computed structures in this work were converted to .xyz (Cartesian coordinate) using Open Babel[56], and stored in the tables that follows this section.

2.9.5.1. Acetonitrile dissociation

61			
exn15b exn15b.fchk			
Ru	-0.39034	-0.88780	0.77296
P	-1.82761	0.39385	-0.66980
C	-2.10705	2.20127	-0.30410
C	-0.79268	2.80609	0.20809
C	-2.68663	2.99075	-1.48180
C	-3.28070	-0.22405	-1.65177
C	-4.53454	-0.16684	-0.76767
C	-2.99122	-1.64326	-2.15375
C	-0.33341	0.29610	-1.72589
N	0.63911	-0.27584	-0.98344
C	1.79161	-0.29649	-1.74314
C	1.48383	0.25970	-2.96606
N	0.14700	0.62825	-2.94272
C	3.09910	-0.83516	-1.22412
C	2.90272	-2.30064	-0.79070
C	4.17153	-0.75615	-2.31879
C	3.52453	0.01413	-0.00925
C	-0.58853	1.24870	-4.03776
C	0.42213	-2.47519	2.05214
C	-1.02778	-2.47580	2.08434
C	-1.46279	-1.22872	2.62614
C	-0.29691	-0.41825	2.84219
C	0.86969	-1.21446	2.52016
H	-2.84200	2.18333	0.52089
H	-0.97301	3.83407	0.56287
H	-0.04889	2.85232	-0.60639
H	-0.35037	2.21725	1.02767
H	-1.97717	3.00992	-2.32620
H	-2.86328	4.03512	-1.17478
H	-3.64393	2.57609	-1.83502
H	-3.41174	0.45706	-2.51024
H	-4.75992	0.86019	-0.43646
H	-4.40943	-0.80261	0.12595
H	-5.40398	-0.54150	-1.33223
H	-2.10318	-1.67337	-2.80694
H	-2.81295	-2.32508	-1.30433
H	-3.85520	-2.02050	-2.72522
H	2.09634	0.41512	-3.84850
H	2.61546	-2.92893	-1.65024
H	3.84355	-2.69205	-0.37050
H	2.11417	-2.37069	-0.02668
H	3.88925	-1.36027	-3.19728
H	4.33368	0.28579	-2.64227
H	5.12577	-1.14428	-1.92966
H	4.44191	-0.40804	0.43392
H	3.72934	1.05361	-0.31494
H	2.73192	0.03642	0.75297
H	-0.46325	0.65125	-4.95311
H	-1.65206	1.28686	-3.76983
H	-0.21984	2.27109	-4.21405
H	1.04738	-3.28997	1.69425
H	-1.66893	-3.29826	1.77392
H	-2.49464	-0.92334	2.78163
H	-0.26877	0.60492	3.20653
H	1.89675	-0.86517	2.57715
N	1.85424	1.92747	2.47440
C	2.64885	2.59176	3.00076
C	3.65004	3.42598	3.66315
H	3.72951	3.14495	4.72557
H	4.63159	3.28953	3.18154
H	3.36074	4.48686	3.59411

61			
exn15a exn15a.fchk			
Ru	-0.09049	-0.30380	1.20161
P	-1.52210	0.77376	-0.39313
C	-2.12949	2.54542	-0.42106
C	-1.25300	3.44646	0.45537
C	-2.27918	3.12871	-1.83051
C	-2.89839	-0.17302	-1.23589
C	-4.10773	-0.28609	-0.29655
C	-2.40112	-1.54148	-1.71611
C	-0.06850	0.57489	-1.48962
N	0.86017	-0.04365	-0.74888
C	1.94443	-0.30330	-1.55108
C	1.63545	0.16230	-2.81668
N	0.36428	0.69912	-2.77094
C	3.20125	-0.97979	-1.06195
C	2.89291	-2.45865	-0.75565
C	4.29021	-0.90105	-2.14154
C	3.68664	-0.27987	0.22218
C	-0.36078	1.25632	-3.90567
C	-0.14409	-2.49197	1.38733
C	-1.41345	-1.97168	1.76224
C	-1.23666	-1.10518	2.90322
C	0.15597	-1.12529	3.22741
C	0.84596	-1.96956	2.30080
H	-3.12911	2.46530	0.04319
H	-1.67476	4.46523	0.47098
H	-0.22964	3.50534	0.04699
H	-1.19173	3.06959	1.48647
H	-1.28972	3.25726	-2.29859
H	-2.75156	4.12336	-1.76955
H	-2.90316	2.50317	-2.48806
H	-3.19378	0.42691	-2.11400
H	-4.49888	0.70228	-0.00533
H	-3.84756	-0.83350	0.62374
H	-4.92003	-0.83378	-0.80235
H	-1.59366	-1.44169	-2.45929
H	-2.01124	-2.13842	-0.87760
H	-3.23347	-2.09589	-2.18004
H	2.21427	0.15960	-3.73452
H	2.55965	-2.98486	-1.66545
H	3.79930	-2.95876	-0.37593
H	2.10408	-2.53790	0.00460
H	3.97383	-1.41623	-3.06393
H	4.53121	0.14647	-2.38746
H	5.20739	-1.39098	-1.77881
H	4.59293	-0.78248	0.59787
H	3.93202	0.77643	0.01901
H	2.90733	-0.31584	0.99882
H	-0.13427	0.66088	-4.80156
H	-1.43722	1.20841	-3.70054
H	-0.07273	2.30469	-4.08090
H	0.04561	-3.16467	0.55413
H	-2.35674	-2.19452	1.27309
H	-2.01725	-0.57619	3.44295
H	0.62431	-0.54633	4.02134
H	1.90751	-2.20054	2.30513
N	0.89077	1.40694	1.69445
C	1.53619	2.31145	2.02749
C	2.32930	3.46139	2.44281
H	2.36523	3.51676	3.54310
H	3.35775	3.37066	2.05638
H	1.87843	4.38916	2.05313

61			
exn15 exn15.fchk			
Ru	-0.49640	-1.05818	1.16061
P	-1.94901	0.17513	-0.31087
C	-2.26764	1.98586	0.00020
C	-0.97350	2.62537	0.52162
C	-2.83859	2.73501	-1.20743
C	-3.38633	-0.50292	-1.27619
C	-4.64283	-0.44527	-0.39586
C	-3.06614	-1.93030	-1.73419
C	-0.45223	0.06879	-1.36371
N	0.52474	-0.49135	-0.61813
C	1.66653	-0.54539	-1.39200
C	1.34893	-0.01874	-2.62519
N	0.01498	0.36012	-2.59615
C	2.97247	-1.09264	-0.87785
C	2.77246	-2.56771	-0.47940
C	4.04978	-0.98957	-1.96562
C	3.39241	-0.27470	0.35962
C	-0.72854	0.95465	-3.70017
C	0.24931	-2.75806	2.31901
C	-1.19961	-2.71354	2.33451
C	-1.60027	-1.49807	2.97341
C	-0.41298	-0.75021	3.26516
C	0.73306	-1.55467	2.89168
H	-3.01734	1.97556	0.81197
H	-1.17591	3.66034	0.84264
H	-0.21269	2.65875	-0.27766
H	-0.54140	2.06704	1.36808
H	-2.11144	2.75044	-2.03655
H	-3.04480	3.78200	-0.92907
H	-3.77878	2.29089	-1.57096
H	-3.53030	0.14876	-2.15524
H	-4.89076	0.58635	-0.09662
H	-4.50593	-1.05039	0.51712
H	-5.50297	-0.85558	-0.94981
H	-2.17703	-1.96143	-2.38580
H	-2.87261	-2.58063	-0.86390
H	-3.92156	-2.34308	-2.29386
H	1.95330	0.11359	-3.51698
H	2.48954	-3.17608	-1.35451
H	3.70997	-2.97002	-0.06186
H	1.97922	-2.65228	0.27784
H	3.77202	-1.57497	-2.85819
H	4.21235	0.05912	-2.26608
H	5.00227	-1.38650	-1.58108
H	4.31463	-0.70147	0.78797
H	3.58626	0.77539	0.08470
H	2.60083	-0.28369	1.12355
H	-0.60572	0.33760	-4.60268
H	-1.79074	0.99516	-3.42763
H	-0.36446	1.97421	-3.90090
H	0.85128	-3.56243	1.90254
H	-1.86215	-3.48958	1.95707
H	-2.62261	-1.16911	3.14261
H	-0.36045	0.24457	3.69919
H	1.77137	-1.24896	2.98610
N	1.65419	1.64022	2.76962
C	2.47241	2.27994	3.29028
C	3.50364	3.08324	3.94484
H	3.59550	2.78738	5.00221
H	4.47322	2.93100	3.44411
H	3.23706	4.15107	3.89387

2.9.5.2. Ru(exo-η³-allyl)

x10-12

67			
x10 | hu110a-huf15b.log | Energy: -907438.9619108			
Ru	-0.38611	-0.81571	0.99070
P	-1.62639	0.62526	-0.48577
C	-2.35177	2.32467	-0.15277
C	-1.31332	3.25543	0.48665
C	-2.99371	2.99414	-1.37587
C	-2.76168	-0.13343	-1.76213
C	-4.15810	-0.34113	-1.15946
C	-2.17574	-1.43317	-2.32165
C	-0.00301	0.77328	-1.31249
N	0.81188	-0.07187	-0.66359
C	2.02177	-0.07841	-1.31368
C	1.92073	0.80837	-2.37148
N	0.64273	1.32921	-2.36692
C	3.16714	-0.99075	-0.94673
C	3.47389	-0.89206	0.55827
C	2.75231	-2.43501	-1.30128
C	4.41801	-0.61193	-1.75272
C	0.11260	2.31433	-3.30105
C	0.45213	-2.79355	1.50803
C	-0.60131	-2.90241	0.52313
C	-1.81293	-2.42995	1.13630
C	-1.51669	-1.99393	2.46921
C	-0.11455	-2.23226	2.68151
H	-3.14139	2.11235	0.59044
H	-1.79820	4.20755	0.75692
H	-0.50062	3.48117	-0.22374
H	-0.86260	2.83477	1.39641
H	-2.24448	3.19169	-2.15931
H	-3.41699	3.96589	-1.07166
H	-3.80685	2.39569	-1.81118
H	-2.83258	0.60621	-2.57725
H	-4.60492	0.60267	-0.80857
H	-4.12165	-1.03847	-0.30637
H	-4.82909	-0.77289	-1.92030
H	-1.14921	-1.29404	-2.69760
H	-2.15280	-2.21662	-1.55115
H	-2.80632	-1.78906	-3.15295
H	2.64799	1.10442	-3.12025
H	2.56867	-1.06274	1.15799
H	4.23436	-1.64298	0.82753
H	3.86944	0.10389	0.81228
H	1.82306	-2.71188	-0.78291
H	2.58629	-2.53524	-2.38670
H	3.54795	-3.13795	-1.00370
H	5.24874	-1.28232	-1.48234
H	4.24143	-0.71276	-2.83659
H	4.72841	0.42456	-1.53955
H	0.70398	2.28036	-4.22587
H	-0.93330	2.07052	-3.53388
H	0.16434	3.32708	-2.87091
H	1.49239	-3.07411	1.37348
H	-0.50499	-3.31808	-0.47643
H	-2.79044	-2.39878	0.66276
H	-2.22341	-1.60169	3.19541
H	0.44023	-1.97361	3.58101
C	0.69135	0.80370	2.49876
C	1.77231	1.55706	2.23525
C	2.01849	2.39703	1.02118
H	0.58061	0.31444	3.46462
H	-0.24335	0.93431	1.88163
H	2.55394	1.60595	3.00490
H	1.21585	2.25019	0.28891
H	2.95735	2.06528	0.54397
C	2.13699	3.88658	1.38532
H	2.37306	4.48740	0.49159
H	2.93619	4.05191	2.12707
H	1.19301	4.25964	1.81621

67			
x11 | hu110t-huf15.log | Energy: -907438.4784775			
Ru	-0.54680	-1.14913	1.29130
P	-1.80717	0.30831	-0.18252
C	-2.56569	2.00801	0.09990
C	-1.53924	2.99346	0.67507
C	-3.24941	2.61426	-1.13409
C	-2.91062	-0.48789	-1.46685
C	-4.30214	-0.74090	-0.87010
C	-2.27972	-1.76807	-2.02241
C	-0.18009	0.46685	-1.00082
N	0.63753	-0.38407	-0.36214
C	1.83724	-0.40258	-1.03273
C	1.72716	0.48214	-2.09090
N	0.45338	1.01341	-2.06748
C	2.98202	-1.32292	-0.68172
C	3.32270	-1.21796	0.81615
C	2.54790	-2.76608	-1.01648
C	4.21950	-0.96239	-1.51640
C	-0.08654	1.99659	-2.99792
C	0.32426	-3.09433	1.85010
C	-0.70814	-3.23460	0.84852
C	-1.94210	-2.77506	1.43036
C	-1.67879	-2.31863	2.76448
C	-0.27648	-2.52517	3.00427
H	-3.33478	1.81096	0.86832
H	-2.04174	3.94828	0.89987
H	-0.74084	3.19758	-0.05849
H	-1.06740	2.63420	1.60001
H	-2.52409	2.78913	-1.94497
H	-3.68035	3.59155	-0.85974
H	-4.06348	1.98605	-1.52258
H	-3.00271	0.24649	-2.28417
H	-4.77794	0.18671	-0.51384
H	-4.24779	-1.44204	-0.02141
H	-4.95820	-1.18681	-1.63589
H	-1.26398	-1.59089	-2.41133
H	-2.21559	-2.54358	-1.24649
H	-2.90489	-2.15491	-2.84400
H	2.44616	0.77358	-2.84942
H	2.42340	-1.34883	1.43560
H	4.05834	-1.99493	1.08054
H	3.76534	-0.23685	1.05012
H	1.63583	-3.03563	-0.46588
H	2.34536	-2.86920	-2.09538
H	3.34953	-3.47186	-0.74278
H	5.05025	-1.63654	-1.25561
H	4.02013	-1.07329	-2.59528
H	4.54232	0.07377	-1.32072
H	0.53253	2.00251	-3.90486
H	-1.11591	1.72056	-3.26712
H	-0.08447	3.00167	-2.54742
H	1.37154	-3.35875	1.73917
H	-0.58522	-3.65829	-0.14505
H	-2.91097	-2.77471	0.93881
H	-2.40525	-1.92921	3.47258
H	0.25631	-2.24205	3.90962
C	0.35453	0.56511	2.89363
C	1.53271	1.11855	2.54793
C	1.79721	1.98788	1.35998
H	0.24358	0.04463	3.84348
H	-0.57401	0.80920	2.34327
H	2.38569	0.97562	3.22439
H	0.92605	1.99576	0.69438
H	2.64051	1.56722	0.78727
C	2.14444	3.42300	1.79381
H	2.39499	4.04195	0.91670
H	3.01037	3.43410	2.47684
H	1.29374	3.88903	2.31853

67			
x12 | hu111a-huf51a.log | Energy: -907458.4305301			
Ru	-0.19528	-0.53522	1.10061
P	-1.54341	0.64042	-0.49995
C	-2.28844	2.37392	-0.41775
C	-1.21643	3.47232	-0.33684
C	-3.26312	2.69605	-1.56205
C	-2.73429	-0.34959	-1.55453
C	-4.02508	-0.62142	-0.76878
C	-2.08632	-1.63738	-2.07316
C	0.01644	0.65632	-1.44408
N	0.87611	-0.09475	-0.74368
C	2.04330	-0.18693	-1.46831
C	1.85905	0.54717	-2.62777
N	0.58002	1.06300	-2.60599
C	3.23270	-1.03959	-1.08798
C	2.81690	-2.52194	-1.19453
C	4.39116	-0.78007	-2.06358
C	3.69857	-0.73513	0.34764
C	-0.02314	1.92046	-3.61717
C	-0.22672	-2.78020	0.88313
C	-1.49504	-2.39386	1.38491
C	-1.30748	-1.71362	2.62910
C	0.10087	-1.73486	2.91830
C	0.77714	-2.37693	1.84076
H	-2.85383	2.36041	0.53117
H	-1.71695	4.45442	-0.33108
H	-0.54984	3.43879	-1.21473
H	-0.59439	3.40766	0.56330
H	-2.74682	2.70571	-2.53646
H	-3.67347	3.70608	-1.39899
H	-4.10757	1.99662	-1.62349
H	-2.97421	0.29134	-2.41814
H	-4.50818	0.30636	-0.42306
H	-3.82802	-1.24401	0.11759
H	-4.74282	-1.15880	-1.41032
H	-1.18289	-1.42814	-2.66805
H	-1.80027	-2.30265	-1.24690
H	-2.80669	-2.17269	-2.71336
H	2.52967	0.73367	-3.45974
H	2.48531	-2.76138	-2.21840
H	3.67489	-3.16764	-0.94519
H	1.99681	-2.74957	-0.50113
H	4.11396	-1.05207	-3.09559
H	4.69604	0.27920	-2.04501
H	5.25891	-1.39317	-1.77449
H	4.43305	-1.49393	0.66331
H	4.18731	0.25054	0.39959
H	2.85140	-0.74187	1.04819
H	0.33829	1.61818	-4.60994
H	-1.11449	1.80255	-3.57962
H	0.23584	2.97626	-3.43838
H	-0.04547	-3.29389	-0.05760
H	-2.44663	-2.55883	0.88907
H	-2.08894	-1.30397	3.26335
H	0.57480	-1.29867	3.79531
H	1.84472	-2.56220	1.77220
C	-0.30010	1.23692	2.40632
C	1.03833	1.08688	2.00012
C	1.72884	2.08548	1.09795
H	-0.62000	0.88374	3.38938
H	-0.90371	2.05349	2.00979
H	1.71534	0.57734	2.69520
H	1.09556	2.32708	0.23382
H	2.64706	1.64272	0.69123
C	2.06874	3.37323	1.86327
H	2.61406	4.08348	1.21945
H	2.69798	3.15647	2.74307
H	1.15010	3.86632	2.22539

x13-15

67
x13 | hu111t-huf51.log | Energy: -907455.0968296

Ru	-0.45332	-0.83156	1.41577
P	-1.70136	0.39053	-0.20138
C	-2.42175	2.12861	-0.03669
C	-1.32766	3.20595	-0.09358
C	-3.52696	2.45899	-1.04996
C	-2.84599	-0.53985	-1.35780
C	-4.09184	-1.00582	-0.58991
C	-2.10702	-1.69117	-2.05154
C	-0.11021	0.45233	-1.07578
N	0.75787	-0.30931	-0.39392
C	1.90218	-0.41390	-1.16141
C	1.68558	0.31945	-2.31807
N	0.41920	0.85134	-2.25477
C	3.15946	-1.20690	-0.84688
C	2.84206	-2.38692	0.07740
C	3.74522	-1.74588	-2.16797
C	4.22800	-0.31722	-0.17552
C	-0.23270	1.66593	-3.27044
C	-0.20306	-3.10329	1.33207
C	-1.58542	-2.80053	1.31255
C	-1.90154	-2.05996	2.50912
C	-0.69224	-1.95795	3.27081
C	0.36839	-2.58372	2.54008
H	-2.86319	2.12599	0.97500
H	-1.78787	4.19233	0.08136
H	-0.85148	3.22765	-1.08704
H	-0.54019	3.06126	0.65684
H	-3.13514	2.47582	-2.08131
H	-3.91728	3.46630	-0.83076
H	-4.36929	1.75415	-1.01237
H	-3.16093	0.18331	-2.12647
H	-4.62311	-0.16546	-0.11402
H	-3.82971	-1.72476	0.20062
H	-4.79218	-1.49878	-1.28420
H	-1.33119	-1.31543	-2.73707
H	-1.61445	-2.35453	-1.32545
H	-2.82582	-2.28778	-2.63712
H	2.32892	0.49057	-3.17461
H	2.15699	-3.09533	-0.41450
H	3.77401	-2.92084	0.32168
H	2.37956	-2.03192	1.00780
H	3.00534	-2.35588	-2.71141
H	4.07763	-0.92639	-2.82629
H	4.62436	-2.37207	-1.94817
H	5.18503	-0.86342	-0.14199
H	4.38067	0.61842	-0.73723
H	3.95268	-0.06831	0.85984
H	-0.12350	1.18779	-4.25504
H	-1.29928	1.74858	-3.02245
H	0.21075	2.67336	-3.30079
H	0.34092	-3.61270	0.54214
H	-2.28309	-3.09031	0.53409
H	-2.88390	-1.70957	2.81511
H	-0.58983	-1.46211	4.23374
H	1.40025	-2.68470	2.86325
C	-0.60868	0.96083	2.69856
C	0.75614	0.68425	2.51180
C	1.64795	1.62436	1.73592
H	-1.12735	0.65243	3.60903
H	-1.04060	1.83719	2.21631
H	1.27122	0.11702	3.29513
H	1.12423	1.99239	0.84108
H	2.53239	1.08895	1.37019
C	2.08380	2.80951	2.61118
H	2.76593	3.47753	2.05931
H	2.60767	2.45962	3.51703
H	1.20834	3.39656	2.93758

67
x14 | hu210a-huf17a.log | Energy: -907457.2769920

Ru	-0.24448	-0.63623	1.00999
P	-1.56273	0.58862	-0.55546
C	-2.22618	2.34376	-0.35275
C	-1.10455	3.38407	-0.49498
C	-3.39038	2.69855	-1.28738
C	-2.78113	-0.31477	-1.65472
C	-3.97807	-0.78811	-0.81701
C	-2.09346	-1.45586	-2.41492
C	-0.00702	0.63205	-1.49322
N	0.88767	-0.09244	-0.80616
C	2.03513	-0.16026	-1.56334
C	1.79709	0.55127	-2.73013
N	0.51076	1.03667	-2.67534
C	3.32039	-0.89206	-1.22653
C	3.24069	-1.60588	0.12790
C	3.58438	-1.94547	-2.32397
C	4.49055	0.11419	-1.21882
C	-0.16793	1.82272	-3.69625
C	0.03258	-2.89757	0.88450
C	-1.35459	-2.60972	0.90453
C	-1.65002	-1.89874	2.12560
C	-0.42364	-1.79008	2.85475
C	0.62756	-2.38834	2.08354
H	-2.59286	2.35768	0.68803
H	-1.50164	4.38011	-0.23902
H	-0.74081	3.42274	-1.53434
H	-0.24449	3.18091	0.15683
H	-3.07116	2.69738	-2.34386
H	-3.73894	3.71706	-1.04995
H	-4.24526	2.01493	-1.18406
H	-3.14007	0.42356	-2.38868
H	-4.47233	0.04803	-0.29543
H	-3.66879	-1.52106	-0.05660
H	-4.72433	-1.26624	-1.47271
H	-1.36559	-1.06924	-3.14556
H	-1.55305	-2.13150	-1.73556
H	-2.85113	-2.04289	-2.95978
H	2.43970	0.74351	-3.58355
H	2.51310	-2.42761	0.08932
H	4.22782	-2.03260	0.36519
H	2.94126	-0.92622	0.93687
H	2.75783	-2.67367	-2.37600
H	3.69247	-1.47151	-3.31321
H	4.51668	-2.48981	-2.10070
H	5.43502	-0.41970	-1.02427
H	4.57963	0.62325	-2.19244
H	4.35887	0.88228	-0.44070
H	-0.10113	1.31008	-4.66743
H	-1.22365	1.92833	-3.41210
H	0.28679	2.82215	-3.77688
H	0.56119	-3.38574	0.06862
H	-2.07025	-2.89578	0.14111
H	-2.62897	-1.56797	2.46266
H	-0.30240	-1.30686	3.82206
H	1.67223	-2.46683	2.36812
C	-0.30352	1.16122	2.29274
C	1.04572	0.82246	2.09327
C	1.98059	1.71859	1.31565
H	-0.82507	0.87509	3.20917
H	-0.69560	2.05905	1.81562
H	1.54049	0.22947	2.87057
H	1.46229	2.14140	0.44131
H	2.82282	1.13410	0.92034
C	2.51436	2.85018	2.20737
H	3.22546	3.48602	1.65411
H	3.03594	2.44307	3.09036
H	1.68770	3.48444	2.56985

67
x15 | hu210t-huf17.log | Energy: -907444.3057375

Ru	-0.62907	-0.59715	1.80738
P	-1.58696	0.33415	-0.19010
C	-1.91639	2.18640	-0.28175
C	-0.59694	2.95489	-0.12367
C	-2.64492	2.65581	-1.54620
C	-3.10013	-0.42957	-0.97614
C	-4.32079	-0.18439	-0.07904
C	-2.93570	-1.90983	-1.34080
C	-0.17944	0.05726	-1.31655
N	1.00083	-0.05081	-0.71042
C	1.94341	-0.22661	-1.69164
C	1.30672	-0.22995	-2.91800
N	-0.03932	-0.03840	-2.67557
C	3.40759	-0.36664	-1.35218
C	3.58131	-1.51259	-0.33581
C	4.22153	-0.66277	-2.61854
C	3.89592	0.94806	-0.71122
C	-1.07933	-0.06045	-3.69680
C	0.41713	-2.59610	1.80659
C	-0.78154	-2.67983	1.05166
C	-1.87686	-2.32323	1.93089
C	-1.32443	-2.04850	3.23045
C	0.09843	-2.21984	3.14840
H	-2.56440	2.38076	0.58995
H	-0.80946	4.03321	-0.04015
H	0.04540	2.79589	-1.00506
H	-0.02666	2.64382	0.76116
H	-2.03134	2.47377	-2.44388
H	-2.80559	3.74480	-1.48056
H	-3.62886	2.18181	-1.67796
H	-3.23812	0.13253	-1.91158
H	-4.49346	0.89028	0.09235
H	-4.19228	-0.66894	0.90285
H	-5.22332	-0.60261	-0.55426
H	-1.97320	-2.11062	-1.83801
H	-3.00841	-2.55681	-0.45620
H	-3.74561	-2.20295	-2.02896
H	1.68338	-0.35554	-3.92856
H	3.23086	-2.46966	-0.75834
H	4.64504	-1.61858	-0.06650
H	3.00770	-1.29779	0.58065
H	3.89147	-1.60344	-3.09039
H	4.11956	0.15335	-3.35339
H	5.28899	-0.76101	-2.36531
H	4.95634	0.85648	-0.42262
H	3.79737	1.78932	-1.41706
H	3.30478	1.17777	0.19044
H	-1.55193	-1.05373	-3.75658
H	-1.84584	0.69136	-3.47145
H	-0.62441	0.18105	-4.66695
H	1.42108	-2.71966	1.40447
H	-0.85002	-2.95331	0.00452
H	-2.93480	-2.31992	1.68642
H	-1.89067	-1.76608	4.11556
H	0.81060	-2.07291	3.95563
C	-1.26367	1.22689	2.93828
C	0.01777	0.80324	3.31636
C	1.26593	1.23976	2.58241
H	-2.10785	1.02581	3.60194
H	-1.37921	2.08124	2.27487
H	0.15957	0.31019	4.28179
H	1.32537	2.34390	2.56597
H	1.17850	0.96464	1.49922
C	2.54898	0.62316	3.13895
H	3.42116	0.92192	2.53742
H	2.48727	-0.47732	3.12194
H	2.72095	0.94403	4.17970

x16-18

67
x16 | hu210z-huf17b.log | Energy: -907448.2268685

Ru	-0.55372	-0.38089	1.63067
P	-1.26690	0.53702	-0.46176
C	-1.60671	2.39454	-0.61833
C	-0.35536	3.22425	-0.28774
C	-2.13375	2.82033	-1.99566
C	-2.78132	-0.21250	-1.27201
C	-4.02595	0.10005	-0.43114
C	-2.65977	-1.70596	-1.60414
C	0.12506	0.25795	-1.62145
N	1.35074	0.22167	-1.10436
C	2.22795	0.07757	-2.14839
C	1.51012	0.02156	-3.32534
N	0.17650	0.14602	-2.99285
C	3.71799	0.00275	-1.91568
C	4.01849	-1.17952	-0.97345
C	4.45527	-0.19337	-3.24698
C	4.18546	1.31139	-1.24891
C	-0.90674	0.06488	-3.96797
C	0.40364	-2.42334	1.75897
C	-0.72655	-2.47972	0.90297
C	-1.89225	-2.10447	1.67972
C	-1.45187	-1.83472	3.01321
C	-0.03247	-2.02335	3.06189
H	-2.39002	2.58976	0.13406
H	-0.53732	4.27558	-0.56439
H	0.52035	2.86700	-0.85370
H	-0.10853	3.20997	0.78100
H	-1.36763	2.65276	-2.77007
H	-2.34089	3.90294	-1.97278
H	-3.06602	2.31461	-2.28610
H	-2.87194	0.32230	-2.22597
H	-4.19380	1.18512	-0.34109
H	-3.93214	-0.31389	0.58576
H	-4.91713	-0.34260	-0.90589
H	-1.66902	-1.96325	-2.01131
H	-2.84646	-2.34090	-0.72911
H	-3.41819	-1.96576	-2.36104
H	1.82026	-0.10414	-4.35814
H	3.71025	-2.13422	-1.43186
H	5.09915	-1.22732	-0.75962
H	3.47543	-1.05763	-0.02160
H	4.14167	-1.12933	-3.73910
H	4.26073	0.64718	-3.93412
H	5.54139	-0.24617	-3.07117
H	5.26589	1.26195	-1.03415
H	3.99954	2.17569	-1.90803
H	3.64485	1.47427	-0.30210
H	-1.45933	-0.88053	-3.86581
H	-1.60053	0.90663	-3.85175
H	-0.46614	0.11225	-4.97260
H	1.43394	-2.60172	1.45755
H	-0.70947	-2.76535	-0.14291
H	-2.92421	-2.09558	1.34581
H	-2.08524	-1.52292	3.84087
H	0.60162	-1.88495	3.93398
C	-1.23213	1.46164	2.68114
C	0.07920	1.06967	3.02648
C	1.19639	1.11688	2.05409
H	-2.01214	1.32479	3.43382
H	-1.41532	2.25904	1.96707
H	0.29200	0.65856	4.01689
H	1.26439	2.04992	1.48444
H	0.98535	0.38985	1.09451
C	2.55082	0.65009	2.57540
H	3.24854	0.47679	1.74235
H	2.44645	-0.28656	3.14556
H	2.98319	1.41702	3.23830

67
x17 | hu220t-huf19.log | Energy: -907444.9225291

Ru	-0.74912	-0.60630	2.02302
P	-1.41318	0.33088	-0.05789
C	-1.76548	2.18926	-0.20901
C	-0.54055	3.04113	0.16438
C	-2.25267	2.61680	-1.60097
C	-2.92491	-0.41683	-0.87647
C	-4.17620	-0.10717	-0.04481
C	-2.79393	-1.90986	-1.20801
C	-0.02870	0.06708	-1.23598
N	1.20396	0.01788	-0.73705
C	2.06942	-0.10093	-1.79439
C	1.33599	-0.12694	-2.96227
N	0.00658	-0.01097	-2.61005
C	3.56233	-0.18813	-1.58631
C	3.87451	-1.42039	-0.71460
C	4.27963	-0.31495	-2.93701
C	4.04245	1.08296	-0.85900
C	-1.08571	-0.09521	-3.57559
C	0.13735	-2.65983	2.28112
C	-0.96759	-2.71669	1.37999
C	-2.15710	-2.34157	2.11344
C	-1.76275	-2.04729	3.44870
C	-0.34697	-2.23411	3.55397
H	-2.57797	2.36938	0.51546
H	-0.72753	4.08687	-0.12948
H	0.36017	2.69433	-0.36877
H	-0.33183	3.04144	1.24188
H	-1.45745	2.46817	-2.34929
H	-2.47828	3.69560	-1.57618
H	-3.16618	2.09933	-1.92757
H	-3.01160	0.11746	-1.83061
H	-4.35540	0.97715	0.03078
H	-4.08344	-0.50741	0.97759
H	-5.06086	-0.56417	-0.51824
H	-1.79471	-2.16439	-1.59666
H	-2.99541	-2.54607	-0.33729
H	-3.53754	-2.17154	-1.97886
H	1.63273	-0.22906	-4.00158
H	3.56057	-2.34845	-1.22109
H	4.95764	-1.47892	-0.51676
H	3.34363	-1.35384	0.24943
H	3.95847	-1.22430	-3.47230
H	4.07599	0.56013	-3.57671
H	5.36802	-0.37753	-2.77961
H	5.12659	1.02155	-0.66754
H	3.84591	1.98087	-1.46826
H	3.52063	1.19561	0.10515
H	-1.63982	-1.03789	-3.45905
H	-1.77535	0.75016	-3.46328
H	-0.65211	-0.06030	-4.58370
H	1.17340	-2.87353	2.02940
H	-0.92064	-3.03358	0.34387
H	-3.17507	-2.33060	1.73907
H	-2.42046	-1.70858	4.24633
H	0.25319	-2.07965	4.44734
C	-1.45522	1.21274	3.05231
C	-0.11252	0.89874	3.40311
C	0.93218	0.85735	2.42359
H	-2.21251	1.06454	3.82601
H	-1.67798	2.00714	2.34644
H	0.10092	0.47454	4.38873
H	0.93644	1.60352	1.63254
H	0.63281	-0.30967	1.24446
C	2.30717	0.37694	2.82861
H	2.85961	-0.00244	1.95606
H	2.24519	-0.41957	3.58678
H	2.88127	1.21909	3.25268

67
x18 | hu220z-huf19b.log | Energy: -907445.2390324

Ru	-0.53073	-0.40824	1.57054
P	-1.18780	0.53744	-0.50814
C	-1.53932	2.39588	-0.65933
C	-0.31911	3.24758	-0.27073
C	-2.00926	2.82260	-2.05748
C	-2.70363	-0.21052	-1.31898
C	-3.95309	0.09835	-0.48468
C	-2.56898	-1.70404	-1.64700
C	0.18613	0.27565	-1.69955
N	1.42088	0.22226	-1.20776
C	2.28144	0.11129	-2.26969
C	1.54193	0.09484	-3.43399
N	0.21387	0.20853	-3.07413
C	3.77494	0.02408	-2.06679
C	4.09028	-1.21112	-1.20048
C	4.48797	-0.09567	-3.42028
C	4.25542	1.29176	-1.33364
C	-0.88381	0.12013	-4.03322
C	0.33376	-2.45612	1.88230
C	-0.76737	-2.52004	0.96971
C	-1.96142	-2.14188	1.68949
C	-1.57783	-1.82977	3.02221
C	-0.16311	-2.01498	3.14302
H	-2.36168	2.57570	0.05387
H	-0.50198	4.29316	-0.56769
H	0.58800	2.89984	-0.79236
H	-0.12327	3.24765	0.80917
H	-1.20465	2.67401	-2.79560
H	-2.23606	3.90118	-2.03552
H	-2.91831	2.30431	-2.39520
H	-2.79381	0.32176	-2.27398
H	-4.13423	1.18247	-0.41076
H	-3.85699	-0.29988	0.53819
H	-4.83827	-0.36119	-0.95469
H	-1.56981	-1.95629	-2.03766
H	-2.76562	-2.33803	-0.77350
H	-3.31395	-1.97104	-2.41470
H	1.83303	-0.00002	-4.47563
H	3.77259	-2.13764	-1.70748
H	5.17445	-1.27111	-1.00887
H	3.56509	-1.14530	-0.23317
H	4.16576	-1.00264	-3.95903
H	4.28165	0.78238	-4.05509
H	5.57692	-0.15811	-3.26672
H	5.34068	1.23161	-1.14825
H	4.05362	2.19333	-1.93579
H	3.73808	1.39551	-0.36594
H	-1.43494	-0.82362	-3.91070
H	-1.57457	0.96432	-3.91913
H	-0.45605	0.15317	-5.04388
H	1.37021	-2.68339	1.64596
H	-0.71384	-2.85245	-0.06139
H	-2.97552	-2.13126	1.30459
H	-2.24147	-1.47847	3.80950
H	0.42857	-1.84793	4.03973
C	-1.27933	1.40152	2.58909
C	0.06051	1.11674	2.98079
C	1.11556	1.07838	2.03330
H	-2.05741	1.23850	3.33879
H	-1.49293	2.19666	1.88160
H	0.24747	0.68610	3.96902
H	1.11107	1.77280	1.19815
H	0.77709	-0.27590	0.67889
C	2.48281	0.57868	2.42435
H	3.00128	0.15180	1.55235
H	2.42312	-0.18589	3.21516
H	3.09453	1.41891	2.79853

x19-21

67
x19 | hu221t-huf45.log | Energy: -907445.1543562

Ru	-0.67318	-0.55317	1.97824
P	-1.35281	0.40433	-0.07526
C	-1.68798	2.26110	-0.23481
C	-0.53691	3.10376	0.33630
C	-1.97442	2.70103	-1.67791
C	-2.91914	-0.32557	-0.80683
C	-4.08887	-0.11461	0.16398
C	-2.79341	-1.79618	-1.23114
C	-0.01462	0.09229	-1.29187
N	1.22832	-0.01043	-0.82967
C	2.05331	-0.19350	-1.90913
C	1.28407	-0.20169	-3.05450
N	-0.02594	-0.01044	-2.66567
C	3.54490	-0.35638	-1.74144
C	3.81367	-1.55011	-0.80398
C	4.20746	-0.60523	-3.10305
C	4.12098	0.92441	-1.10697
C	-1.14641	-0.03731	-3.60091
C	0.49181	-2.48476	1.94123
C	-0.68196	-2.60527	1.13448
C	-1.83450	-2.48407	1.99343
C	-1.35484	-2.26130	3.31609
C	0.07695	-2.25677	3.28496
H	-2.59877	2.42748	0.36476
H	-0.62692	4.13929	-0.02967
H	0.44487	2.71543	0.01681
H	-0.56489	3.14616	1.43311
H	-1.09680	2.52398	-2.32052
H	-2.17552	3.78472	-1.68081
H	-2.85381	2.20783	-2.11753
H	-3.11155	0.26627	-1.71188
H	-4.26555	0.95278	0.37159
H	-3.89288	-0.62069	1.12283
H	-5.01225	-0.53137	-0.27080
H	-1.82800	-2.01515	-1.71297
H	-2.90988	-2.47640	-0.37796
H	-3.59612	-2.03462	-1.94804
H	1.54344	-0.33351	-4.10057
H	3.42108	-2.48565	-1.23714
H	4.89816	-1.66748	-0.64375
H	3.33011	-1.38359	0.17311
H	3.81534	-1.52269	-3.57335
H	4.03449	0.24215	-3.78760
H	5.29510	-0.72349	-2.97524
H	5.20583	0.81030	-0.94571
H	3.95538	1.79511	-1.76313
H	3.63870	1.12205	-0.13567
H	-1.86083	0.75892	-3.36862
H	-0.75222	0.13383	-4.61166
H	-1.65961	-1.01014	-3.57795
H	1.51591	-2.52314	1.57892
H	-0.68992	-2.79749	0.06699
H	-2.87579	-2.57913	1.70349
H	-1.97025	-2.09962	4.19887
H	0.73345	-2.09641	4.13614
C	-1.87346	1.02033	2.97181
C	-0.61203	0.85985	3.61112
C	0.59431	1.07804	2.90066
H	-2.75924	0.67963	3.51342
H	-2.03933	1.86351	2.30516
H	-0.55902	0.33592	4.57053
H	0.62989	1.87037	2.16011
H	0.62889	-0.11308	1.18858
C	1.92846	0.72045	3.50452
H	2.64145	0.40709	2.72606
H	1.83562	-0.09032	4.24355
H	2.35769	1.60231	4.01289

67
x20 | hu230a-huf55a.log | Energy: -907449.8992377

Ru	-0.41190	-0.19256	1.61084
P	-1.08467	0.63106	-0.48272
C	-1.40695	2.48849	-0.53353
C	-0.08668	3.23003	-0.78589
C	-2.51927	2.95000	-1.48318
C	-2.59758	-0.18690	-1.23567
C	-3.76828	-0.22536	-0.24790
C	-2.27437	-1.58919	-1.76559
C	0.26893	0.32398	-1.68620
N	1.42811	-0.17604	-1.27178
C	2.23298	-0.29879	-2.37574
C	1.53866	0.13706	-3.48514
N	0.29046	0.52529	-3.04871
C	3.63098	-0.86150	-2.27507
C	3.54851	-2.31874	-1.77931
C	4.31747	-0.82389	-3.64731
C	4.44015	-0.02627	-1.26488
C	-0.71099	1.12278	-3.91961
C	1.25109	-1.71380	1.52176
C	0.14857	-2.16776	0.73277
C	-0.97657	-2.36530	1.59976
C	-0.56103	-2.00942	2.92327
C	0.81544	-1.61266	2.87595
H	-1.73992	2.72475	0.48908
H	-0.23630	4.31214	-0.63782
H	0.26538	3.06728	-1.81732
H	0.71227	2.89030	-0.10665
H	-2.28083	2.73650	-2.53451
H	-2.64068	4.04160	-1.38456
H	-3.48613	2.48093	-1.24574
H	-2.88932	0.45533	-2.08054
H	-4.04490	0.77809	0.11128
H	-3.51605	-0.84421	0.62660
H	-4.64911	-0.66320	-0.74547
H	-1.43492	-1.58309	-2.47852
H	-2.02317	-2.27347	-0.94088
H	-3.16143	-1.99768	-2.27723
H	1.81170	0.20258	-4.53392
H	2.98590	-2.94470	-2.49212
H	4.56189	-2.73945	-1.67025
H	3.04348	-2.36701	-0.80076
H	3.76328	-1.42876	-4.38472
H	4.39100	0.20983	-4.02458
H	5.33695	-1.23340	-3.56821
H	5.45260	-0.44807	-1.15219
H	4.53231	1.01860	-1.60519
H	3.94512	-0.02666	-0.27987
H	-1.71455	0.77541	-3.64670
H	-0.67601	2.22250	-3.86468
H	-0.50475	0.81196	-4.95286
H	2.22673	-1.44916	1.12614
H	0.17926	-2.32443	-0.34028
H	-1.95710	-2.73282	1.30999
H	-1.18611	-2.02947	3.81380
H	1.41618	-1.28143	3.71939
C	-2.24383	0.73682	2.42347
C	-1.11315	1.07074	3.22109
C	-0.04395	1.79802	2.65202
H	-2.97476	0.04241	2.84399
H	-2.66486	1.47421	1.74229
H	-0.96011	0.58315	4.18836
H	-0.28133	2.54920	1.89820
H	0.78021	0.66401	1.01218
C	1.23672	2.02787	3.41147
H	2.09706	2.10864	2.72955
H	1.43096	1.20949	4.12239
H	1.17164	2.97242	3.98111

67
x21 | hu230t-huf55.log | Energy: -907441.2988063

Ru	-0.60443	-0.51507	1.90835
P	-1.44748	0.42736	-0.05404
C	-1.68567	2.30603	-0.21070
C	-0.40251	2.98753	-0.71691
C	-2.88555	2.73473	-1.06417
C	-2.97972	-0.34795	-0.79707
C	-4.09001	-0.35343	0.26317
C	-2.70735	-1.75791	-1.33352
C	-0.08107	0.11700	-1.25327
N	1.07995	-0.19332	-0.68055
C	2.04252	-0.29906	-1.66123
C	1.42173	-0.02941	-2.86356
N	0.08874	0.22549	-2.59157
C	3.45909	-0.73176	-1.37452
C	3.47122	-2.26345	-1.18187
C	4.36787	-0.35735	-2.55462
C	3.96063	-0.05430	-0.08782
C	-0.91382	0.62764	-3.57087
C	0.85210	-2.22323	1.92082
C	-0.28357	-2.55099	1.10644
C	-1.44859	-2.60076	1.94801
C	-1.02740	-2.26404	3.26821
C	0.38589	-2.03297	3.25544
H	-1.86146	2.64027	0.82356
H	-0.49504	4.07791	-0.58490
H	-0.25283	2.78866	-1.79022
H	0.50141	2.64850	-0.18927
H	-2.76087	2.42428	-2.11476
H	-2.95989	3.83479	-1.05022
H	-3.83668	2.32579	-0.69318
H	-3.29051	0.29683	-1.63363
H	-4.31630	0.66028	0.63127
H	-3.78695	-0.96369	1.12857
H	-5.01305	-0.77536	-0.16708
H	-1.89415	-1.77189	-2.07764
H	-2.43899	-2.44731	-0.52075
H	-3.62005	-2.14706	-1.81442
H	1.80539	-0.01201	-3.87935
H	3.14024	-2.77659	-2.09957
H	4.49176	-2.60315	-0.93990
H	2.80190	-2.56197	-0.35811
H	4.04041	-0.85534	-3.48260
H	4.37219	0.73230	-2.72118
H	5.39939	-0.68184	-2.34605
H	4.99445	-0.37318	0.11948
H	3.94658	1.04387	-0.18531
H	3.33342	-0.33387	0.77364
H	-1.89553	0.24441	-3.26484
H	-0.95630	1.72555	-3.65141
H	-0.65002	0.20051	-4.54793
H	1.88010	-2.13921	1.57989
H	-0.25312	-2.75845	0.04025
H	-2.45742	-2.86385	1.64473
H	-1.67534	-2.17068	4.13718
H	0.99530	-1.75691	4.11229
C	-1.92503	0.85604	3.03729
C	-0.56312	1.00274	3.42965
C	0.40341	1.41366	2.47601
H	-2.60622	0.37207	3.74158
H	-2.39652	1.60590	2.40276
H	-0.22340	0.58316	4.38161
H	0.08985	2.16701	1.75361
H	0.71736	-0.25496	0.67529
C	1.87219	1.43155	2.81954
H	2.49227	1.32172	1.91701
H	2.12660	0.61218	3.51176
H	2.15202	2.38655	3.30118

x22-24

67			
x22 | hu310a-huf57a.log | Energy: -907454.5222757			
Ru	-0.65318	-0.27226	1.54030
P	-1.34881	0.64992	-0.43460
C	-1.61309	2.52990	-0.61077
C	-0.37408	3.24228	-1.17530
C	-2.87896	2.96804	-1.35733
C	-2.80357	-0.14631	-1.32282
C	-3.97686	-0.23407	-0.33554
C	-2.45981	-1.53894	-1.86649
C	0.03837	0.37785	-1.67219
N	1.24032	0.01509	-1.19884
C	2.16664	-0.12924	-2.21076
C	1.48224	0.16905	-3.36167
N	0.17642	0.48153	-3.00818
C	3.58203	-0.57491	-1.95694
C	3.55748	-2.05388	-1.51462
C	4.40173	-0.43041	-3.24663
C	4.19637	0.28890	-0.83821
C	-0.88104	0.82987	-3.95381
C	0.91494	-1.89419	1.57957
C	-0.14372	-2.27300	0.69637
C	-1.35971	-2.40571	1.45968
C	-1.04728	-2.06970	2.80945
C	0.34751	-1.74941	2.88714
H	-1.72326	2.84462	0.43776
H	-0.48973	4.33104	-1.04626
H	-0.25557	3.04472	-2.25334
H	0.55439	2.93532	-0.66868
H	-2.83570	2.73092	-2.43317
H	-2.97864	4.06306	-1.27167
H	-3.79146	2.51345	-0.94702
H	-3.08010	0.51090	-2.16172
H	-4.26106	0.74889	0.07077
H	-3.70146	-0.87491	0.51656
H	-4.85596	-0.66405	-0.84348
H	-1.60265	-1.52952	-2.55953
H	-2.22558	-2.23238	-1.04680
H	-3.33095	-1.94357	-2.40809
H	1.81204	0.18523	-4.39499
H	3.13643	-2.69452	-2.30627
H	4.58406	-2.39126	-1.29989
H	2.95495	-2.18843	-0.60080
H	3.98290	-1.05298	-4.05463
H	4.43063	0.61878	-3.58325
H	5.43488	-0.76350	-3.06416
H	5.23022	-0.03923	-0.64828
H	4.21323	1.35387	-1.12151
H	3.63430	0.18696	0.10599
H	-1.54675	1.56600	-3.49019
H	-0.42098	1.26737	-4.84960
H	-1.45533	-0.06759	-4.22879
H	1.96622	-1.77947	1.32402
H	-0.03886	-2.47691	-0.36700
H	-2.32553	-2.73502	1.08844
H	-1.75050	-2.04709	3.63899
H	0.88521	-1.46121	3.78697
C	-1.94968	1.12667	2.64198
C	-0.57791	1.26230	3.01516
C	0.40085	1.62673	2.04362
H	-2.62695	0.68353	3.37691
H	-2.42130	1.87503	2.00322
H	-0.24085	0.86445	3.97790
H	0.12730	2.41240	1.33793
H	1.34982	-0.11933	-0.18226
C	1.86916	1.60484	2.40738
H	2.50518	1.48900	1.51272
H	2.09389	0.77031	3.09180
H	2.17797	2.54444	2.90285

67			
x23 | hu310t-huf57.log | Energy: -907445.8448237			
Ru	-0.47307	-0.62754	2.12235
P	-1.13757	0.40115	0.16715
C	-0.80444	2.26752	0.17852
C	0.61425	2.53243	0.69197
C	-1.06778	3.01275	-1.13212
C	-2.84678	0.29812	-0.61807
C	-3.94157	0.96171	0.23246
C	-3.18687	-1.14173	-1.02468
C	-0.09496	-0.04566	-1.35252
N	1.15481	-0.49764	-1.14642
C	1.84709	-0.70300	-2.32050
C	0.96018	-0.36360	-3.30414
N	-0.22458	0.04075	-2.70044
C	3.27177	-1.18863	-2.35685
C	3.34876	-2.59437	-1.72721
C	3.74891	-1.24219	-3.81499
C	4.15214	-0.21310	-1.54885
C	-1.38422	0.46108	-3.49468
C	1.77719	-0.59607	1.94707
C	1.30794	-1.94594	1.67217
C	0.66899	-2.42209	2.84824
C	0.73456	-1.39191	3.84153
C	1.42361	-0.26735	3.28394
H	-1.51726	2.62157	0.94142
H	0.77482	3.61776	0.80126
H	1.36895	2.15437	-0.02147
H	0.77300	2.04155	1.66283
H	-0.37098	2.68101	-1.92128
H	-0.89703	4.09190	-0.98260
H	-2.10225	2.89070	-1.48977
H	-2.77456	0.90336	-1.52957
H	-3.69510	2.01200	0.45648
H	-4.12054	0.44475	1.18450
H	-4.88531	0.95335	-0.33831
H	-2.40653	-1.57847	-1.67137
H	-3.28657	-1.80538	-0.15478
H	-4.14063	-1.15444	-1.57916
H	1.06600	-0.37762	-4.38299
H	2.70459	-3.30713	-2.26683
H	4.38761	-2.95776	-1.77138
H	3.04746	-2.57608	-0.66675
H	3.13669	-1.94246	-4.40683
H	3.70546	-0.24551	-4.28407
H	4.79232	-1.59103	-3.84645
H	5.19726	-0.55984	-1.56874
H	4.11131	0.80334	-1.97267
H	3.83583	-0.16859	-0.49223
H	-1.66390	1.48945	-3.23824
H	-1.09489	0.41817	-4.55228
H	-2.22842	-0.21778	-3.32097
H	2.38691	0.04536	1.31124
H	1.45826	-2.53232	0.76891
H	0.20117	-3.39639	2.96596
H	0.33970	-1.45831	4.85166
H	1.64500	0.66807	3.79133
C	-2.48007	-1.44734	2.48268
C	-2.12562	-0.47115	3.46262
C	-1.82878	0.86991	3.08186
H	-2.53228	-2.48872	2.81170
H	-3.18801	-1.19256	1.70039
H	-1.85302	-0.79505	4.47111
H	-2.48786	1.32830	2.34240
H	1.49304	-0.66777	-0.20596
C	-1.26084	1.84614	4.08567
H	-0.63161	2.60493	3.58996
H	-0.63818	1.32717	4.83269
H	-2.06349	2.38384	4.62408

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x24 | hu320a-huf59a.log | Energy: -907448.9033613			
Ru	-0.18665	-0.26738	1.60424
P	-1.05486	0.72259	-0.28583
C	-1.14163	2.60442	-0.11926
C	0.26423	3.21415	-0.20099
C	-2.14766	3.37199	-0.98530
C	-2.63097	0.26599	-1.23938
C	-3.90283	0.34466	-0.38157
C	-2.50122	-1.09858	-1.93315
C	0.13609	0.39390	-1.70949
N	0.96828	-0.64967	-1.56422
C	1.69326	-0.90032	-2.70802
C	1.27094	0.04743	-3.60397
N	0.31177	0.83046	-2.97578
C	2.73392	-1.98537	-2.79140
C	2.15323	-3.29532	-2.22393
C	3.14629	-2.18325	-4.25695
C	3.95992	-1.55466	-1.95728
C	-0.38791	1.93130	-3.63530
C	1.94013	0.35782	1.26701
C	1.92692	-1.07033	1.44138
C	1.40668	-1.32404	2.74988
C	1.14330	-0.06580	3.38000
C	1.48655	0.98273	2.47087
H	-1.47369	2.67559	0.93025
H	0.21887	4.28685	0.04944
H	0.68693	3.12660	-1.21696
H	0.95435	2.72649	0.50130
H	-1.87593	3.37273	-2.05024
H	-2.16607	4.42401	-0.65413
H	-3.16923	2.97650	-0.89219
H	-2.71478	1.04230	-2.01756
H	-3.99692	1.30859	0.14233
H	-3.93977	-0.45494	0.37167
H	-4.78070	0.23079	-1.03935
H	-1.72816	-1.09099	-2.71892
H	-2.25152	-1.89900	-1.22004
H	-3.46093	-1.35604	-2.41155
H	1.57165	0.23411	-4.62927
H	1.26967	-3.61999	-2.79708
H	2.91643	-4.08710	-2.27888
H	1.86200	-3.18561	-1.16473
H	2.28533	-2.48715	-4.87445
H	3.57754	-1.25892	-4.67605
H	3.91258	-2.97105	-4.31923
H	4.72272	-2.34914	-1.98792
H	4.40253	-0.62907	-2.35953
H	3.68810	-1.38083	-0.90303
H	-1.47200	1.80535	-3.52087
H	-0.07985	2.89269	-3.20222
H	-0.13084	1.90983	-4.70192
H	2.28471	0.88182	0.37790
H	2.33170	-1.81822	0.76315
H	1.24771	-2.30418	3.19380
H	0.74232	0.06710	4.38121
H	1.42338	2.05020	2.66322
C	-1.71312	-1.85747	1.60470
C	-1.82152	-1.01134	2.74955
C	-2.08048	0.38189	2.59839
H	-1.36580	-2.88106	1.76925
H	-2.42549	-1.74932	0.78963
H	-1.47466	-1.37414	3.72296
H	-2.81936	0.67304	1.85207
H	0.96913	-1.16441	-0.67199
C	-2.01049	1.31817	3.78206
H	-1.69856	2.33026	3.47193
H	-1.28991	0.96032	4.53406
H	-2.99658	1.41416	4.27337

x25-27

67
x25 | hu320t-huf59.log | Energy: -907448.1589845

Ru	-0.10720	-0.23754	2.06794
P	-0.97348	0.77011	0.18770
C	-0.91509	2.66609	0.33271
C	0.46232	3.22638	-0.04814
C	-2.05617	3.47018	-0.30331
C	-2.57602	0.41284	-0.77580
C	-3.82374	0.41443	0.11866
C	-2.50587	-0.88585	-1.59637
C	0.19030	0.34216	-1.23249
N	1.01844	-0.69913	-1.05619
C	1.71167	-1.00796	-2.20677
C	1.27034	-0.10321	-3.13775
N	0.33662	0.71759	-2.51959
C	2.74364	-2.10238	-2.25715
C	2.13341	-3.40040	-1.69202
C	3.18971	-2.31717	-3.70991
C	3.95127	-1.67798	-1.39405
C	-0.45997	1.71482	-3.22652
C	2.00288	0.41859	1.69810
C	2.04356	-0.95727	2.08979
C	1.49060	-1.03604	3.40865
C	1.14853	0.29085	3.82957
C	1.47095	1.20160	2.78048
H	-1.01654	2.75387	1.42622
H	0.52198	4.28657	0.24927
H	0.64020	3.17767	-1.13497
H	1.27698	2.68699	0.45598
H	-2.03374	3.46694	-1.40500
H	-1.96521	4.52204	0.01567
H	-3.04566	3.10878	0.01167
H	-2.66000	1.25750	-1.47870
H	-3.88115	1.30156	0.76801
H	-3.85494	-0.48050	0.75793
H	-4.72150	0.40430	-0.52165
H	-1.75610	-0.83859	-2.40176
H	-2.27157	-1.75908	-0.96907
H	-3.48749	-1.06460	-2.06640
H	1.54612	0.03203	-4.17821
H	1.26392	-3.72236	-2.28772
H	2.88971	-4.20050	-1.71549
H	1.81166	-3.27334	-0.64364
H	2.34071	-2.61758	-4.34553
H	3.64026	-1.40080	-4.12602
H	3.94796	-3.11423	-3.74728
H	4.70785	-2.47882	-1.40057
H	4.41230	-0.75764	-1.78770
H	3.65267	-1.49793	-0.34779
H	-1.31301	1.22584	-3.72245
H	-0.82321	2.45579	-2.50998
H	0.17147	2.21066	-3.97637
H	2.36633	0.81410	0.75223
H	2.46568	-1.78375	1.52208
H	1.36711	-1.94322	3.99533
H	0.70470	0.55722	4.78465
H	1.36674	2.28265	2.80684
C	-1.45337	-1.97579	1.82456
C	-1.65551	-1.31223	3.07151
C	-2.07065	0.04899	3.11067
H	-1.00910	-2.97447	1.85066
H	-2.17846	-1.82135	1.02684
H	-1.27533	-1.76670	3.99236
H	-2.81680	0.36837	2.38708
H	1.03898	-1.16765	-0.13844
C	-2.13132	0.79467	4.42388
H	-1.86566	1.85802	4.29873
H	-1.44280	0.35751	5.16467
H	-3.15092	0.75836	4.85035

67
x26 | hu410a-huf61b.log | Energy: -907452.8045689

Ru	-0.14101	-0.17690	1.60296
P	-0.99225	0.95140	-0.22018
C	-0.44118	2.76444	-0.37429
C	1.03493	2.85005	-0.78962
C	-1.28776	3.66719	-1.27910
C	-2.78779	1.00583	-0.77575
C	-3.65465	1.63798	0.32529
C	-3.31539	-0.35271	-1.25799
C	-0.14298	0.23564	-1.76101
N	0.93347	-0.52783	-1.51929
C	1.54788	-0.94519	-2.67690
C	0.80017	-0.39938	-3.68754
N	-0.23746	0.32091	-3.10767
C	2.76512	-1.82972	-2.66316
C	2.40333	-3.15983	-1.97023
C	3.22423	-2.09203	-4.10351
C	3.88398	-1.12350	-1.86999
C	-1.22595	1.05746	-3.89504
C	1.99522	0.51074	1.75344
C	1.82920	-0.67868	2.52691
C	0.88599	-0.40666	3.57024
C	0.46632	0.95890	3.45760
C	1.13390	1.51569	2.33088
H	-0.54314	3.11945	0.66383
H	1.39868	3.88184	-0.65379
H	1.14953	2.59450	-1.85733
H	1.67806	2.17691	-0.20848
H	-1.26095	3.32919	-2.32693
H	-0.86950	4.68740	-1.25382
H	-2.33807	3.72796	-0.96143
H	-2.80732	1.69948	-1.62923
H	-3.28080	2.63405	0.61149
H	-3.68870	1.02439	1.23544
H	-4.68476	1.75841	-0.04967
H	-2.70127	-0.76090	-2.07852
H	-3.33692	-1.10699	-0.45896
H	-4.34580	-0.23135	-1.63283
H	0.90635	-0.47198	-4.76474
H	1.60536	-3.68640	-2.51824
H	3.29240	-3.80924	-1.93415
H	2.06138	-2.99024	-0.93496
H	2.43736	-2.60245	-4.68306
H	3.48837	-1.15072	-4.61319
H	4.11509	-2.73855	-4.09437
H	4.77733	-1.76716	-1.84114
H	4.15749	-0.16436	-2.33896
H	3.57275	-0.93007	-0.82867
H	-2.20280	1.00838	-3.40333
H	-0.91539	2.10524	-4.01740
H	-1.29849	0.58305	-4.88283
H	2.70307	0.65594	0.94080
H	2.33291	-1.62863	2.36012
H	0.55205	-1.11603	4.32301
H	-0.23696	1.47265	4.10748
H	1.04348	2.54268	1.99005
C	-0.60739	-2.11203	0.64299
C	-1.21217	-1.99392	1.93132
C	-2.14919	-0.95407	2.17836
H	0.19027	-2.85334	0.53146
H	-1.22454	-1.98289	-0.25014
H	-0.79758	-2.55446	2.77487
H	-2.85288	-0.73499	1.38012
H	1.14513	-0.77164	-0.53708
C	-2.67731	-0.69792	3.56966
H	-2.98137	0.35510	3.69017
H	-1.91290	-0.91765	4.33250
H	-3.56224	-1.32565	3.78465

67
x27 | hu410t-huf61.log | Energy: -907440.1372360

Ru	0.01011	-0.27909	1.95067
P	-0.95525	0.91232	0.14932
C	-0.45466	2.73909	0.08084
C	1.01374	2.86377	-0.35348
C	-1.33288	3.64306	-0.79367
C	-2.76482	0.93065	-0.34464
C	-3.64074	1.53258	0.76589
C	-3.26090	-0.43317	-0.84463
C	-0.08237	0.19784	-1.32600
N	0.94154	-0.59200	-1.01344
C	1.56592	-0.99576	-2.16793
C	0.88285	-0.42168	-3.21847
N	-0.15208	0.32330	-2.67919
C	2.76702	-1.90629	-2.14750
C	2.37501	-3.23748	-1.47673
C	3.25325	-2.16463	-3.57976
C	3.88509	-1.23432	-1.32565
C	-1.08775	1.11203	-3.47314
C	2.10808	0.48488	2.12986
C	1.98010	-0.72354	2.88649
C	1.03067	-0.48666	3.93060
C	0.57683	0.87053	3.83156
C	1.23575	1.46265	2.72004
H	-0.55491	3.06477	1.12917
H	1.36227	3.89624	-0.18674
H	1.11248	2.64180	-1.42915
H	1.67845	2.17801	0.18736
H	-1.31441	3.32352	-1.84724
H	-0.93374	4.67032	-0.75435
H	-2.37930	3.67659	-0.45942
H	-2.80347	1.63123	-1.19242
H	-3.26352	2.51412	1.09451
H	-3.70207	0.88678	1.65246
H	-4.66375	1.67689	0.38053
H	-2.64120	-0.80706	-1.67642
H	-3.25796	-1.20128	-0.05725
H	-4.29750	-0.33296	-1.20787
H	1.02917	-0.48779	-4.29250
H	1.57281	-3.74184	-2.04025
H	3.24934	-3.90742	-1.43656
H	2.02227	-3.06286	-0.44695
H	2.46914	-2.65367	-4.18157
H	3.54321	-1.22319	-4.07553
H	4.13272	-2.82704	-3.56154
H	4.76584	-1.89537	-1.28067
H	4.18867	-0.27720	-1.78118
H	3.54357	-1.04049	-0.29483
H	-2.08392	1.08132	-3.01589
H	-0.74790	2.15588	-3.55636
H	-1.14739	0.67363	-4.47862
H	2.76886	0.63790	1.28089
H	2.51378	-1.65326	2.70377
H	0.71455	-1.21064	4.67713
H	-0.15066	1.35409	4.47818
H	1.11167	2.48690	2.38265
C	-0.53538	-2.23692	1.08696
C	-1.11268	-2.06316	2.37477
C	-2.02013	-0.99270	2.58572
H	0.25855	-2.97788	0.97300
H	-1.14116	-2.07917	0.19300
H	-0.69873	-2.60102	3.23231
H	-2.71049	-0.77988	1.77560
H	0.77935	-0.72853	0.42070
C	-2.53230	-0.65702	3.96483
H	-2.79852	0.40980	4.04177
H	-1.77935	-0.87746	4.73827
H	-3.44077	-1.24205	4.19872

x28-30

67
x28 | hu420a-huf63a.log | Energy: -907443.2637894

Ru	-0.05048	-0.20762	1.64215
P	-0.86685	0.87319	-0.32789
C	-0.28751	2.67350	-0.38161
C	1.22785	2.71668	-0.62937
C	-0.99291	3.58806	-1.38958
C	-2.68053	0.97804	-0.80058
C	-3.49354	1.68392	0.29244
C	-3.29728	-0.35775	-1.25259
C	-0.06466	0.11454	-1.79986
N	1.04467	-0.59238	-1.61142
C	1.50642	-0.97483	-2.84390
C	0.64839	-0.48141	-3.80464
N	-0.34352	0.21550	-3.14572
C	2.75735	-1.80558	-2.99893
C	2.58025	-3.12470	-2.22225
C	3.01255	-2.10612	-4.48213
C	3.95083	-1.02719	-2.41219
C	-1.47395	0.82730	-3.83775
C	1.95920	0.62794	2.20870
C	1.68429	-0.52580	3.01285
C	0.53011	-0.23449	3.80226
C	0.09003	1.09783	3.49574
C	0.97738	1.62353	2.51501
H	-0.51553	3.04006	0.63261
H	1.60267	3.73821	-0.45100
H	1.44354	2.44952	-1.67641
H	1.78643	2.01729	0.00518
H	-0.75692	3.28991	-2.42306
H	-0.61098	4.61440	-1.25875
H	-2.08449	3.62005	-1.25982
H	-2.66975	1.63828	-1.67827
H	-3.08946	2.68588	0.50997
H	-3.50356	1.11256	1.23201
H	-4.53652	1.80683	-0.04372
H	-2.60283	-0.94556	-1.87395
H	-3.60918	-0.99214	-0.41039
H	-4.20159	-0.15260	-1.84942
H	0.64560	-0.56979	-4.88677
H	1.74033	-3.71092	-2.63138
H	3.49811	-3.73120	-2.29570
H	2.37852	-2.91855	-1.15829
H	2.17365	-2.67110	-4.92222
H	3.14953	-1.17486	-5.05720
H	3.92652	-2.71132	-4.59005
H	4.86889	-1.63352	-2.48543
H	4.11078	-0.08357	-2.96017
H	3.76893	-0.78938	-1.35136
H	-2.39839	0.25755	-3.66473
H	-1.62060	1.86446	-3.51298
H	-1.25372	0.82888	-4.91340
H	2.77763	0.73185	1.50173
H	2.25393	-1.45179	3.02142
H	0.06568	-0.90938	4.51614
H	-0.76018	1.61265	3.93529
H	0.92808	2.61487	2.07771
C	-0.41621	-2.21775	0.77391
C	-1.15025	-2.03964	1.97262
C	-2.11595	-1.00185	2.04680
H	0.42082	-2.91757	0.77157
H	-0.89321	-2.06797	-0.19536
H	-0.82138	-2.54126	2.88710
H	-2.69724	-0.81473	1.15210
H	0.86364	-0.64940	0.41078
C	-2.81867	-0.66919	3.33931
H	-3.12066	0.39000	3.36831
H	-2.18309	-0.86938	4.21542
H	-3.73731	-1.27503	3.44197

67
x29 | hu420t-huf63.log | Energy: -907442.5727697

Ru	-0.00700	-0.21612	2.13455
P	-0.81851	0.87710	0.16225
C	-0.27083	2.68863	0.11402
C	1.23755	2.75674	-0.16869
C	-1.01483	3.61632	-0.85377
C	-2.63064	0.94634	-0.32460
C	-3.46695	1.60938	0.77800
C	-3.20657	-0.39849	-0.80079
C	0.00698	0.11790	-1.29747
N	1.08949	-0.62784	-1.09814
C	1.55408	-1.01775	-2.32746
C	0.72746	-0.48917	-3.29691
N	-0.24902	0.23612	-2.64641
C	2.77938	-1.88793	-2.47180
C	2.55375	-3.20201	-1.69920
C	3.03880	-2.19530	-3.95291
C	3.99185	-1.14911	-1.87292
C	-1.35725	0.87792	-3.34604
C	2.02125	0.62186	2.62967
C	1.75814	-0.52310	3.45266
C	0.62788	-0.22086	4.27341
C	0.18468	1.10857	3.96489
C	1.05182	1.61986	2.95617
H	-0.47998	3.03535	1.13885
H	1.60469	3.77942	0.01904
H	1.43054	2.51122	-1.22556
H	1.81994	2.05255	0.43931
H	-0.78281	3.36725	-1.90080
H	-0.66167	4.64792	-0.68781
H	-2.10524	3.61138	-0.71167
H	-2.63647	1.62140	-1.19129
H	-3.09156	2.61806	1.01520
H	-3.46302	1.02202	1.70771
H	-4.51190	1.70951	0.44037
H	-2.50810	-0.93600	-1.46178
H	-3.46479	-1.07248	0.02869
H	-4.13660	-0.21237	-1.36348
H	0.73835	-0.56817	-4.37970
H	1.69636	-3.75879	-2.11329
H	3.45073	-3.83929	-1.76903
H	2.35523	-2.99160	-0.63536
H	2.18632	-2.73239	-4.40172
H	3.21102	-1.26828	-4.52527
H	3.93397	-2.82923	-4.05313
H	4.89063	-1.78456	-1.93815
H	4.18710	-0.21072	-2.41833
H	3.80757	-0.90600	-0.81367
H	-2.28564	0.29918	-3.22942
H	-1.51732	1.89679	-2.97560
H	-1.10264	0.93222	-4.41280
H	2.81952	0.71555	1.89867
H	2.32109	-1.45369	3.45438
H	0.17873	-0.88812	5.00430
H	-0.64981	1.63335	4.42242
H	0.99224	2.60742	2.51218
C	-0.30349	-2.21563	1.20873
C	-1.03791	-2.06537	2.43047
C	-2.04171	-1.06781	2.52344
H	0.50705	-2.94879	1.19457
H	-0.82203	-2.10794	0.25389
H	-0.69507	-2.58486	3.32968
H	-2.63480	-0.88382	1.63515
H	0.75765	-0.97033	0.91535
C	-2.74443	-0.78291	3.82737
H	-3.08652	0.26353	3.87384
H	-2.08954	-0.96819	4.69275
H	-3.63712	-1.42586	3.93298

67
x30 | hu430a-huf65a.log | Energy: -907446.0969005

Ru	-0.10148	-0.22805	1.66344
P	-0.91731	0.92177	-0.28736
C	-0.39394	2.74313	-0.33677
C	1.10083	2.84064	-0.67768
C	-1.18535	3.67175	-1.26699
C	-2.72507	0.96445	-0.79519
C	-3.59304	1.62661	0.28466
C	-3.26386	-0.39946	-1.25709
C	-0.06351	0.16214	-1.72763
N	1.01623	-0.58115	-1.50213
C	1.50631	-0.96838	-2.72279
C	0.70077	-0.44212	-3.71116
N	-0.29114	0.28082	-3.08215
C	2.73810	-1.83386	-2.83949
C	2.49282	-3.15716	-2.08875
C	3.04504	-2.12436	-4.31480
C	3.92905	-1.09909	-2.19419
C	-1.38564	0.92329	-3.80101
C	1.96992	0.54641	1.93972
C	1.77968	-0.61789	2.76172
C	0.75252	-0.33699	3.71005
C	0.27530	0.99694	3.47053
C	1.04693	1.53787	2.39697
H	-0.56822	3.07956	0.69829
H	1.45407	3.87026	-0.50195
H	1.25677	2.60092	-1.74203
H	1.72229	2.14850	-0.09629
H	-0.97904	3.44668	-2.32469
H	-0.84722	4.70697	-1.09260
H	-2.27086	3.64324	-1.09760
H	-2.73461	1.62750	-1.67155
H	-3.23093	2.63771	0.52990
H	-3.61454	1.04687	1.21832
H	-4.62876	1.71992	-0.08235
H	-2.57270	-0.89686	-1.95594
H	-3.44844	-1.09273	-0.42365
H	-4.22728	-0.25169	-1.77314
H	0.73663	-0.51935	-4.79355
H	1.65111	-3.71204	-2.53639
H	3.39361	-3.79124	-2.13637
H	2.25974	-2.95841	-1.02953
H	2.20880	-2.65904	-4.79591
H	3.23152	-1.19052	-4.87131
H	3.94500	-2.75453	-4.39414
H	4.83154	-1.73119	-2.23727
H	4.13878	-0.15390	-2.72218
H	3.70927	-0.86863	-1.13878
H	-2.31572	0.34257	-3.70638
H	-1.55524	1.93943	-3.42712
H	-1.11031	0.98478	-4.86225
H	2.68988	0.64881	1.13311
H	2.32001	-1.55795	2.66813
H	0.37497	-1.02300	4.46402
H	-0.50745	1.51065	4.02233
H	0.93855	2.53728	1.99039
C	-0.57631	-2.30055	0.71059
C	-1.20765	-2.00381	2.01841
C	-2.18151	-0.99899	2.13566
H	0.04301	-3.20692	0.71503
H	-1.24823	-2.26658	-0.15558
H	-0.86895	-2.55479	2.89947
H	-2.78961	-0.78297	1.26533
H	0.26918	-1.49325	0.40010
C	-2.80001	-0.65244	3.46584
H	-3.08090	0.41234	3.50699
H	-2.10700	-0.85663	4.29740
H	-3.71884	-1.24312	3.63417

x31-33

67
x31 | hu430t-huf65.log | Energy: -907442.1321263

Ru	0.07544	-0.20957	1.98104
P	-0.87839	1.00079	0.13984
C	-0.37878	2.82872	0.10668
C	1.09502	2.94768	-0.31189
C	-1.23605	3.76627	-0.75328
C	-2.68641	1.00924	-0.36185
C	-3.56158	1.60201	0.75255
C	-3.19038	-0.35784	-0.84946
C	0.00613	0.23772	-1.26829
N	1.06828	-0.50967	-0.97634
C	1.58801	-0.95355	-2.16613
C	0.81941	-0.45437	-3.19875
N	-0.17956	0.30613	-2.62753
C	2.80845	-1.84106	-2.20917
C	2.51149	-3.13457	-1.42541
C	3.16473	-2.18466	-3.66168
C	3.98707	-1.10542	-1.54250
C	-1.24082	0.96225	-3.38028
C	2.15262	0.54779	2.22861
C	1.96645	-0.64997	3.01858
C	0.96192	-0.39387	3.98959
C	0.46012	0.93909	3.77178
C	1.24630	1.52325	2.71885
H	-0.49344	3.13871	1.15885
H	1.45345	3.97261	-0.12027
H	1.19512	2.74479	-1.39067
H	1.74870	2.23820	0.21253
H	-1.11696	3.54907	-1.82647
H	-0.88640	4.80069	-0.59801
H	-2.30519	3.73324	-0.50097
H	-2.72370	1.69867	-1.21848
H	-3.21854	2.60501	1.05246
H	-3.56694	0.96906	1.65202
H	-4.60087	1.69401	0.39577
H	-2.49646	-0.82139	-1.56802
H	-3.33976	-1.07087	-0.02564
H	-4.16633	-0.22683	-1.34596
H	0.89299	-0.56680	-4.27616
H	1.67296	-3.68655	-1.88226
H	3.39990	-3.78758	-1.42318
H	2.24779	-2.89848	-0.38119
H	2.33740	-2.72096	-4.15613
H	3.38789	-1.27270	-4.24045
H	4.05554	-2.83202	-3.68702
H	4.87994	-1.75231	-1.53333
H	4.23153	-0.17952	-2.08928
H	3.73300	-0.84113	-0.50263
H	-2.16662	0.36632	-3.36073
H	-1.44355	1.95598	-2.96400
H	-0.91031	1.07888	-4.42113
H	2.84733	0.66415	1.40122
H	2.50174	-1.58814	2.88613
H	0.58968	-1.10125	4.72584
H	-0.31363	1.43735	4.35008
H	1.12824	2.53074	2.33464
C	-0.69351	-2.61288	0.99410
C	-1.02735	-2.04889	2.35258
C	-1.98461	-1.05552	2.54087
H	-0.42869	-3.68003	1.05926
H	-1.51047	-2.46819	0.27274
H	-0.61329	-2.56193	3.22496
H	-2.64301	-0.83153	1.70767
H	0.21076	-2.12110	0.54846
C	-2.49764	-0.65676	3.90040
H	-2.73994	0.41751	3.93986
H	-1.76286	-0.87523	4.69072
H	-3.42336	-1.21285	4.13587

67
x32 | hu510a-huf67a.log | Energy: -907459.5048891

Ru	0.20886	-0.20870	1.11637
P	-1.21284	1.13654	-0.25078
C	-0.69280	2.94430	-0.40626
C	0.73890	3.02070	-0.95408
C	-1.63240	3.83385	-1.22801
C	-3.06005	1.14012	-0.56624
C	-3.77837	1.59230	0.71385
C	-3.62543	-0.16842	-1.13157
C	-0.37795	0.24473	-1.60087
N	0.57530	-0.49373	-1.02150
C	1.28076	-1.12645	-2.02081
C	0.70285	-0.75660	-3.22388
N	-0.33549	0.10926	-2.94612
C	2.52469	-1.95646	-1.79819
C	2.29309	-3.02895	-0.71780
C	2.94028	-2.63567	-3.11202
C	3.65597	-1.00690	-1.34845
C	-1.22334	0.74340	-3.91124
C	2.16531	0.81211	1.53369
C	2.21595	-0.55576	1.99430
C	1.23695	-0.69720	3.01552
C	0.55434	0.55887	3.17450
C	1.16125	1.49024	2.27267
H	-0.69564	3.29774	0.63955
H	1.11540	4.05242	-0.86304
H	0.75501	2.74372	-2.02153
H	1.42085	2.34554	-0.42153
H	-1.72063	3.47047	-2.26672
H	-1.21507	4.85356	-1.26997
H	-2.64081	3.90110	-0.79294
H	-3.20220	1.91444	-1.33577
H	-3.41322	2.57297	1.06281
H	-3.63283	0.86319	1.52764
H	-4.86020	1.68293	0.52255
H	-3.05761	-0.51628	-2.00941
H	-3.63432	-0.98050	-0.39151
H	-4.66800	0.00648	-1.44552
H	0.95102	-1.03597	-4.24237
H	1.63884	-3.83117	-1.09393
H	3.25827	-3.48272	-0.43972
H	1.82979	-2.59240	0.17907
H	2.14107	-3.29585	-3.48719
H	3.17971	-1.89093	-3.88917
H	3.84043	-3.24658	-2.94157
H	4.58494	-1.58059	-1.19613
H	3.84344	-0.23454	-2.11260
H	3.39671	-0.50725	-0.40523
H	-1.82018	-0.01738	-4.43753
H	-1.89686	1.42301	-3.37185
H	-0.63593	1.31843	-4.64293
H	2.79395	1.24448	0.76000
H	2.90034	-1.32525	1.65030
H	1.03034	-1.61156	3.56379
H	-0.23776	0.77343	3.88492
H	0.87037	2.52994	2.14175
C	-1.17279	-2.76087	-0.28265
C	-0.78027	-2.20966	1.06861
C	-1.62992	-1.33424	1.76670
H	-1.80622	-3.65588	-0.14215
H	-1.75261	-2.02620	-0.85858
H	-0.14601	-2.87131	1.67026
H	-2.48805	-0.96174	1.20741
H	-0.30522	-3.05591	-0.88433
C	-1.89778	-1.40340	3.25141
H	-2.16043	-0.42037	3.67402
H	-1.04840	-1.81225	3.81634
H	-2.75917	-2.07522	3.42315

67
x33 | hu510t-huf67.log | Energy: -907439.1703067

Ru	0.43809	0.18567	1.52042
P	-1.03266	1.45344	0.09672
C	-0.51447	3.21751	-0.28676
C	0.93034	3.22129	-0.80364
C	-1.44516	3.95953	-1.25241
C	-2.89113	1.42254	-0.08715
C	-3.50553	2.13443	1.12694
C	-3.44081	0.00360	-0.26159
C	-0.27363	0.41247	-1.19544
N	0.69502	-0.28403	-0.58342
C	1.37556	-0.99293	-1.54441
C	0.76533	-0.72753	-2.75795
N	-0.26864	0.15875	-2.52450
C	2.62216	-1.79399	-1.25625
C	2.39631	-2.75409	-0.07274
C	3.03338	-2.59563	-2.49939
C	3.74236	-0.78865	-0.90723
C	-1.15547	0.74265	-3.52239
C	2.20238	1.27758	2.03831
C	2.43270	-0.09531	2.42681
C	1.45525	-0.44341	3.38916
C	0.61026	0.69993	3.64143
C	1.09075	1.76575	2.81686
H	-0.54466	3.71689	0.69792
H	1.30673	4.25599	-0.84741
H	0.97422	2.79763	-1.82132
H	1.59448	2.62502	-0.16352
H	-1.50025	3.44165	-2.22553
H	-1.04465	4.97018	-1.43684
H	-2.46537	4.06880	-0.85519
H	-3.11823	2.00358	-0.99599
H	-3.13958	3.16993	1.22803
H	-3.26700	1.59057	2.05715
H	-4.60229	2.17070	1.02286
H	-3.00254	-0.50143	-1.13708
H	-3.24790	-0.62068	0.62425
H	-4.53269	0.05560	-0.40614
H	0.97861	-1.09938	-3.75483
H	1.73832	-3.58801	-0.36209
H	3.36249	-3.18057	0.24260
H	1.93819	-2.23351	0.78146
H	2.23983	-3.30148	-2.79608
H	3.25117	-1.92927	-3.35066
H	3.94472	-3.17429	-2.28171
H	4.66588	-1.33110	-0.64557
H	3.95421	-0.13238	-1.76751
H	3.44842	-0.15658	-0.05652
H	-1.55771	-0.04978	-4.17045
H	-1.98527	1.24217	-3.00435
H	-0.61229	1.47769	-4.13699
H	2.81295	1.85591	1.35009
H	3.19684	-0.75609	2.02898
H	1.33418	-1.43273	3.82376
H	-0.21153	0.75217	4.35024
H	0.67810	2.77156	2.77291
C	-1.17692	-2.87048	-0.44285
C	-1.16534	-2.93921	1.05189
C	-1.22212	-1.91361	1.91781
H	-2.01559	-3.47727	-0.82886
H	-1.29303	-1.84378	-0.80788
H	-1.18646	-3.94971	1.48172
H	-1.35905	-0.87984	1.51031
H	-0.25620	-3.29259	-0.87644
C	-1.47742	-2.08683	3.39139
H	-0.78507	-1.52103	4.02775
H	-1.41816	-3.15185	3.66833
H	-2.49438	-1.73213	3.64101

x34-36

67			
x34 | hu510z-huf67b.log | Energy: -907439.7136546			
Ru	0.22767	0.14383	1.18938
P	-1.16031	1.39057	-0.28511
C	-0.58770	3.14039	-0.66621
C	0.80854	3.09407	-1.30531
C	-1.55808	3.94892	-1.53468
C	-3.01512	1.38274	-0.47284
C	-3.61640	2.07275	0.76115
C	-3.56206	-0.03578	-0.65720
C	-0.38456	0.32995	-1.54850
N	0.56049	-0.37067	-0.90438
C	1.23510	-1.12022	-1.83790
C	0.65346	-0.86431	-3.06803
N	-0.36073	0.05183	-2.87147
C	2.43435	-1.97955	-1.51784
C	2.20721	-2.76535	-0.21453
C	2.69914	-2.95923	-2.67099
C	3.65278	-1.04516	-1.35482
C	-1.22579	0.62799	-3.89220
C	1.65584	1.60023	1.86131
C	2.27309	0.30522	2.00540
C	1.50288	-0.46455	2.90981
C	0.39057	0.35176	3.35648
C	0.50682	1.62784	2.73928
H	-0.51232	3.61313	0.32875
H	1.24429	4.10623	-1.31887
H	0.73807	2.73898	-2.34719
H	1.48918	2.41871	-0.76729
H	-1.69912	3.47046	-2.51946
H	-1.13754	4.95278	-1.71139
H	-2.54421	4.07285	-1.06269
H	-3.24890	1.97991	-1.36933
H	-3.23642	3.10033	0.88819
H	-3.38189	1.50130	1.67563
H	-4.71275	2.12615	0.66099
H	-3.17489	-0.50761	-1.57396
H	-3.30387	-0.68362	0.19569
H	-4.66139	0.00590	-0.73055
H	0.87013	-1.26738	-4.05186
H	1.37222	-3.47464	-0.31898
H	3.11881	-3.33348	0.03070
H	1.96989	-2.08912	0.61951
H	1.83779	-3.62990	-2.82724
H	2.90492	-2.42392	-3.61292
H	3.58024	-3.57691	-2.43664
H	4.53997	-1.62985	-1.06014
H	3.87418	-0.52590	-2.30175
H	3.45913	-0.28297	-0.58414
H	-1.71340	-0.17355	-4.46696
H	-1.99393	1.23662	-3.39571
H	-0.64075	1.26400	-4.57463
H	2.04190	2.43250	1.28001
H	3.15474	-0.04077	1.47259
H	1.70296	-1.49372	3.19642
H	-0.38280	0.05098	4.05714
H	-0.16751	2.46837	2.88732
C	-1.38785	-2.90626	-0.96412
C	-1.29903	-3.05937	0.52109
C	-1.23222	-2.09890	1.45591
H	-2.25565	-3.47273	-1.34576
H	-1.49211	-1.85915	-1.26756
H	-1.33316	-4.09333	0.88999
H	-1.39173	-1.02961	1.13266
H	-0.49409	-3.32420	-1.45816
C	-1.29527	-2.38616	2.93274
H	-0.32047	-2.26607	3.42897
H	-1.63382	-3.42046	3.10336
H	-2.00190	-1.70503	3.43577

67			
x35 | gu210t-guf15.log | Energy: -907442.7350876			
Ru	-0.53600	-0.68321	1.91091
P	-1.51825	0.16832	-0.11274
C	-1.85200	2.01603	-0.26964
C	-0.51623	2.77027	-0.25592
C	-2.68239	2.42200	-1.49256
C	-3.07754	-0.60829	-0.79085
C	-4.23313	-0.35899	0.18824
C	-2.93691	-2.08648	-1.17250
C	-0.15218	-0.13314	-1.28898
N	1.05312	-0.20793	-0.72812
C	1.96516	-0.32620	-1.74541
C	1.28695	-0.33214	-2.94850
N	-0.05583	-0.20709	-2.65541
C	3.44382	-0.43120	-1.46100
C	3.69378	-1.64493	-0.54436
C	4.22763	-0.59631	-2.76963
C	3.90144	0.84961	-0.73474
C	-1.10765	-0.13473	-3.66160
C	0.25038	-2.28473	3.23384
C	0.55174	-2.65705	1.88446
C	-0.65953	-2.77008	1.15817
C	-1.74638	-2.44069	2.05961
C	-1.17428	-2.15481	3.34683
H	-2.42604	2.26325	0.63872
H	-0.70090	3.85096	-0.14226
H	0.02314	2.60805	-1.20339
H	0.14416	2.44067	0.55637
H	-2.19728	2.10207	-2.42851
H	-2.76200	3.52152	-1.52102
H	-3.70410	2.01470	-1.46607
H	-3.28787	-0.04147	-1.71002
H	-4.39204	0.71735	0.36324
H	-4.03905	-0.83433	1.16300
H	-5.16636	-0.77802	-0.22269
H	-2.02248	-2.27757	-1.75779
H	-2.92279	-2.73863	-0.28919
H	-3.80392	-2.38414	-1.78522
H	1.63103	-0.43251	-3.97350
H	3.37253	-2.58006	-1.03338
H	4.76757	-1.72510	-0.30758
H	3.13401	-1.52890	0.39849
H	3.92120	-1.51265	-3.30155
H	4.06825	0.26709	-3.43713
H	5.30582	-0.66833	-2.55608
H	4.97369	0.78062	-0.48693
H	3.74574	1.73738	-1.36997
H	3.33216	0.98487	0.20000
H	-0.79459	-0.71490	-4.54108
H	-2.03340	-0.57012	-3.26821
H	-1.29209	0.90671	-3.96952
H	0.97614	-2.11886	4.02605
H	1.54895	-2.75981	1.46073
H	-0.74318	-3.03523	0.10959
H	-2.80843	-2.47293	1.83820
H	-1.72904	-1.88642	4.24348
C	-1.17053	1.18882	2.97196
C	0.07435	0.71763	3.41297
C	1.33738	1.04505	2.65581
H	-2.04969	1.05846	3.60678
H	-1.21060	2.01803	2.26809
H	0.16795	0.25622	4.39817
H	2.16496	0.42517	3.03081
H	1.20411	0.74005	1.57444
C	1.73364	2.53210	2.66808
H	2.57953	2.71394	1.98634
H	2.03163	2.82856	3.68665
H	0.89272	3.17250	2.36304

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x36 | gu220a-guf13a.log | Energy: -907447.1331195			
Ru	-0.42884	-0.30262	1.63988
P	-1.14281	0.47552	-0.49625
C	-1.38985	2.33927	-0.68655
C	-0.03899	3.00193	-0.99082
C	-2.46598	2.76786	-1.69084
C	-2.72598	-0.30519	-1.12489
C	-3.81200	-0.22575	-0.04523
C	-2.51266	-1.74066	-1.61921
C	0.17369	0.08501	-1.71269
N	1.39242	-0.20783	-1.26783
C	2.20179	-0.33247	-2.36950
C	1.44964	-0.11036	-3.50490
N	0.16334	0.15255	-3.08839
C	3.66368	-0.69400	-2.24843
C	3.78167	-2.13051	-1.70177
C	4.34361	-0.61506	-3.62264
C	4.34921	0.28026	-1.27256
C	-0.91455	0.50263	-4.00258
C	0.78860	-1.73571	2.81922
C	1.19769	-1.84930	1.44546
C	0.07407	-2.26498	0.69028
C	-1.05642	-2.39680	1.57665
C	-0.59442	-2.09014	2.90018
H	-1.72592	2.66741	0.30669
H	-0.12896	4.09474	-0.88005
H	0.27437	2.78128	-2.02408
H	0.75992	2.64707	-0.32212
H	-2.23280	2.43037	-2.71120
H	-2.51723	3.86944	-1.70827
H	-3.46274	2.38913	-1.41762
H	-3.05026	0.31283	-1.97523
H	-3.99451	0.81235	0.27664
H	-3.51861	-0.80694	0.84238
H	-4.75712	-0.63159	-0.44199
H	-1.71794	-1.80357	-2.37943
H	-2.24830	-2.41559	-0.79301
H	-3.44895	-2.11429	-2.06589
H	1.70509	-0.12967	-4.56001
H	3.31059	-2.85215	-2.38990
H	4.84311	-2.40430	-1.58182
H	3.28787	-2.21543	-0.72026
H	3.88425	-1.32187	-4.33411
H	4.27131	0.40236	-4.04190
H	5.41015	-0.87381	-3.52845
H	5.40976	0.00522	-1.14941
H	4.29826	1.31460	-1.65183
H	3.85804	0.24772	-0.28648
H	-1.87907	0.18733	-3.59082
H	-0.93268	1.58746	-4.19422
H	-0.75388	-0.02283	-4.95457
H	1.41975	-1.43148	3.65172
H	2.17026	-1.60279	1.03085
H	0.06504	-2.40029	-0.38666
H	-2.05369	-2.73600	1.31353
H	-1.20382	-2.09544	3.80175
C	-2.03106	0.94485	2.56971
C	-0.80530	0.98689	3.26353
C	0.36901	1.70183	2.68961
H	-2.85806	0.39083	3.01901
H	-2.32522	1.75448	1.90425
H	-0.69082	0.49831	4.23313
H	1.26610	1.51457	3.29425
H	0.66189	1.20400	1.63365
C	0.22045	3.19263	2.37367
H	1.07071	3.56218	1.78191
H	0.18752	3.74778	3.32478
H	-0.70729	3.40356	1.82725

x37-39

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x37 | gu220t-guf13.log | Energy: -907442.5355772

Ru	-0.49398	-0.40710	2.14225
P	-1.19783	0.36011	0.00725
C	-1.55676	2.20415	-0.22686
C	-0.27782	2.92981	-0.66891
C	-2.74400	2.55368	-1.13380
C	-2.73286	-0.50873	-0.64483
C	-3.84110	-0.50520	0.41451
C	-2.44989	-1.92265	-1.16557
C	0.13743	-0.00607	-1.19698
N	1.34028	-0.37485	-0.76866
C	2.13386	-0.52068	-1.87924
C	1.38819	-0.23262	-3.00380
N	0.12038	0.08875	-2.57109
C	3.57405	-0.96457	-1.77434
C	3.61538	-2.40477	-1.22615
C	4.24181	-0.92559	-3.15607
C	4.32461	-0.03012	-0.80731
C	-0.94727	0.52315	-3.45951
C	0.71344	-1.87649	3.32495
C	1.12701	-1.96599	1.95851
C	0.00377	-2.38298	1.19141
C	-1.11565	-2.56887	2.07472
C	-0.66860	-2.25234	3.39433
H	-1.82085	2.54773	0.78175
H	-0.41726	4.01879	-0.56999
H	-0.04914	2.70554	-1.72299
H	0.59692	2.63313	-0.07141
H	-2.59136	2.21551	-2.16875
H	-2.85677	3.65051	-1.15614
H	-3.68850	2.12569	-0.76564
H	-3.07532	0.10540	-1.49013
H	-4.07842	0.51367	0.75976
H	-3.54004	-1.09634	1.29246
H	-4.75848	-0.94389	-0.01141
H	-1.62488	-1.93979	-1.89526
H	-2.20011	-2.61293	-0.34790
H	-3.35552	-2.31236	-1.65941
H	1.63672	-0.23574	-4.06065
H	3.09652	-3.09918	-1.90802
H	4.66062	-2.73876	-1.11710
H	3.12794	-2.45943	-0.23927
H	3.73308	-1.60356	-3.86204
H	4.22539	0.09453	-3.57471
H	5.29225	-1.24681	-3.07395
H	5.36860	-0.36599	-0.69355
H	4.32997	1.00480	-1.18821
H	3.84197	-0.03209	0.18357
H	-1.90803	0.10348	-3.13776
H	-1.01587	1.62220	-3.48590
H	-0.72943	0.15691	-4.47202
H	1.33602	-1.57352	4.16426
H	2.09843	-1.70932	1.54836
H	0.00699	-2.51767	0.11503
H	-2.10592	-2.91969	1.80028
H	-1.27718	-2.27816	4.29614
C	-2.18595	0.74118	3.01358
C	-1.00874	0.81305	3.80210
C	0.17899	1.44302	3.28088
H	-3.02128	0.15465	3.40180
H	-2.46747	1.56871	2.36411
H	-0.93555	0.23950	4.72914
H	1.07807	1.22246	3.86595
H	0.68451	0.67131	1.87829
C	0.17838	2.85229	2.72882
H	1.01852	3.02596	2.04166
H	0.28656	3.54538	3.58124
H	-0.75879	3.09976	2.21818

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x38 | gu220z-guf13b.log | Energy: -907444.1177545

Ru	-0.37098	-0.17521	1.66077
P	-1.09481	0.56250	-0.46538
C	-1.46066	2.40340	-0.69372
C	-0.18121	3.13563	-1.12173
C	-2.64776	2.74886	-1.60231
C	-2.61862	-0.32321	-1.12294
C	-3.74289	-0.33232	-0.08182
C	-2.31446	-1.73717	-1.63165
C	0.23762	0.19467	-1.67619
N	1.43741	-0.19576	-1.26031
C	2.21944	-0.35446	-2.37668
C	1.46907	-0.05277	-3.49408
N	0.21021	0.28955	-3.05042
C	3.65349	-0.81934	-2.28153
C	3.67851	-2.25208	-1.71334
C	4.30615	-0.80913	-3.67089
C	4.42829	0.11712	-1.33557
C	-0.85319	0.74499	-3.93373
C	0.85930	-1.63389	2.87150
C	1.26243	-1.72159	1.50778
C	0.13532	-2.15709	0.74516
C	-0.96868	-2.36413	1.63956
C	-0.51780	-2.03006	2.95140
H	-1.72782	2.74221	0.31540
H	-0.33342	4.22393	-1.03493
H	0.07017	2.90430	-2.16914
H	0.68249	2.85385	-0.50097
H	-2.49140	2.41862	-2.63899
H	-2.76918	3.84482	-1.61787
H	-3.58961	2.31114	-1.23861
H	-2.95588	0.28595	-1.97411
H	-3.99453	0.68171	0.26632
H	-3.45255	-0.92985	0.79529
H	-4.64910	-0.77582	-0.52612
H	-1.48546	-1.75099	-2.35658
H	-2.06112	-2.41571	-0.80470
H	-3.21265	-2.14273	-2.12625
H	1.70889	-0.05617	-4.55292
H	3.14201	-2.94813	-2.37976
H	4.71965	-2.60038	-1.61043
H	3.20090	-2.28481	-0.72064
H	3.77857	-1.48762	-4.36238
H	4.30178	0.20575	-4.10243
H	5.35217	-1.14606	-3.59610
H	5.46821	-0.23303	-1.22793
H	4.44521	1.14639	-1.73104
H	3.95647	0.13690	-0.33968
H	-1.81783	0.32572	-3.62321
H	-0.91442	1.84458	-3.94240
H	-0.63391	0.39427	-4.95130
H	1.48151	-1.31242	3.70381
H	2.22885	-1.45768	1.09060
H	0.13898	-2.30925	-0.32866
H	-1.95666	-2.72882	1.37351
H	-1.11723	-2.06354	3.85885
C	-2.15727	0.88994	2.47326
C	-1.05113	0.96910	3.35741
C	0.15351	1.60741	2.95159
H	-3.00102	0.26338	2.76826
H	-2.41329	1.73497	1.83674
H	-1.03907	0.33602	4.24780
H	1.02139	1.36902	3.57436
H	0.79079	0.71019	1.04829
C	0.22431	2.98241	2.33556
H	1.09256	3.08723	1.66965
H	0.33385	3.72204	3.14930
H	-0.68392	3.23938	1.77855

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x39 | gu230t-guf11.log | Energy: -907435.8845165

Ru	-0.48460	-0.55514	2.01300
P	-1.40584	0.38072	0.03821
C	-1.76401	2.24760	-0.23102
C	-0.68932	2.94556	-1.08303
C	-3.14874	2.58622	-0.80119
C	-2.90478	-0.48507	-0.70521
C	-4.03609	-0.57289	0.32935
C	-2.57312	-1.86166	-1.29513
C	-0.03818	0.06430	-1.16169
N	1.13322	-0.22281	-0.59954
C	2.08507	-0.32654	-1.58962
C	1.44640	-0.09339	-2.78975
N	0.11488	0.15424	-2.50425
C	3.52546	-0.65167	-1.28708
C	3.61129	-2.10692	-0.78474
C	4.37532	-0.49237	-2.55519
C	4.03486	0.29966	-0.18706
C	-0.92573	0.40919	-3.49217
C	0.20728	-2.15590	3.43996
C	0.77428	-2.39279	2.15080
C	-0.30261	-2.62593	1.23900
C	-1.53691	-2.58229	1.98543
C	-1.21659	-2.28185	3.33334
H	-1.71604	2.66634	0.78422
H	-0.81590	4.03651	-0.98633
H	-0.81092	2.69239	-2.14717
H	0.33420	2.69149	-0.78132
H	-3.25145	2.24982	-1.84639
H	-3.26203	3.68305	-0.80284
H	-3.97743	2.16457	-0.21726
H	-3.24159	0.16094	-1.52957
H	-4.32432	0.41312	0.72284
H	-3.73611	-1.18835	1.18883
H	-4.92593	-1.02712	-0.13700
H	-1.74916	-1.81678	-2.02432
H	-2.29826	-2.58551	-0.51717
H	-3.46545	-2.25384	-1.81093
H	1.81926	-0.08531	-3.80972
H	3.26301	-2.81156	-1.55772
H	4.65432	-2.35506	-0.52889
H	2.99113	-2.24357	0.11591
H	4.03459	-1.17741	-3.34953
H	4.32872	0.54127	-2.93593
H	5.42672	-0.73054	-2.33069
H	5.08192	0.05890	0.05759
H	3.98670	1.34934	-0.52082
H	3.43031	0.19817	0.72917
H	-1.80005	0.83719	-2.98761
H	-0.55421	1.12717	-4.23737
H	-1.21641	-0.52610	-3.99597
H	0.76247	-1.93248	4.34769
H	1.83278	-2.38937	1.90629
H	-0.19682	-2.85272	0.18181
H	-2.52948	-2.78391	1.59840
H	-1.92984	-2.14412	4.14320
C	-1.39454	1.11870	3.17380
C	-0.03861	0.89293	3.52592
C	1.00060	1.02026	2.55182
H	-2.15982	0.85321	3.90704
H	-1.65968	1.93923	2.51028
H	0.18011	0.38915	4.47062
H	1.95135	0.57150	2.86185
H	0.79065	-0.32894	0.76593
C	1.18104	2.23328	1.67454
H	1.66012	1.96879	0.72018
H	1.83652	2.96269	2.18399
H	0.22598	2.73243	1.47023

x40-42

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x40 | gu230z-guf11b.log | Energy: -907447.8471876

Ru	-0.49554	-0.35111	1.62314
P	-1.26878	0.57935	-0.35391
C	-1.61141	2.44813	-0.66873
C	-0.52080	3.15441	-1.49277
C	-2.98431	2.79005	-1.26424
C	-2.72796	-0.28124	-1.19892
C	-3.90251	-0.37822	-0.21404
C	-2.38660	-1.66330	-1.77202
C	0.10480	0.28820	-1.60196
N	1.32105	-0.00658	-1.11872
C	2.25504	-0.12612	-2.12614
C	1.55829	0.10267	-3.28553
N	0.23774	0.35924	-2.94089
C	3.70012	-0.44177	-1.84957
C	3.79073	-1.84377	-1.21275
C	4.49125	-0.41081	-3.16411
C	4.25895	0.60873	-0.86782
C	-0.83228	0.61516	-3.90156
C	0.26870	-1.94264	2.98173
C	0.84026	-2.15210	1.68436
C	-0.23107	-2.40307	0.77901
C	-1.46924	-2.39582	1.52553
C	-1.15316	-2.10195	2.87914
H	-1.58469	2.86312	0.34841
H	-0.65180	4.24458	-1.39283
H	-0.61411	2.91215	-2.56279
H	0.49687	2.90687	-1.16599
H	-3.07338	2.45763	-2.31223
H	-3.09661	3.88719	-1.26436
H	-3.82302	2.36806	-0.69562
H	-3.02866	0.36807	-2.03361
H	-4.20869	0.60251	0.17803
H	-3.63183	-1.00044	0.65006
H	-4.77024	-0.82965	-0.72334
H	-1.50012	-1.64970	-2.42625
H	-2.20895	-2.39795	-0.97687
H	-3.24197	-2.02343	-2.36782
H	1.88858	0.10460	-4.31893
H	3.39595	-2.61459	-1.89424
H	4.84307	-2.07934	-0.98806
H	3.22337	-1.88775	-0.26799
H	4.10784	-1.16107	-3.87534
H	4.44014	0.58499	-3.63425
H	5.54849	-0.64167	-2.96269
H	5.31379	0.38099	-0.64755
H	4.20123	1.62185	-1.29772
H	3.70416	0.60262	0.08611
H	-1.63209	1.17447	-3.40484
H	-0.42960	1.21409	-4.72972
H	-1.23021	-0.33603	-4.28653
H	0.82162	-1.71888	3.89080
H	1.90057	-2.14023	1.44384
H	-0.12495	-2.62431	-0.27997
H	-2.45541	-2.63037	1.13973
H	-1.86525	-2.00885	3.69593
C	-1.38424	1.33391	2.77284
C	-0.02686	1.08761	3.11463
C	1.01706	1.19131	2.13198
H	-2.14394	1.09597	3.52143
H	-1.64150	2.16242	2.11361
H	0.18647	0.59154	4.06534
H	1.95832	0.73377	2.46474
H	1.42793	-0.11503	-0.09522
C	1.24984	2.44413	1.31647
H	1.76763	2.23071	0.36637
H	1.89061	3.14919	1.87831
H	0.31133	2.96613	1.09175

67
x41 | gu310t-guf23.log | Energy: -907436.9503476

Ru	-0.26406	-0.37762	2.25449
P	-1.06091	0.53639	0.25799
C	-0.80141	2.40063	0.07891
C	0.59137	2.76728	0.60113
C	-1.05790	3.00982	-1.30101
C	-2.75715	0.27362	-0.54603
C	-3.95490	0.96890	0.11614
C	-3.01397	-1.21512	-0.81175
C	-0.05442	-0.03817	-1.26887
N	1.16744	-0.55559	-1.06035
C	1.82071	-0.88489	-2.22767
C	0.93771	-0.54923	-3.21527
N	-0.20735	-0.03364	-2.62102
C	3.19124	-1.50966	-2.26517
C	3.08273	-2.98535	-1.82569
C	3.73624	-1.43880	-3.69952
C	4.12993	-0.75242	-1.30625
C	-1.36553	0.34082	-3.44124
C	1.69787	0.11589	3.25419
C	1.97973	-0.30801	1.92977
C	1.55609	-1.69322	1.78963
C	0.98578	-2.08746	3.02844
C	1.07246	-0.97833	3.93189
H	-1.55223	2.79591	0.77956
H	0.70886	3.86345	0.61830
H	1.37806	2.35692	-0.05822
H	0.74374	2.36791	1.61510
H	-0.33332	2.63389	-2.04344
H	-0.92903	4.10367	-1.24675
H	-2.08088	2.81913	-1.66230
H	-2.64750	0.77990	-1.50993
H	-3.76632	2.04123	0.27898
H	-4.24697	0.51840	1.07481
H	-4.81907	0.88067	-0.56379
H	-2.19356	-1.67634	-1.38775
H	-3.11561	-1.78430	0.12302
H	-3.94697	-1.33122	-1.38931
H	1.02059	-0.63627	-4.29269
H	2.41643	-3.54912	-2.49805
H	4.08175	-3.44925	-1.85098
H	2.69689	-3.07140	-0.79652
H	3.08658	-1.99075	-4.39889
H	3.82198	-0.39446	-4.04111
H	4.73568	-1.89875	-3.73416
H	5.13635	-1.19625	-1.35498
H	4.20480	0.31286	-1.57952
H	3.78691	-0.82918	-0.26075
H	-2.19978	-0.34680	-3.24871
H	-1.66412	1.37393	-3.23594
H	-1.06445	0.25855	-4.49332
H	1.91641	1.09484	3.67225
H	2.51321	0.30437	1.20447
H	1.71059	-2.36049	0.94480
H	0.56553	-3.06488	3.25298
H	0.72969	-0.97027	4.96318
C	-2.31426	-1.18157	2.59932
C	-1.82821	-0.42954	3.69995
C	-1.45184	0.95064	3.57196
H	-2.43097	-2.25988	2.73397
H	-3.01825	-0.72822	1.90888
H	-1.50193	-0.98098	4.58571
H	-0.82488	1.29082	4.40594
H	1.49906	-0.70447	-0.11423
C	-2.37470	2.04757	3.09700
H	-1.80667	2.94606	2.80570
H	-3.05199	2.35059	3.91795
H	-3.00133	1.73719	2.25477

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x42 | gu320a-guf25a.log | Energy: -907441.0337839

Ru	-0.11034	-0.12054	1.67961
P	-1.04322	0.77919	-0.24922
C	-1.14535	2.66574	-0.22753
C	0.26199	3.27447	-0.30168
C	-2.13830	3.36438	-1.16445
C	-2.54681	0.21223	-1.28840
C	-3.93115	0.37112	-0.64544
C	-2.36275	-1.22892	-1.79309
C	0.16724	0.37304	-1.65603
N	0.92355	-0.72385	-1.48868
C	1.60529	-1.07240	-2.63276
C	1.23802	-0.12933	-3.55589
N	0.35280	0.74781	-2.94309
C	2.56479	-2.23177	-2.69504
C	1.94345	-3.45142	-1.98777
C	2.85803	-2.56937	-4.16421
C	3.87435	-1.82630	-1.98412
C	-0.27229	1.86054	-3.65631
C	1.63261	1.13374	2.35979
C	2.00591	0.44154	1.16435
C	2.00105	-0.97431	1.41448
C	1.55603	-1.15694	2.75873
C	1.33627	0.13417	3.33848
H	-1.50238	2.81366	0.80344
H	0.20278	4.36368	-0.14178
H	0.73764	3.10548	-1.28268
H	0.91702	2.84884	0.47105
H	-1.85881	3.28797	-2.22351
H	-2.16303	4.43790	-0.91183
H	-3.15966	2.97429	-1.05457
H	-2.51374	0.89578	-2.15258
H	-4.07668	1.34485	-0.15862
H	-4.12367	-0.41815	0.09657
H	-4.69124	0.26771	-1.43791
H	-1.51465	-1.33257	-2.48797
H	-2.20829	-1.92683	-0.95524
H	-3.27290	-1.54034	-2.33224
H	1.53606	0.00043	-4.59064
H	0.99842	-3.75191	-2.46882
H	2.64527	-4.29832	-2.03640
H	1.74366	-3.24650	-0.92158
H	1.93763	-2.85809	-4.69730
H	3.31745	-1.71231	-4.68421
H	3.56637	-3.41065	-4.21268
H	4.57770	-2.67442	-1.99776
H	4.34759	-0.97137	-2.49348
H	3.69302	-1.54698	-0.93334
H	-1.36337	1.73705	-3.67143
H	-0.01472	2.81327	-3.17769
H	0.10528	1.85731	-4.68662
H	1.59911	2.20969	2.50475
H	2.29802	0.91815	0.23112
H	2.36250	-1.75991	0.75522
H	1.41834	-2.11174	3.26110
H	0.98534	0.32109	4.35092
C	-1.74679	-1.63678	1.76030
C	-1.58588	-0.92682	2.98041
C	-1.75901	0.49655	3.02919
H	-1.47757	-2.69594	1.74672
H	-2.54717	-1.35427	1.07817
H	-1.09272	-1.43319	3.81581
H	-1.34226	0.95447	3.93383
H	0.90555	-1.20619	-0.57971
C	-3.01489	1.19133	2.56003
H	-2.82763	2.22427	2.22307
H	-3.74006	1.25659	3.39302
H	-3.49937	0.63788	1.75089

x43-45

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x43 | gu320t-guf25.log | Energy: -907439.3409642

Ru	0.02747	-0.08822	2.19422
P	-0.93192	0.86624	0.29367
C	-0.78741	2.76983	0.31642
C	0.59084	3.26662	-0.14586
C	-1.91114	3.58148	-0.34273
C	-2.50216	0.54311	-0.76555
C	-3.85914	0.78216	-0.08480
C	-2.50877	-0.83621	-1.44636
C	0.22052	0.32228	-1.11318
N	0.99038	-0.75493	-0.89224
C	1.64819	-1.16641	-2.03065
C	1.24801	-0.28854	-3.00404
N	0.37181	0.61818	-2.42225
C	2.61877	-2.31703	-2.03203
C	1.97609	-3.52616	-1.32456
C	2.97724	-2.68100	-3.47951
C	3.89036	-1.88550	-1.27005
C	-0.35834	1.61956	-3.19329
C	1.56801	1.47089	2.67593
C	2.10469	0.58766	1.66677
C	2.21350	-0.72559	2.21354
C	1.70778	-0.67128	3.55195
C	1.32756	0.68236	3.83478
H	-0.85115	2.93557	1.40346
H	0.69283	4.33504	0.10779
H	0.71726	3.17617	-1.23628
H	1.41516	2.72594	0.33614
H	-1.93469	3.48135	-1.43989
H	-1.74548	4.64933	-0.12213
H	-2.90520	3.31135	0.03755
H	-2.39204	1.30860	-1.54842
H	-3.84732	1.58578	0.66241
H	-4.21394	-0.13331	0.41083
H	-4.59759	1.04144	-0.86160
H	-1.64171	-1.00703	-2.10315
H	-2.54287	-1.65185	-0.70869
H	-3.41670	-0.91566	-2.06808
H	1.51826	-0.22355	-4.05273
H	1.05893	-3.84878	-1.84359
H	2.68802	-4.36619	-1.31731
H	1.72192	-3.29379	-0.27562
H	2.08240	-2.98865	-4.04476
H	3.45061	-1.82997	-3.99682
H	3.69268	-3.51760	-3.48155
H	4.60299	-2.72517	-1.23692
H	4.37743	-1.03231	-1.76931
H	3.65544	-1.59357	-0.23298
H	-1.20852	1.14443	-3.70680
H	-0.72177	2.40043	-2.52155
H	0.32114	2.06363	-3.93393
H	1.41852	2.54269	2.58513
H	2.43298	0.88441	0.67373
H	2.63993	-1.59982	1.72652
H	1.64644	-1.50689	4.24458
H	0.90307	1.03923	4.77002
C	-1.26217	-1.89280	1.91751
C	-1.26726	-1.40567	3.25394
C	-1.72368	-0.07662	3.53905
H	-0.80488	-2.86822	1.73096
H	-2.10007	-1.64317	1.26630
H	-0.70717	-1.95732	4.01378
H	-1.43858	0.27896	4.53563
H	1.00297	-1.16950	0.05230
C	-3.06604	0.44684	3.08873
H	-3.03377	1.51738	2.82745
H	-3.81315	0.32643	3.89564
H	-3.42556	-0.11704	2.22252

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x44 | gu410a-guf27b.log | Energy: -907442.7737108

Ru	-0.06116	-0.00458	1.66945
P	-1.01944	0.96930	-0.23611
C	-0.51218	2.80437	-0.44661
C	0.88512	2.93489	-1.07058
C	-1.49303	3.75186	-1.15168
C	-2.73189	0.94243	-1.06494
C	-3.84130	1.62298	-0.23363
C	-3.16600	-0.44062	-1.56793
C	-0.07888	0.15510	-1.67593
N	0.82778	-0.78258	-1.36817
C	1.44321	-1.30147	-2.48363
C	0.87347	-0.63795	-3.53912
N	-0.05955	0.25365	-3.02503
C	2.50242	-2.36626	-2.38887
C	1.88283	-3.62892	-1.75500
C	3.03388	-2.68676	-3.79205
C	3.64687	-1.84951	-1.49253
C	-0.89706	1.11200	-3.85912
C	0.93168	1.21255	3.29679
C	1.39089	1.68156	2.03792
C	2.09115	0.61033	1.36827
C	2.03713	-0.53113	2.22209
C	1.31285	-0.16583	3.40519
H	-0.45784	3.11903	0.60579
H	1.24733	3.96965	-0.95150
H	0.85449	2.71682	-2.15125
H	1.61888	2.25945	-0.61097
H	-1.61642	3.52248	-2.22192
H	-1.08722	4.77560	-1.08850
H	-2.48831	3.75703	-0.68973
H	-2.55790	1.57348	-1.94678
H	-3.44810	2.29294	0.54671
H	-4.47409	0.87858	0.26517
H	-4.48266	2.22191	-0.90000
H	-2.40725	-0.91412	-2.21267
H	-3.38315	-1.13072	-0.73919
H	-4.09389	-0.33457	-2.15553
H	1.05269	-0.71827	-4.60602
H	1.06105	-4.02017	-2.37622
H	2.65412	-4.40977	-1.66064
H	1.48732	-3.41620	-0.74711
H	2.22793	-3.06187	-4.44425
H	3.48415	-1.79520	-4.25886
H	3.80803	-3.46634	-3.72384
H	4.42465	-2.62439	-1.40443
H	4.10404	-0.94109	-1.91767
H	3.28420	-1.61721	-0.47626
H	-1.92222	0.71582	-3.90043
H	-0.90470	2.12815	-3.44918
H	-0.46957	1.13396	-4.86983
H	0.38304	1.78943	4.03642
H	1.28048	2.69502	1.66564
H	2.62738	0.67964	0.42508
H	2.47816	-1.50636	2.02453
H	1.10178	-0.81978	4.24788
C	-0.85464	-1.97961	1.00876
C	-1.09029	-1.72130	2.38900
C	-1.87547	-0.59755	2.79722
H	-0.15792	-2.78845	0.76575
H	-1.65777	-1.84520	0.28277
H	-0.47647	-2.24857	3.12467
H	-1.76837	-0.35002	3.85981
H	0.94995	-1.02832	-0.37128
C	-3.26083	-0.33100	2.26724
H	-3.52088	0.73515	2.32942
H	-4.00891	-0.89363	2.85797
H	-3.35484	-0.65243	1.22298

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x45 | gu410t-guf27.log | Energy: -907429.4696692

Ru	0.12901	-0.06404	2.11617
P	-0.91264	0.97910	0.19872
C	-0.43909	2.82327	0.07503
C	0.96692	2.97673	-0.52571
C	-1.41871	3.76578	-0.63913
C	-2.64222	0.93803	-0.57872
C	-3.76423	1.60188	0.24688
C	-3.04950	-0.45174	-1.08629
C	0.03926	0.16541	-1.17812
N	0.90260	-0.77792	-0.81606
C	1.50772	-1.28496	-1.93986
C	0.97905	-0.61789	-3.02348
N	0.05748	0.29175	-2.53532
C	2.55609	-2.36551	-1.85947
C	1.92909	-3.62777	-1.23568
C	3.08797	-2.68599	-3.26268
C	3.70796	-1.87417	-0.96020
C	-0.75892	1.15969	-3.37404
C	1.02949	1.21550	3.78089
C	1.51517	1.69373	2.53683
C	2.24638	0.63760	1.89264
C	2.20910	-0.50560	2.75357
C	1.44571	-0.15245	3.91143
H	-0.41155	3.12195	1.13408
H	1.32128	4.01028	-0.37652
H	0.94734	2.77991	-1.60986
H	1.69901	2.29002	-0.08043
H	-1.52119	3.53551	-1.71092
H	-1.02327	4.79280	-0.56653
H	-2.42104	3.76009	-0.19264
H	-2.47357	1.57107	-1.46146
H	-3.38675	2.30013	1.00955
H	-4.37580	0.84997	0.76138
H	-4.42607	2.16825	-0.42789
H	-2.28510	-0.89913	-1.74123
H	-3.24293	-1.15265	-0.25977
H	-3.98642	-0.36264	-1.66189
H	1.17665	-0.70274	-4.08786
H	1.10024	-4.00437	-1.85741
H	2.68995	-4.42060	-1.14878
H	1.53847	-3.40875	-0.22819
H	2.27881	-3.04711	-3.91921
H	3.54697	-1.79625	-3.72509
H	3.85445	-3.47427	-3.20074
H	4.47610	-2.65951	-0.87096
H	4.17939	-0.97082	-1.38195
H	3.33477	-1.63607	0.04997
H	-1.79428	0.78882	-3.42553
H	-0.75139	2.18145	-2.97462
H	-0.32953	1.17216	-4.38450
H	0.43418	1.77796	4.49552
H	1.37399	2.69645	2.14744
H	2.75627	0.69328	0.93504
H	2.67968	-1.46726	2.56329
H	1.22773	-0.80482	4.75365
C	-0.71551	-2.04202	1.53269
C	-0.93733	-1.74691	2.90125
C	-1.70415	-0.59864	3.26997
H	-0.02033	-2.84630	1.28451
H	-1.49700	-1.86765	0.79327
H	-0.32911	-2.26172	3.64941
H	-1.58246	-0.30735	4.31946
H	0.68756	-0.80915	0.66230
C	-3.07923	-0.31114	2.73021
H	-3.30930	0.76229	2.76638
H	-3.83756	-0.83659	3.34092
H	-3.18568	-0.65839	1.69624

x46-48

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x46 | gu420a-guf35a.log | Energy: -907430.0476933

Ru	0.00555	-0.06327	1.65973
P	-0.98104	0.92745	-0.33033
C	-0.53867	2.78107	-0.42874
C	0.87091	2.95895	-1.01410
C	-1.52884	3.72116	-1.13229
C	-2.70866	0.86622	-1.10915
C	-3.84556	1.53241	-0.30457
C	-3.09630	-0.53226	-1.60778
C	-0.01091	0.12238	-1.69387
N	0.84614	-0.84247	-1.37665
C	1.41203	-1.31016	-2.53513
C	0.87515	-0.60290	-3.58903
N	-0.02181	0.30096	-3.05429
C	2.44366	-2.41114	-2.52020
C	1.81582	-3.67684	-1.90449
C	2.91988	-2.70860	-3.94829
C	3.63724	-1.96463	-1.65308
C	-0.83575	1.19669	-3.86357
C	0.84349	1.28984	3.30839
C	1.36983	1.72447	2.06482
C	2.11960	0.64904	1.48133
C	2.06247	-0.46165	2.38571
C	1.26236	-0.06990	3.50434
H	-0.52703	3.06886	0.63306
H	1.21303	3.99398	-0.84692
H	0.86484	2.77510	-2.10028
H	1.60559	2.27171	-0.57219
H	-1.64202	3.50054	-2.20429
H	-1.13859	4.74988	-1.05461
H	-2.52661	3.70666	-0.67615
H	-2.53742	1.49231	-1.99539
H	-3.48166	2.20756	0.48465
H	-4.48663	0.78067	0.17331
H	-4.47615	2.12480	-0.98664
H	-2.31994	-0.97589	-2.25075
H	-3.29040	-1.22716	-0.77574
H	-4.02898	-0.45945	-2.19237
H	1.05026	-0.65331	-4.65948
H	0.96347	-4.02697	-2.51011
H	2.56529	-4.48396	-1.85570
H	1.45659	-3.47006	-0.88269
H	2.08109	-3.03757	-4.58441
H	3.37998	-1.81685	-4.40603
H	3.67255	-3.51256	-3.93293
H	4.39067	-2.76804	-1.60551
H	4.11361	-1.06361	-2.07455
H	3.30235	-1.73711	-0.62716
H	-1.86786	0.82186	-3.94986
H	-0.84274	2.20088	-3.42374
H	-0.39306	1.25800	-4.86671
H	0.22486	1.87668	3.98257
H	1.24007	2.71158	1.63489
H	2.64758	0.66850	0.53212
H	2.53998	-1.42818	2.24388
H	1.02102	-0.69098	4.36376
C	-0.82487	-2.06747	1.12587
C	-1.07345	-1.72347	2.47814
C	-1.85607	-0.56764	2.78744
H	-0.12537	-2.87904	0.91707
H	-1.58509	-1.90837	0.36177
H	-0.48083	-2.21153	3.25597
H	-1.75893	-0.23912	3.82837
H	0.51705	-0.89504	0.36845
C	-3.22137	-0.31459	2.20934
H	-3.47076	0.75446	2.22178
H	-3.98253	-0.84243	2.81429
H	-3.29863	-0.68246	1.18012

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x47 | gu420t-guf35.log | Energy: -907429.9850239

Ru	0.12313	-0.01536	2.19850
P	-0.85660	0.96644	0.19761
C	-0.45542	2.82985	0.10359
C	0.95129	3.04943	-0.47452
C	-1.46791	3.74983	-0.59575
C	-2.57551	0.86661	-0.59965
C	-3.73641	1.50758	0.19136
C	-2.92665	-0.54108	-1.09983
C	0.13564	0.16572	-1.15056
N	0.95708	-0.83197	-0.83778
C	1.51781	-1.29876	-1.99913
C	1.01627	-0.55927	-3.04845
N	0.14377	0.36479	-2.50952
C	2.51510	-2.43147	-1.99272
C	1.84481	-3.68572	-1.39891
C	2.99181	-2.72479	-3.42154
C	3.71621	-2.03429	-1.11223
C	-0.64759	1.28194	-3.31667
C	0.98126	1.32329	3.84341
C	1.46206	1.78489	2.59071
C	2.21644	0.73240	1.96891
C	2.20554	-0.38872	2.86017
C	1.43220	-0.02963	4.00845
H	-0.45442	3.11362	1.16643
H	1.26076	4.09400	-0.30313
H	0.95944	2.86849	-1.56076
H	1.70430	2.38531	-0.02942
H	-1.58289	3.52950	-1.66752
H	-1.09850	4.78615	-0.51746
H	-2.46287	3.71416	-0.13496
H	-2.40818	1.49388	-1.48601
H	-3.39723	2.18542	0.98910
H	-4.36957	0.74126	0.65677
H	-4.36868	2.09109	-0.49675
H	-2.13537	-0.96789	-1.73586
H	-3.11306	-1.23895	-0.26835
H	-3.85581	-0.48980	-1.69223
H	1.20316	-0.59779	-4.11737
H	0.98584	-4.00091	-2.01434
H	2.56858	-4.51634	-1.35688
H	1.48577	-3.48231	-0.37639
H	2.14769	-3.01873	-4.06770
H	3.48269	-1.84184	-3.86409
H	3.71903	-3.55196	-3.41221
H	4.44289	-2.86227	-1.06877
H	4.22461	-1.14454	-1.52000
H	3.38102	-1.80676	-0.08647
H	-1.67253	0.90201	-3.45477
H	-0.68151	2.26892	-2.84220
H	-0.16889	1.38379	-4.29998
H	0.37008	1.88815	4.54274
H	1.30041	2.77608	2.18136
H	2.71840	0.77263	1.00666
H	2.69206	-1.34615	2.68860
H	1.22901	-0.66722	4.86565
C	-0.65346	-2.03396	1.65027
C	-0.92487	-1.68436	3.00806
C	-1.73529	-0.54826	3.31159
H	0.02982	-2.86802	1.47034
H	-1.42292	-1.91168	0.88766
H	-0.33580	-2.16694	3.79202
H	-1.65758	-0.22559	4.35600
H	0.52128	-0.99617	0.95947
C	-3.09695	-0.31636	2.71571
H	-3.36372	0.74850	2.72669
H	-3.85792	-0.85780	3.30868
H	-3.15315	-0.68208	1.68437

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x48 | gu420z-guf35b.log | Energy: -907434.0714220

Ru	-0.00050	-0.05609	1.66784
P	-0.95851	0.96383	-0.33651
C	-0.61793	2.84320	-0.41002
C	0.77682	3.13863	-0.98318
C	-1.66406	3.72755	-1.10847
C	-2.65984	0.80372	-1.16719
C	-3.86758	1.42894	-0.43460
C	-2.95606	-0.63057	-1.62484
C	0.07342	0.17750	-1.65455
N	0.87605	-0.83320	-1.33178
C	1.44280	-1.29437	-2.49239
C	0.96807	-0.54292	-3.54644
N	0.10102	0.38849	-3.01537
C	2.42682	-2.43958	-2.48394
C	1.74049	-3.68624	-1.89265
C	2.90597	-2.73922	-3.91062
C	3.62994	-2.05819	-1.59954
C	-0.67329	1.31186	-3.83113
C	1.02161	1.05206	3.28455
C	1.32267	1.66015	2.02976
C	2.03783	0.70160	1.21999
C	2.16870	-0.48957	1.99111
C	1.55172	-0.28141	3.26179
H	-0.62853	3.11979	0.65541
H	0.99513	4.21304	-0.86441
H	0.82269	2.90168	-2.05726
H	1.57511	2.57229	-0.48947
H	-1.78279	3.49289	-2.17692
H	-1.32235	4.77411	-1.04388
H	-2.65358	3.67149	-0.63981
H	-2.48578	1.40636	-2.06904
H	-3.58169	2.12497	0.36679
H	-4.50266	0.65387	0.01452
H	-4.48337	1.98703	-1.15773
H	-2.13257	-1.06296	-2.21428
H	-3.15553	-1.29470	-0.76890
H	-3.86510	-0.62753	-2.24965
H	1.17273	-0.57523	-4.61232
H	0.88028	-3.99125	-2.51169
H	2.45417	-4.52560	-1.84841
H	1.38004	-3.47750	-0.87169
H	2.06079	-3.02184	-4.56044
H	3.40982	-1.86256	-4.35111
H	3.62279	-3.57551	-3.89879
H	4.34518	-2.89586	-1.54991
H	4.15262	-1.17619	-2.00607
H	3.29176	-1.82245	-0.57697
H	-1.67369	0.90363	-4.04909
H	-0.77437	2.27424	-3.31825
H	-0.14072	1.47628	-4.77797
H	0.48368	1.51732	4.10696
H	1.07996	2.68117	1.75454
H	2.41589	0.83393	0.21233
H	2.62381	-1.41525	1.64481
H	1.48285	-1.00878	4.06674
C	-0.95290	-2.17059	1.27289
C	-1.10924	-1.58199	2.62500
C	-1.90112	-0.43565	2.84895
H	-0.45291	-3.14824	1.27770
H	-1.85305	-2.17359	0.64910
H	-0.55046	-2.04127	3.44269
H	-1.81594	-0.03144	3.86339
H	-0.16439	-1.55369	0.60591
C	-3.23923	-0.18866	2.20890
H	-3.46373	0.88369	2.14715
H	-4.03233	-0.65853	2.82078
H	-3.29271	-0.61502	1.20083

x49-51

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x49 | gu430t-guf37.log | Energy: -907431.6503838

Ru	0.16845	-0.02476	2.11662
P	-0.88405	1.03373	0.16678
C	-0.41481	2.88058	0.05384
C	0.98040	3.03813	-0.57150
C	-1.41046	3.82178	-0.64014
C	-2.61844	0.98716	-0.59042
C	-3.73033	1.62883	0.26650
C	-3.00957	-0.40924	-1.08933
C	0.09490	0.19286	-1.14793
N	0.97574	-0.73584	-0.78486
C	1.55746	-1.21800	-1.93015
C	1.01196	-0.55996	-3.01284
N	0.08674	0.33412	-2.51503
C	2.61711	-2.29187	-1.87839
C	2.01219	-3.56074	-1.24613
C	3.12412	-2.60704	-3.29190
C	3.78536	-1.79949	-1.00192
C	-0.74737	1.19080	-3.34469
C	1.01506	1.21820	3.68620
C	1.55037	1.68352	2.43922
C	2.27710	0.62751	1.82376
C	2.21923	-0.50518	2.71508
C	1.48108	-0.13030	3.87396
H	-0.37354	3.18160	1.11221
H	1.33857	4.07010	-0.41990
H	0.93937	2.84881	-1.65583
H	1.72008	2.34384	-0.14995
H	-1.52808	3.59663	-1.71127
H	-1.01948	4.85051	-0.56773
H	-2.40573	3.80786	-0.17783
H	-2.47973	1.62582	-1.47374
H	-3.34512	2.32772	1.02525
H	-4.31953	0.86445	0.78911
H	-4.41723	2.19093	-0.38634
H	-2.26076	-0.82917	-1.77893
H	-3.13921	-1.11893	-0.25771
H	-3.97437	-0.34646	-1.62034
H	1.19910	-0.63857	-4.07946
H	1.17921	-3.94482	-1.85830
H	2.78057	-4.34783	-1.16858
H	1.63074	-3.34141	-0.23509
H	2.30418	-2.97019	-3.93401
H	3.56843	-1.71339	-3.76137
H	3.89648	-3.39118	-3.24839
H	4.56015	-2.58051	-0.92944
H	4.24345	-0.89237	-1.43081
H	3.42752	-1.56463	0.01411
H	-1.77367	0.79644	-3.41131
H	-0.77102	2.20742	-2.93278
H	-0.31322	1.23197	-4.35259
H	0.42155	1.79995	4.38699
H	1.39511	2.67449	2.02708
H	2.76549	0.64511	0.85437
H	2.65670	-1.48344	2.52514
H	1.25526	-0.76862	4.72485
C	-0.93431	-2.37389	1.56085
C	-0.89426	-1.73514	2.91864
C	-1.69343	-0.65801	3.31082
H	-0.59652	-3.42101	1.59453
H	-1.91492	-2.30047	1.07169
H	-0.24928	-2.21283	3.65996
H	-1.53551	-0.32361	4.34186
H	-0.19823	-1.87251	0.86167
C	-3.04998	-0.31959	2.76168
H	-3.23540	0.76251	2.78538
H	-3.82510	-0.80190	3.38689
H	-3.17655	-0.67051	1.73185

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x50 | gu430z-guf37b.log | Energy: -907455.7227013

Ru	0.31502	-0.12388	1.10899
P	-1.16104	1.19604	-0.34535
C	-0.51609	2.97441	-0.55378
C	0.90797	2.94672	-1.12676
C	-1.38356	3.92671	-1.38601
C	-2.96420	1.33974	-0.89808
C	-3.82287	1.98377	0.19937
C	-3.60079	0.06887	-1.47234
C	-0.30190	0.23127	-1.62881
N	0.61747	-0.52416	-1.01846
C	1.30220	-1.21853	-1.99331
C	0.75380	-0.85880	-3.21173
N	-0.24791	0.05829	-2.96998
C	2.47742	-2.13289	-1.73860
C	2.15384	-3.12330	-0.60732
C	2.81652	-2.91210	-3.01878
C	3.69395	-1.27085	-1.34126
C	-1.09011	0.70175	-3.96935
C	0.72931	0.81491	3.07241
C	1.34631	1.64718	2.08103
C	2.31264	0.87639	1.38743
C	2.33540	-0.44890	1.95903
C	1.37681	-0.46962	3.00785
H	-0.48106	3.34945	0.48308
H	1.36570	3.94481	-1.03066
H	0.87971	2.68669	-2.19815
H	1.54620	2.21226	-0.62293
H	-1.46365	3.58266	-2.43174
H	-0.89957	4.91729	-1.40554
H	-2.39711	4.05507	-0.98050
H	-2.89060	2.05613	-1.73008
H	-3.36685	2.90715	0.59262
H	-3.97732	1.29311	1.04031
H	-4.81035	2.24625	-0.21509
H	-2.94582	-0.43118	-2.20238
H	-3.86703	-0.66260	-0.69671
H	-4.53536	0.35024	-1.98594
H	0.99719	-1.18053	-4.21870
H	1.32797	-3.79350	-0.89437
H	3.04163	-3.74010	-0.39346
H	1.86260	-2.58568	0.30475
H	1.96202	-3.52602	-3.34766
H	3.10055	-2.23163	-3.83866
H	3.66934	-3.58152	-2.82635
H	4.56291	-1.91979	-1.14280
H	3.95826	-0.57278	-2.15262
H	3.48248	-0.68629	-0.43532
H	-1.79485	-0.02381	-4.40458
H	-1.65425	1.50983	-3.48600
H	-0.46150	1.12505	-4.76664
H	-0.03445	1.11595	3.78431
H	1.08941	2.68159	1.86838
H	2.93447	1.21769	0.56416
H	2.99302	-1.26380	1.67240
H	1.14870	-1.32931	3.63375
C	-1.39903	-2.56081	-0.14430
C	-0.70125	-2.12084	1.11774
C	-1.30878	-1.32409	2.10154
H	-2.04031	-3.43666	0.06528
H	-2.03741	-1.76960	-0.55691
H	0.08550	-2.80111	1.45760
H	-0.94081	-1.44913	3.12222
H	-0.67621	-2.85043	-0.92000
C	-2.72977	-0.83139	2.06511
H	-2.83818	0.12171	2.60605
H	-3.38376	-1.57226	2.56334
H	-3.09422	-0.69558	1.04323

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x51 | gu510t-guf39.log | Energy: -907440.4980791

Ru	0.47793	0.22515	1.53851
P	-0.81622	1.48825	-0.02335
C	-0.04011	3.13077	-0.50388
C	1.44568	2.92673	-0.82902
C	-0.75789	3.84691	-1.65384
C	-2.64449	1.72149	-0.28577
C	-3.15236	2.71246	0.77245
C	-3.38353	0.38664	-0.21953
C	-0.11169	0.29317	-1.21177
N	0.80764	-0.39505	-0.51970
C	1.47121	-1.21713	-1.40137
C	0.90802	-1.01826	-2.64948
N	-0.08233	-0.06234	-2.51699
C	2.61592	-2.11410	-0.99734
C	2.16980	-3.06019	0.13358
C	3.08834	-2.93589	-2.20460
C	3.77265	-1.23037	-0.48942
C	-0.91047	0.48188	-3.58534
C	0.94782	-0.07938	3.66753
C	0.45508	1.24701	3.47616
C	1.34913	1.89657	2.55077
C	2.38461	0.96489	2.19658
C	2.14372	-0.26810	2.89734
H	-0.12786	3.74139	0.41261
H	1.93792	3.90613	-0.94247
H	1.55760	2.37640	-1.77853
H	1.96228	2.35237	-0.04770
H	-0.76078	3.22355	-2.56465
H	-0.22357	4.78129	-1.89355
H	-1.79727	4.10804	-1.40505
H	-2.77258	2.16477	-1.28721
H	-2.64472	3.68865	0.70591
H	-2.99742	2.30778	1.78763
H	-4.23289	2.88086	0.63424
H	-3.04227	-0.30278	-1.00549
H	-3.22326	-0.10112	0.75382
H	-4.46555	0.55373	-0.35094
H	1.12310	-1.48259	-3.60642
H	1.40183	-3.76630	-0.22177
H	3.03352	-3.64500	0.48954
H	1.76101	-2.48527	0.98021
H	2.27684	-3.57327	-2.59359
H	3.44327	-2.28012	-3.01697
H	3.92296	-3.58861	-1.90483
H	4.62479	-1.86445	-0.19466
H	4.10934	-0.53397	-1.27507
H	3.44957	-0.64658	0.38406
H	-1.35589	-0.33920	-4.16646
H	-1.71151	1.08371	-3.13558
H	-0.30760	1.11681	-4.25334
H	0.46250	-0.84279	4.27377
H	-0.41975	1.68337	3.95037
H	1.27222	2.92173	2.19646
H	3.21178	1.16805	1.52030
H	2.76153	-1.16157	2.86997
C	-2.63781	-2.78975	-0.01709
C	-1.34567	-2.42007	0.64124
C	-1.16596	-1.91357	1.87829
H	-2.71254	-3.89225	-0.06524
H	-3.52174	-2.41164	0.51438
H	-0.44421	-2.65247	0.07070
H	-0.12656	-1.91355	2.24119
H	-2.66921	-2.43294	-1.06043
C	-2.23042	-1.55873	2.87971
H	-2.06609	-0.54460	3.27933
H	-2.20670	-2.25629	3.73641
H	-3.24069	-1.60029	2.44536

x52-54

67
x52 | gu510z-guf39b.log | Energy: -907441.7243832

Ru	0.38706	0.13032	1.20962
P	-0.96371	1.37449	-0.33840
C	-0.22657	3.04090	-0.80650
C	1.25637	2.86704	-1.16270
C	-0.97259	3.76883	-1.93076
C	-2.79544	1.56458	-0.63417
C	-3.35930	2.50715	0.43953
C	-3.52885	0.22350	-0.65895
C	-0.23780	0.20348	-1.53459
N	0.69196	-0.47862	-0.85418
C	1.31589	-1.33342	-1.73327
C	0.72308	-1.15250	-2.97035
N	-0.25168	-0.18137	-2.83111
C	2.43200	-2.26379	-1.32830
C	1.94361	-3.18928	-0.19711
C	2.87412	-3.10612	-2.53273
C	3.61863	-1.42150	-0.82040
C	-1.09781	0.35697	-3.88825
C	0.91091	-0.16066	3.31754
C	0.40973	1.16469	3.14080
C	1.28421	1.82232	2.19978
C	2.31466	0.90095	1.82181
C	2.09089	-0.33820	2.51718
H	-0.30660	3.63345	0.12239
H	1.73368	3.85612	-1.25382
H	1.35810	2.34811	-2.13074
H	1.79435	2.27554	-0.40929
H	-0.98950	3.15963	-2.85118
H	-0.44883	4.71020	-2.16616
H	-2.00835	4.01972	-1.65775
H	-2.89457	2.04670	-1.62074
H	-2.86405	3.49204	0.42954
H	-3.23748	2.06736	1.44433
H	-4.43609	2.66649	0.26578
H	-3.10483	-0.46042	-1.40976
H	-3.47606	-0.27403	0.31922
H	-4.59046	0.39463	-0.90361
H	0.90856	-1.63723	-3.92326
H	1.11505	-3.82969	-0.54049
H	2.76993	-3.83983	0.13280
H	1.59748	-2.59649	0.66432
H	2.04230	-3.72178	-2.91381
H	3.24378	-2.46586	-3.35091
H	3.69026	-3.78175	-2.23294
H	4.44057	-2.08572	-0.50680
H	3.99259	-0.75224	-1.61280
H	3.31150	-0.81039	0.04041
H	-1.53590	-0.46817	-4.46883
H	-1.90404	0.94353	-3.42766
H	-0.51139	1.00445	-4.55904
H	0.44680	-0.92926	3.93354
H	-0.45627	1.59672	3.63478
H	1.19143	2.84650	1.84701
H	3.12281	1.10596	1.12339
H	2.71089	-1.22917	2.46912
C	-2.96059	-3.02642	-0.29578
C	-1.64918	-2.42709	0.11043
C	-1.37818	-1.76272	1.24689
H	-2.87479	-4.12759	-0.33561
H	-3.78215	-2.76862	0.38730
H	-0.81988	-2.57517	-0.58715
H	-0.27333	-1.64858	1.45525
H	-3.23963	-2.69906	-1.31260
C	-2.31264	-1.46894	2.38659
H	-2.46899	-0.38204	2.49467
H	-1.88416	-1.82431	3.33903
H	-3.29161	-1.95357	2.25485

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x53 | au210a-auf73a | Energy: -907456.2407166

Ru	-0.44406	-0.46576	1.36875
P	-1.65824	0.64023	-0.32015
C	-2.59525	2.23279	-0.05918
C	-3.26695	2.78615	-1.32086
C	-3.61071	2.05012	1.08216
C	-2.59888	-0.34078	-1.61137
C	-3.88392	-0.93281	-1.01593
C	-1.69918	-1.41533	-2.23734
C	-0.03676	0.87426	-1.10918
N	0.81259	0.06224	-0.45411
C	1.91843	-0.10837	-1.26277
C	1.71348	0.64817	-2.40600
N	0.48060	1.24686	-2.30424
C	3.10790	-1.01337	-1.00083
C	2.71240	-2.12934	-0.02718
C	3.54834	-1.65045	-2.33469
C	4.29983	-0.21060	-0.43957
C	-0.16110	2.08674	-3.30805
C	0.05079	-1.98519	2.95305
C	-0.12821	-2.69396	1.73445
C	-1.44710	-2.45486	1.25062
C	-2.11076	-1.58874	2.20044
C	-1.18522	-1.29110	3.24125
H	-1.81796	2.93636	0.27770
H	-3.72500	3.76250	-1.09184
H	-4.06971	2.11684	-1.67071
H	-2.55179	2.93348	-2.14498
H	-4.44443	1.39909	0.77377
H	-4.03698	3.02988	1.35264
H	-3.14386	1.61221	1.97782
H	-2.87890	0.38590	-2.39257
H	-4.41849	-1.50463	-1.79240
H	-4.56459	-0.15171	-0.64444
H	-3.65796	-1.61822	-0.18426
H	-0.87584	-0.97219	-2.81852
H	-1.25127	-2.06059	-1.46684
H	-2.29987	-2.04433	-2.91460
H	2.34616	0.80163	-3.27407
H	1.94726	-2.78053	-0.48119
H	3.59569	-2.74136	0.21443
H	2.29858	-1.71275	0.89954
H	2.71993	-2.20809	-2.80128
H	3.90565	-0.88847	-3.04683
H	4.38070	-2.34779	-2.14853
H	5.17641	-0.87372	-0.35164
H	4.56219	0.61984	-1.11544
H	4.08543	0.20071	0.55481
H	0.40918	2.01548	-4.24350
H	-1.18695	1.73089	-3.48400
H	-0.18862	3.13616	-2.97704
H	0.95099	-1.97395	3.56043
H	0.63063	-3.28498	1.23082
H	-1.88937	-2.89788	0.36428
H	-3.13848	-1.23797	2.14692
H	-1.38333	-0.66708	4.10969
C	-0.20812	1.64670	2.00627
C	0.79876	0.90867	2.64265
C	2.26646	1.07565	2.33688
H	-1.09877	1.95460	2.55633
H	0.08948	2.30397	1.18281
H	0.59860	0.58466	3.66852
H	2.56295	2.07432	2.71217
H	2.41968	1.09858	1.24848
C	3.14649	0.02447	3.01532
H	4.21413	0.20559	2.81372
H	2.90431	-0.99228	2.67024
H	3.00263	0.05345	4.10916

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x54 | au210t-auf73 | Energy: -907441.2590159

Ru	-0.66574	-0.53731	1.95104
P	-1.52267	0.37550	-0.11233
C	-2.18479	2.15732	-0.06168
C	-1.09458	3.16115	-0.47143
C	-3.48806	2.42800	-0.82593
C	-2.79202	-0.58486	-1.12286
C	-4.02686	-0.98763	-0.30231
C	-2.17055	-1.78727	-1.84742
C	-0.06324	0.36530	-1.20917
N	1.08503	-0.09923	-0.72959
C	1.98713	-0.08843	-1.76641
C	1.35539	0.38891	-2.89765
N	0.05663	0.68019	-2.53826
C	3.42080	-0.52108	-1.57295
C	3.44660	-1.92349	-0.93625
C	4.15272	-0.54743	-2.92170
C	4.11796	0.47671	-0.62633
C	-0.97977	1.12077	-3.45805
C	-0.32901	-2.07129	3.52934
C	-0.38087	-2.76915	2.28050
C	-1.64058	-2.53345	1.67850
C	-2.39181	-1.64803	2.54551
C	-1.57738	-1.38619	3.70008
H	-2.39936	2.29479	1.00867
H	-1.41369	4.17977	-0.19566
H	-0.92829	3.14043	-1.55968
H	-0.12372	2.95830	0.00679
H	-3.36573	2.34308	-1.91765
H	-3.80669	3.46283	-0.61700
H	-4.30420	1.75701	-0.52180
H	-3.11661	0.13747	-1.88707
H	-4.85738	-1.22517	-0.98696
H	-4.36659	-0.18863	0.37586
H	-3.83029	-1.88671	0.29813
H	-1.43661	-1.47700	-2.60476
H	-1.64939	-2.46586	-1.15591
H	-2.96783	-2.35833	-2.35206
H	1.71035	0.55180	-3.91075
H	2.96561	-2.66363	-1.59738
H	4.48909	-2.23668	-0.76105
H	2.91258	-1.91784	0.02805
H	3.67208	-1.25362	-3.61915
H	4.16381	0.45294	-3.38624
H	5.19723	-0.86501	-2.77527
H	5.16050	0.16355	-0.44938
H	4.12678	1.48998	-1.06128
H	3.59587	0.51832	0.34229
H	-1.43954	0.26204	-3.97438
H	-1.75256	1.66374	-2.90344
H	-0.53937	1.79802	-4.20348
H	0.50941	-2.06143	4.22014
H	0.43373	-3.34094	1.83967
H	-1.98144	-2.95443	0.74017
H	-3.41211	-1.30788	2.39959
H	-1.85953	-0.76362	4.54677
C	-0.57614	1.56126	2.71275
C	0.49494	0.79887	3.19411
C	1.76624	0.64590	2.40049
H	-1.41722	1.79065	3.37158
H	-0.40034	2.26657	1.90313
H	0.50254	0.46236	4.23402
H	2.12927	1.63801	2.07445
H	1.53297	0.14307	1.42173
C	2.85749	-0.14306	3.12108
H	3.73780	-0.27403	2.47324
H	2.49270	-1.14400	3.40502
H	3.17930	0.37812	4.03799

x55-57

67
x55 | au210z-auf73b | Energy: -907445.5822298

Ru	-0.54578	-0.32972	1.69838
P	-1.19345	0.50515	-0.46388
C	-1.88361	2.28063	-0.46274
C	-0.77656	3.29203	-0.80036
C	-3.14995	2.54810	-1.28906
C	-2.44141	-0.46933	-1.49058
C	-3.73382	-0.81281	-0.73343
C	-1.81840	-1.70493	-2.15504
C	0.26167	0.50569	-1.59070
N	1.44921	0.08726	-1.16832
C	2.30330	0.13278	-2.24185
C	1.60711	0.58384	-3.34338
N	0.31487	0.82498	-2.92911
C	3.76116	-0.23927	-2.11188
C	3.87348	-1.65609	-1.51829
C	4.44337	-0.19784	-3.48614
C	4.44759	0.76702	-1.16641
C	-0.75769	1.23146	-3.82401
C	-0.41455	-1.82682	3.35727
C	-0.37838	-2.56016	2.12944
C	-1.58040	-2.30249	1.42370
C	-2.38625	-1.39307	2.21167
C	-1.65915	-1.11773	3.41199
H	-2.16507	2.41192	0.59221
H	-1.12406	4.31121	-0.56347
H	-0.51905	3.25867	-1.87034
H	0.15497	3.10402	-0.24284
H	-2.99030	2.45076	-2.37338
H	-3.47133	3.58635	-1.10141
H	-3.98122	1.88563	-1.00971
H	-2.70743	0.24052	-2.28745
H	-4.54207	-0.99201	-1.46108
H	-4.05989	-0.00637	-0.05854
H	-3.62132	-1.72992	-0.14005
H	-1.03310	-1.43239	-2.87527
H	-1.35869	-2.38575	-1.42283
H	-2.60343	-2.26241	-2.69319
H	1.90964	0.76024	-4.37099
H	3.41740	-2.40038	-2.19214
H	4.93372	-1.92049	-1.37133
H	3.35686	-1.70911	-0.54631
H	3.96938	-0.90742	-4.18476
H	4.39268	0.81349	-3.92352
H	5.50555	-0.47186	-3.38581
H	5.50738	0.49495	-1.02839
H	4.40038	1.78780	-1.58094
H	3.95608	0.76907	-0.18055
H	-1.38872	0.37199	-4.10147
H	-1.37588	2.00040	-3.34804
H	-0.31219	1.65611	-4.73368
H	0.36318	-1.81391	4.11673
H	0.44541	-3.17777	1.77787
H	-1.85417	-2.73844	0.47049
H	-3.38673	-1.04573	1.97844
H	-1.98690	-0.46400	4.21760
C	-0.46541	1.76313	2.46075
C	0.65507	0.99308	2.82876
C	1.62062	0.58191	1.79223
H	-1.20205	2.01648	3.22673
H	-0.37462	2.46981	1.64015
H	0.81378	0.65991	3.85724
H	1.85333	1.37161	1.06569
H	1.10401	-0.17824	0.98129
C	2.84689	-0.18412	2.26829
H	3.36352	-0.65748	1.42094
H	2.56014	-0.96704	2.98829
H	3.55054	0.50555	2.76226

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x56 | au211t-aug51 | Energy: -907444.4125898

Ru	-0.75862	-0.55997	2.13876
P	-1.36365	0.26720	-0.03220
C	-2.01598	2.06434	0.00480
C	-0.98127	3.05729	-0.55358
C	-3.37934	2.30768	-0.65811
C	-2.61166	-0.72344	-1.04863
C	-3.95941	-1.03297	-0.37797
C	-1.96444	-2.00847	-1.58464
C	0.05411	0.32427	-1.19962
N	1.28792	0.08439	-0.77837
C	2.12132	0.21129	-1.86192
C	1.36455	0.53789	-2.96697
N	0.05372	0.61763	-2.54608
C	3.61374	0.01681	-1.73713
C	3.89412	-1.37362	-1.13566
C	4.27874	0.12941	-3.11592
C	4.18644	1.09861	-0.80011
C	-1.06327	0.88078	-3.44118
C	-1.06328	-1.65961	4.07553
C	-1.05465	-2.61906	3.01879
C	-2.11920	-2.32029	2.12478
C	-2.80323	-1.14765	2.63381
C	-2.14476	-0.74847	3.83707
H	-2.12572	2.24816	1.08399
H	-1.28644	4.08182	-0.28379
H	-0.93013	2.99905	-1.65176
H	0.03687	2.88540	-0.17503
H	-3.37917	2.05300	-1.72994
H	-3.61915	3.38134	-0.57932
H	-4.19498	1.75176	-0.17697
H	-2.82476	-0.05965	-1.89730
H	-4.69438	-1.26969	-1.16467
H	-4.35976	-0.19361	0.20620
H	-3.89839	-1.91050	0.27792
H	-1.09668	-1.80027	-2.22851
H	-1.61871	-2.65288	-0.75986
H	-2.70651	-2.57468	-2.17207
H	1.63292	0.72014	-4.00297
H	3.51236	-2.17086	-1.79491
H	4.97975	-1.51620	-1.00594
H	3.40570	-1.47326	-0.15254
H	3.88811	-0.63606	-3.80705
H	4.10511	1.12448	-3.55904
H	5.36652	-0.01600	-3.02130
H	5.27492	0.96272	-0.68728
H	3.99973	2.10753	-1.20374
H	3.72452	1.03388	0.19909
H	-1.56111	-0.05611	-3.73865
H	-1.79085	1.54287	-2.95565
H	-0.68036	1.38443	-4.33913
H	-0.36817	-1.62354	4.91031
H	-0.33062	-3.42201	2.89507
H	-2.38140	-2.89998	1.24705
H	-3.69374	-0.68761	2.22120
H	-2.41651	0.10120	4.45952
C	-0.02842	1.51714	2.54352
C	0.79803	0.51988	3.09242
C	1.60314	-0.33163	2.19326
H	-0.64354	2.12093	3.21421
H	0.25938	1.98524	1.60484
H	0.85213	0.34931	4.16997
H	2.09437	0.22663	1.38790
H	0.86932	-0.94193	1.43319
C	2.48969	-1.37263	2.85975
H	2.88302	-2.08707	2.12047
H	1.93595	-1.93188	3.63053
H	3.34606	-0.87287	3.34153

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x57 | au211z-aug51b | Energy: -907448.2669161

Ru	-0.53912	-0.24116	1.67634
P	-1.08380	0.37226	-0.56620
C	-2.26530	1.83636	-0.49494
C	-1.45830	3.11707	-0.24105
C	-3.29080	2.02076	-1.62336
C	-1.93210	-0.98673	-1.54823
C	-3.22562	-1.48708	-0.89934
C	-0.95156	-2.14578	-1.77143
C	0.31046	0.76284	-1.69517
N	1.54186	0.40725	-1.34100
C	2.36588	0.65359	-2.40864
C	1.60737	1.16357	-3.44093
N	0.30499	1.22099	-2.99384
C	3.84660	0.36644	-2.34321
C	4.05695	-1.13985	-2.09256
C	4.52176	0.76804	-3.66165
C	4.46026	1.16454	-1.17665
C	-0.79235	1.73972	-3.79552
C	-1.12105	0.20516	3.74467
C	-1.11588	-1.21644	3.59398
C	-2.11835	-1.56256	2.62500
C	-2.72627	-0.35706	2.18248
C	-2.10549	0.75163	2.85445
H	-2.82956	1.60497	0.42051
H	-2.14485	3.96299	-0.07100
H	-0.82670	3.36042	-1.11234
H	-0.80366	3.01234	0.63850
H	-2.86012	2.54049	-2.48824
H	-4.11355	2.65144	-1.24711
H	-3.72893	1.07115	-1.96588
H	-2.17699	-0.53379	-2.52362
H	-3.72256	-2.19823	-1.57949
H	-3.93657	-0.67296	-0.68620
H	-3.00352	-2.01859	0.03842
H	-0.02530	-1.81744	-2.26776
H	-0.68214	-2.60880	-0.80631
H	-1.42929	-2.91869	-2.39573
H	1.87153	1.49366	-4.44078
H	3.62296	-1.73968	-2.90984
H	5.13466	-1.36377	-2.02879
H	3.58347	-1.44651	-1.14522
H	4.10471	0.19957	-4.51000
H	4.39026	1.84470	-3.86129
H	5.60194	0.55915	-3.60883
H	5.53611	0.93882	-1.09072
H	4.34296	2.24890	-1.33927
H	3.96773	0.90030	-0.22648
H	-1.69940	1.14521	-3.63405
H	-1.00052	2.79232	-3.54645
H	-0.51128	1.67230	-4.85530
H	-0.46899	0.78030	4.39877
H	-0.46973	-1.91319	4.12269
H	-2.36675	-2.56597	2.28793
H	-3.51838	-0.28543	1.44439
H	-2.37098	1.80031	2.75280
C	1.15110	1.22176	1.63718
C	1.51894	-0.04296	2.13718
C	1.56295	-1.23051	1.26141
H	1.05909	2.03937	2.35674
H	1.37851	1.48671	0.60867
H	1.72465	-0.19008	3.20189
H	1.96174	-0.99859	0.26617
H	0.41531	-1.52336	0.88587
C	2.07436	-2.51372	1.90101
H	1.85949	-3.39011	1.27039
H	1.61752	-2.67311	2.89092
H	3.16696	-2.44536	2.03065

x58-60

67
x58 | au220t-auf69 | Energy: -907424.5165675

Ru	-0.78788	-0.29682	2.16808
P	-1.40289	0.20587	-0.03496
C	-2.54895	1.70342	-0.07382
C	-1.74517	3.00147	0.08077
C	-3.59601	1.81088	-1.19164
C	-2.25606	-1.13543	-1.03688
C	-3.52167	-1.62892	-0.32633
C	-1.28697	-2.29770	-1.28763
C	0.04303	0.54369	-1.16843
N	1.28089	0.16175	-0.80837
C	2.16806	0.39247	-1.83025
C	1.44153	0.94012	-2.85879
N	0.12524	1.01989	-2.44097
C	3.62864	0.05210	-1.69196
C	3.76236	-1.46190	-1.42632
C	4.37246	0.43012	-2.97926
C	4.20632	0.83212	-0.49302
C	-0.94947	1.55267	-3.27122
C	-1.20505	-0.15240	4.33442
C	-1.18071	-1.53603	3.96978
C	-2.23953	-1.78051	3.03706
C	-2.89959	-0.52869	2.81087
C	-2.27032	0.48145	3.60890
H	-3.08930	1.53201	0.87221
H	-2.43806	3.85407	0.17325
H	-1.10565	3.18229	-0.80049
H	-1.10487	2.97359	0.97389
H	-3.17058	2.20043	-2.12561
H	-4.37036	2.52791	-0.87127
H	-4.09677	0.85579	-1.40648
H	-2.54099	-0.68029	-2.00059
H	-4.05486	-2.33789	-0.98067
H	-4.21570	-0.81145	-0.07521
H	-3.25312	-2.15533	0.60074
H	-0.40016	-1.98648	-1.86292
H	-0.94718	-2.72524	-0.32860
H	-1.80046	-3.09283	-1.85289
H	1.74252	1.28060	-3.84368
H	3.34904	-2.04792	-2.26376
H	4.82675	-1.72216	-1.31025
H	3.23538	-1.74599	-0.50001
H	3.97404	-0.12408	-3.84556
H	4.29132	1.51116	-3.18146
H	5.43989	0.18100	-2.87626
H	5.27129	0.57849	-0.36771
H	4.12223	1.91965	-0.65247
H	3.67487	0.57058	0.43711
H	-1.83892	0.91754	-3.18401
H	-1.19957	2.57923	-2.96583
H	-0.60997	1.55469	-4.31518
H	-0.52629	0.33602	5.02977
H	-0.46836	-2.27475	4.33045
H	-2.50412	-2.74075	2.60339
H	-3.74907	-0.37360	2.15122
H	-2.56657	1.52486	3.67809
C	0.68126	1.33999	2.02745
C	1.31640	0.12636	2.41567
C	1.38638	-1.04714	1.58876
H	0.60222	2.11449	2.79528
H	0.78700	1.72589	1.01587
H	1.71697	0.03893	3.43335
H	1.52892	-0.42874	0.19794
H	0.42978	-1.27546	0.99001
C	2.00325	-2.29462	2.18778
H	1.64748	-3.20224	1.67472
H	1.78409	-2.40320	3.26666
H	3.10160	-2.26500	2.07731

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x59 | au410a-auf67a | Energy: -907446.7054028

Ru	-0.61545	-0.15522	-1.69622
P	-1.11528	-0.04206	0.54084
C	0.30398	0.26577	1.76511
N	0.44082	0.86001	2.97820
C	1.76959	0.79685	3.38088
C	2.47753	0.15032	2.40645
N	1.54289	-0.15874	1.44471
C	3.93272	-0.19289	2.23849
C	-0.58198	1.50727	3.80545
C	-1.82955	-1.60817	1.30753
C	-0.89190	-2.79429	1.05882
C	-2.21211	-1.49337	2.78551
C	-2.31368	1.29541	1.09604
C	-1.78013	2.66485	0.66417
C	-3.73759	1.04236	0.58343
C	4.46672	0.53967	0.98875
C	4.06933	-1.71654	2.04144
C	4.70829	0.25150	3.48543
H	-2.36784	1.24540	2.18905
H	-2.74238	-1.75620	0.70372
H	2.09308	1.22144	4.32448
H	-0.66162	-2.89398	-0.01198
H	-1.36378	-3.72431	1.41644
H	0.05571	-2.66897	1.61313
H	-2.67527	-2.43486	3.12473
H	-2.93193	-0.68111	2.97308
H	-1.31495	-1.32946	3.40793
H	-1.66980	2.70008	-0.43152
H	-0.78692	2.87446	1.09891
H	-2.47298	3.46192	0.98223
H	-3.80709	1.14978	-0.50549
H	-4.41398	1.78661	1.03567
H	-4.10567	0.04206	0.86220
H	4.38561	1.63223	1.10838
H	3.91262	0.24584	0.08060
H	5.52683	0.28084	0.83892
H	5.13187	-1.97409	1.90890
H	3.68128	-2.26616	2.91427
H	3.52797	-2.05505	1.14091
H	5.77394	0.00506	3.36215
H	4.62499	1.34046	3.63685
H	4.33881	-0.26382	4.38740
H	-0.96004	2.40756	3.30298
H	-0.11183	1.79025	4.75570
H	-1.40287	0.80768	4.00286
C	-2.74971	-0.53970	-2.25206
C	-1.93525	-1.44634	-2.98785
C	-1.06150	-0.66426	-3.81293
C	-1.36707	0.72190	-3.60497
C	-2.41398	0.81164	-2.64476
H	-3.52813	-0.82304	-1.54850
H	-1.96428	-2.53113	-2.92647
H	-0.30426	-1.05554	-4.48873
H	-0.87521	1.56149	-4.08953
H	-2.90097	1.72559	-2.31879
C	1.12410	-1.44840	-1.44495
C	1.48843	-0.18470	-2.02865
C	1.21153	1.09267	-1.45117
H	1.35186	-1.76894	-0.42519
H	1.18528	-2.30503	-2.12358
H	1.72409	-0.18970	-3.09827
H	1.39116	1.26945	-0.39170
H	1.75925	-0.60228	0.55565
C	1.41175	2.33527	-2.29086
H	1.26071	2.11950	-3.36082
H	0.70145	3.12708	-2.00023
H	2.43243	2.74460	-2.16939

67
x60 | au410t-auf67 | Energy: -907428.8658796

Ru	-0.80262	-0.32102	-2.16120
P	-1.35356	-0.11037	0.09675
C	0.11087	0.11589	1.23714
N	0.25562	0.67919	2.47135
C	1.58489	0.58088	2.84401
C	2.25824	-0.05022	1.82844
N	1.32477	-0.32605	0.85973
C	3.71071	-0.40652	1.65186
C	-0.74842	1.33671	3.30937
C	-2.16192	-1.64351	0.81755
C	-1.26104	-2.86246	0.58209
C	-2.56244	-1.52538	2.29057
C	-2.48064	1.30326	0.57748
C	-1.82678	2.63996	0.21417
C	-3.85061	1.15531	-0.09580
C	4.26487	0.38257	0.44675
C	3.82609	-1.91779	1.36900
C	4.48958	-0.04440	2.92317
H	-2.63534	1.24305	1.66248
H	-3.07004	-1.75017	0.19846
H	1.93196	0.96845	3.79559
H	-1.04189	-2.99656	-0.48805
H	-1.75877	-3.77134	0.95799
H	-0.30482	-2.75378	1.12298
H	-3.09120	-2.44013	2.60548
H	-3.23189	-0.67113	2.47879
H	-1.66641	-1.42865	2.92713
H	-1.67657	2.70023	-0.87434
H	-0.84163	2.76739	0.69342
H	-2.47682	3.47342	0.52800
H	-3.76487	1.26408	-1.18593
H	-4.51995	1.95014	0.27205
H	-4.32415	0.18580	0.12846
H	4.19532	1.46871	0.62264
H	3.70804	0.13593	-0.47222
H	5.32407	0.12076	0.29198
H	4.88563	-2.18532	1.22869
H	3.42459	-2.50923	2.20834
H	3.27923	-2.18678	0.44976
H	5.55167	-0.30240	2.79123
H	4.42541	1.03624	3.13416
H	4.10699	-0.60003	3.79555
H	-1.06811	2.28257	2.85028
H	-0.29002	1.54389	4.28476
H	-1.61266	0.67800	3.45290
C	-2.90117	-0.77023	-2.74262
C	-2.08473	-1.83635	-3.21970
C	-1.13812	-1.27112	-4.14045
C	-1.39421	0.13085	-4.24739
C	-2.47783	0.45730	-3.36697
H	-3.71740	-0.86745	-2.03207
H	-2.16471	-2.88360	-2.93985
H	-0.35606	-1.81678	-4.66403
H	-0.84668	0.83249	-4.87121
H	-2.93575	1.43530	-3.24766
C	1.38227	-1.09576	-1.70832
C	1.28680	0.17588	-2.38316
C	0.66688	1.33499	-1.84421
H	0.44097	-1.45182	-1.15488
H	1.75697	-1.90813	-2.33952
H	1.66627	0.23205	-3.41042
H	0.75924	1.52407	-0.77481
H	1.55472	-0.76997	-0.21234
C	0.58121	2.58567	-2.68946
H	0.55111	2.33751	-3.76235
H	-0.32012	3.17498	-2.45602
H	1.45494	3.24091	-2.51558

x61-63

67
x61 | au411a-aug61a | Energy: -907452.6442026

Ru	-0.57248	-0.24472	-1.70688
P	-1.06176	0.10969	0.59262
C	0.37434	0.37091	1.70635
N	0.51801	1.06446	2.89029
C	1.79640	0.80822	3.34070
C	2.39055	-0.03373	2.42563
N	1.49244	-0.29164	1.42153
C	3.78315	-0.61713	2.41389
C	-0.42137	1.90942	3.62049
C	-1.88204	-1.39083	1.36555
C	-1.00219	-2.63195	1.17475
C	-2.22552	-1.16875	2.84279
C	-2.23208	1.51891	0.97366
C	-1.67318	2.83030	0.41424
C	-3.67098	1.26696	0.50668
C	4.53711	-0.09325	1.17549
C	3.68660	-2.15278	2.33884
C	4.53822	-0.20670	3.68571
H	-2.26469	1.57460	2.06788
H	-2.81300	-1.51891	0.78658
H	2.16350	1.25297	4.26019
H	-0.84208	-2.84715	0.10637
H	-1.48997	-3.50613	1.63650
H	-0.01734	-2.48939	1.64866
H	-2.71758	-2.06762	3.24954
H	-2.90828	-0.31667	2.98906
H	-1.30790	-0.99430	3.42947
H	-1.65844	2.79801	-0.68606
H	-0.64154	3.01712	0.75604
H	-2.30441	3.67702	0.73114
H	-3.75844	1.28603	-0.58735
H	-4.31673	2.06923	0.90030
H	-4.06746	0.30852	0.87686
H	4.62530	1.00559	1.20544
H	4.01052	-0.37456	0.24892
H	5.55136	-0.52446	1.14192
H	4.69711	-2.59199	2.29978
H	3.16428	-2.55638	3.22220
H	3.13431	-2.46302	1.43676
H	5.55227	-0.63656	3.67474
H	4.63327	0.89014	3.75391
H	4.02038	-0.57167	4.58846
H	-0.73657	2.76640	3.00864
H	0.08731	2.28583	4.51763
H	-1.30240	1.33027	3.93372
C	-1.98110	-1.66798	-2.74672
C	-1.11121	-1.04987	-3.71049
C	-1.34550	0.35918	-3.67240
C	-2.33467	0.62728	-2.66956
C	-2.73564	-0.64550	-2.11688
H	-2.03960	-2.73129	-2.52532
H	-0.40495	-1.56554	-4.35747
H	-0.84012	1.10712	-4.27836
H	-2.75664	1.59960	-2.43555
H	-3.47898	-0.79588	-1.33967
C	1.59380	-1.12713	-1.50562
C	1.45211	0.17284	-2.19514
C	1.06851	1.33021	-1.49639
H	0.52616	-1.55324	-1.10685
H	1.93858	-1.93459	-2.16223
H	1.62639	0.21759	-3.27382
H	1.29543	1.37730	-0.43165
H	2.08622	-1.07892	-0.52727
C	0.93594	2.64956	-2.21279
H	0.71429	2.50824	-3.28258
H	0.14149	3.27126	-1.77296
H	1.87885	3.22104	-2.13428

67
x62 | au411t-aug61 | Energy: -907451.2900434

Ru	-0.70940	-0.30335	-2.23098
P	-1.16404	0.09379	0.06966
C	0.26576	0.23681	1.20767
N	0.36115	0.78942	2.47136
C	1.61420	0.46199	2.94335
C	2.23843	-0.28392	1.96656
N	1.38470	-0.41315	0.90006
C	3.61481	-0.90621	1.97011
C	-0.59356	1.57152	3.25237
C	-2.07808	-1.39626	0.77073
C	-1.16924	-2.63173	0.70875
C	-2.60181	-1.19412	2.19600
C	-2.24277	1.56515	0.48901
C	-1.51029	2.89388	0.26485
C	-3.56971	1.53584	-0.27513
C	4.44389	-0.32202	0.81022
C	3.47558	-2.42864	1.77838
C	4.32142	-0.61389	3.30133
H	-2.46914	1.46029	1.55811
H	-2.93190	-1.53911	0.08736
H	1.94551	0.79358	3.92230
H	-0.77531	-2.80029	-0.30434
H	-1.73876	-3.52230	1.02228
H	-0.30967	-2.51162	1.38712
H	-3.14107	-2.10034	2.51819
H	-3.29700	-0.34443	2.28018
H	-1.76188	-1.04563	2.89424
H	-1.42863	3.11518	-0.80675
H	-0.49336	2.89187	0.68834
H	-2.08062	3.71214	0.73507
H	-3.39728	1.62734	-1.35896
H	-4.19387	2.38703	0.04283
H	-4.13925	0.61245	-0.08050
H	4.54558	0.77157	0.90952
H	3.96920	-0.54438	-0.15920
H	5.45229	-0.76780	0.80760
H	4.47309	-2.89687	1.73860
H	2.91238	-2.87808	2.61333
H	2.94304	-2.65070	0.83943
H	5.32114	-1.07622	3.30399
H	4.44601	0.47132	3.45473
H	3.75146	-1.02597	4.15088
H	-0.82025	2.52702	2.76061
H	-0.14015	1.77793	4.23069
H	-1.52339	1.00902	3.41068
C	-2.07266	-2.00787	-2.66414
C	-1.18184	-1.83630	-3.77786
C	-1.40565	-0.54583	-4.34115
C	-2.42443	0.10805	-3.56870
C	-2.84376	-0.80550	-2.55275
H	-2.17472	-2.89746	-2.04993
H	-0.45069	-2.56363	-4.12577
H	-0.87959	-0.12025	-5.19203
H	-2.82113	1.10551	-3.73880
H	-3.61820	-0.61102	-1.81899
C	1.62132	-0.46622	-2.12678
C	1.06478	0.65129	-2.91187
C	0.36889	1.70495	-2.29475
H	0.75915	-1.15462	-1.60785
H	2.17261	-1.19640	-2.73113
H	1.17343	0.63580	-3.99890
H	0.61402	1.95039	-1.26022
H	2.12624	-0.19392	-1.19389
C	-0.19884	2.81308	-3.14962
H	-0.31740	2.47755	-4.19278
H	-1.18421	3.15453	-2.79740
H	0.47342	3.68976	-3.14531

67
x63 | au420a-auf65a | Energy: -907451.3940531

Ru	-0.49447	-0.14912	-1.75179
P	-0.98928	0.24161	0.53863
C	0.44260	0.34693	1.67468
N	0.55286	0.88260	2.94351
C	1.79823	0.51893	3.40963
C	2.40069	-0.23322	2.42319
N	1.54260	-0.32950	1.35706
C	3.75781	-0.89601	2.41640
C	-0.38380	1.68093	3.72975
C	-1.92376	-1.24558	1.22408
C	-0.99743	-2.47013	1.23834
C	-2.52758	-1.02886	2.61512
C	-2.06536	1.71246	0.96894
C	-1.34661	3.05778	0.79595
C	-3.37548	1.68468	0.17501
C	4.56943	-0.38356	1.21156
C	3.56613	-2.41969	2.28701
C	4.50845	-0.57649	3.71664
H	-2.30982	1.58149	2.03149
H	-2.73898	-1.41091	0.50026
H	2.14103	0.83398	4.39017
H	-0.49027	-2.61796	0.27360
H	-1.58556	-3.37208	1.47622
H	-0.21779	-2.35128	2.00697
H	-3.06162	-1.94266	2.92470
H	-3.24624	-0.19559	2.64715
H	-1.73037	-0.85025	3.35498
H	-1.30370	3.34756	-0.26131
H	-0.31629	3.04020	1.18533
H	-1.90582	3.84151	1.33345
H	-3.17621	1.78805	-0.90377
H	-4.01416	2.52719	0.48714
H	-3.94119	0.75367	0.34356
H	4.71058	0.70897	1.26695
H	4.05365	-0.62501	0.26821
H	5.56195	-0.86324	1.19497
H	4.54698	-2.92127	2.23803
H	3.01316	-2.81895	3.15370
H	3.00047	-2.65886	1.37184
H	5.49465	-1.06704	3.71020
H	4.66601	0.50959	3.82740
H	3.95135	-0.94228	4.59551
H	-0.58132	2.64887	3.25014
H	0.06900	1.86112	4.71354
H	-1.33074	1.14392	3.87532
C	-1.82501	-1.90539	-2.04891
C	-0.87681	-1.89129	-3.11931
C	-1.04667	-0.68703	-3.86395
C	-2.10065	0.06894	-3.24914
C	-2.58822	-0.68701	-2.13950
H	-1.97079	-2.70622	-1.33154
H	-0.13190	-2.65993	-3.31703
H	-0.46752	-0.38628	-4.73343
H	-2.46696	1.04064	-3.57051
H	-3.40844	-0.39485	-1.49254
C	1.84539	-0.03738	-1.66596
C	1.15180	0.98736	-2.47086
C	0.35391	1.96231	-1.84892
H	1.08207	-0.80053	-1.11261
H	2.47426	-0.71443	-2.25628
H	1.25187	0.96938	-3.55830
H	0.59845	2.23854	-0.82271
H	2.34027	0.32545	-0.75871
C	-0.35519	3.00152	-2.68367
H	-0.43289	2.67358	-3.73296
H	-1.37518	3.20265	-2.32020
H	0.19596	3.95872	-2.66336

x64-65

67			
x64 | au420t-auf65 | Energy: -907445.7776049			
Ru	-0.55861	-0.32285	-2.05953
P	-1.27829	0.18945	0.15228
C	0.19897	0.23987	1.21378
N	0.38744	0.68534	2.50027
C	1.65227	0.28169	2.86870
C	2.18743	-0.41269	1.80171
N	1.26726	-0.42613	0.78072
C	3.52511	-1.10754	1.69839
C	-0.48837	1.49347	3.34196
C	-2.27467	-1.25415	0.85439
C	-1.33969	-2.45370	1.07098
C	-3.05972	-0.96233	2.13742
C	-2.30353	1.69591	0.56146
C	-1.54024	3.02374	0.45466
C	-3.57814	1.68614	-0.29300
C	4.32228	-0.53275	0.51275
C	3.28524	-2.61198	1.46458
C	4.32193	-0.90687	2.99554
H	-2.59311	1.55566	1.61282
H	-2.99484	-1.48756	0.05256
H	2.05695	0.52755	3.84547
H	-0.67976	-2.63469	0.20957
H	-1.93926	-3.35920	1.26235
H	-0.69349	-2.27721	1.94586
H	-3.62560	-1.86487	2.42311
H	-3.78078	-0.13888	2.02370
H	-2.37690	-0.73370	2.97143
H	-1.44622	3.35393	-0.58621
H	-0.52757	2.95797	0.88270
H	-2.09546	3.80377	1.00149
H	-3.32993	1.74627	-1.36509
H	-4.20912	2.55312	-0.03741
H	-4.17408	0.77348	-0.12602
H	4.47635	0.55314	0.62899
H	3.79335	-0.71396	-0.43498
H	5.30905	-1.02111	0.45566
H	4.24988	-3.13431	1.35218
H	2.74334	-3.05873	2.31488
H	2.69012	-2.76823	0.55017
H	5.29124	-1.42460	2.92190
H	4.51795	0.16287	3.17955
H	3.77941	-1.31935	3.86267
H	-0.55049	2.52695	2.97045
H	-0.07409	1.50330	4.35881
H	-1.49639	1.06169	3.38015
C	-1.80423	-2.15752	-2.26617
C	-0.67338	-2.32498	-3.11602
C	-0.65711	-1.27976	-4.08441
C	-1.77888	-0.42175	-3.81948
C	-2.49499	-0.96582	-2.69592
H	-2.09520	-2.82112	-1.45973
H	0.08414	-3.10011	-3.01160
H	0.08750	-1.14410	-4.86412
H	-2.05373	0.47210	-4.37366
H	-3.41479	-0.56248	-2.27970
C	2.16388	0.36520	-2.33685
C	0.93641	1.00050	-2.94026
C	0.08565	1.85348	-2.23044
H	1.94353	-0.12176	-1.36305
H	2.60553	-0.37932	-3.01482
H	0.86276	1.00679	-4.03084
H	0.39911	2.17073	-1.23338
H	2.92563	1.13175	-2.10315
C	-0.86207	2.77130	-2.97193
H	-0.94616	2.46990	-4.02809
H	-1.87536	2.77930	-2.54320
H	-0.48550	3.80976	-2.94699

67			
x65 | au420z-auf65b | Energy: -907457.4863668			
Ru	0.06064	-0.19709	-1.07514
P	-1.38676	0.50455	0.68587
C	0.17114	0.67605	1.60832
N	0.64096	0.88556	2.86070
C	1.88224	0.29036	2.92347
C	2.13180	-0.30429	1.69646
N	1.06126	-0.01562	0.87897
C	3.21357	-1.31439	1.38021
C	-0.04060	1.59087	3.93853
C	-2.22493	-0.94642	1.56356
C	-1.17453	-1.98961	1.97315
C	-3.08291	-0.55737	2.77402
C	-2.53398	1.94564	0.99989
C	-1.92206	3.33478	0.78968
C	-3.81874	1.74868	0.18058
C	3.72643	-1.19719	-0.06210
C	2.57898	-2.70988	1.58721
C	4.38988	-1.15468	2.35596
H	-2.78566	1.84691	2.06842
H	-2.87779	-1.37917	0.78480
H	2.48703	0.33260	3.82339
H	-0.48129	-2.22667	1.15608
H	-1.68253	-2.91397	2.29257
H	-0.57607	-1.61893	2.82173
H	-3.48584	-1.47232	3.23907
H	-3.93453	0.08424	2.50454
H	-2.47807	-0.03754	3.53687
H	-1.78067	3.55891	-0.27581
H	-0.95149	3.44109	1.30163
H	-2.61192	4.08930	1.20291
H	-3.60902	1.80726	-0.89990
H	-4.54186	2.54245	0.42944
H	-4.29726	0.77742	0.38720
H	4.36849	-0.31137	-0.17325
H	2.89375	-1.12026	-0.77666
H	4.32952	-2.08632	-0.30683
H	3.31700	-3.49540	1.35525
H	2.24702	-2.83531	2.63079
H	1.70324	-2.84309	0.93401
H	5.16656	-1.89907	2.12018
H	4.83603	-0.14996	2.27582
H	4.07387	-1.32086	3.39918
H	0.57557	2.43317	4.28785
H	-0.23268	0.90514	4.77808
H	-0.99461	1.97660	3.55535
C	-0.90412	-2.17342	-1.44943
C	0.49380	-2.35511	-1.64216
C	0.92917	-1.48654	-2.68487
C	-0.22908	-0.77252	-3.16563
C	-1.35981	-1.18856	-2.40783
H	-1.52298	-2.70801	-0.73477
H	1.13660	-3.00955	-1.05961
H	1.94295	-1.40100	-3.06656
H	-0.23675	-0.04578	-3.97272
H	-2.38300	-0.85007	-2.55081
C	2.64386	1.82885	-1.10829
C	1.37331	1.47157	-1.83578
C	0.13140	2.00621	-1.46776
H	2.49316	1.90017	-0.02122
H	3.44625	1.10929	-1.30822
H	1.51291	1.23993	-2.89657
H	0.13881	2.55816	-0.52349
H	2.98796	2.81595	-1.46999
C	-0.90116	2.47181	-2.47094
H	-0.76732	1.97427	-3.44243
H	-1.93145	2.28373	-2.13255
H	-0.79788	3.56053	-2.63668

2.9.5.3. Ru(endo-η³-allyl)

n10-12

67			
n10 | iu110a-iuf19b | Energy: -907439.4365778			
Ru	-0.47726	-0.75497	0.87814
P	-1.68336	0.71488	-0.59000
C	-0.04056	0.90385	-1.37082
N	0.62595	1.47991	-2.40298
C	1.89455	0.93581	-2.41090
C	1.96740	0.01233	-1.38212
N	0.75055	0.02135	-0.74471
C	0.12263	2.49662	-3.31802
H	-0.91714	2.26394	-3.58714
H	0.73885	2.49048	-4.22707
H	0.16488	3.49531	-2.85518
H	2.63510	1.24212	-3.14249
C	-2.44735	2.38662	-0.22897
C	-3.01700	3.10846	-1.45715
C	-1.45292	3.27950	0.52194
C	-2.76495	-0.02218	-1.92483
C	-2.14679	-1.30374	-2.49166
C	-4.18056	-0.25327	-1.37871
H	-3.28005	2.13467	0.45239
H	-2.81198	0.73557	-2.72516
H	-3.79115	2.52173	-1.97287
H	-2.22124	3.35232	-2.17908
H	-3.47377	4.05923	-1.13554
H	-0.58136	3.51128	-0.11492
H	-1.94055	4.23231	0.78480
H	-1.08845	2.81415	1.44854
H	-2.13511	-2.10131	-1.73533
H	-2.74791	-1.65120	-3.34797
H	-1.11157	-1.14426	-2.83416
H	-4.65044	0.68170	-1.03416
H	-4.81755	-0.68271	-2.16954
H	-4.16825	-0.96074	-0.53310
C	3.08879	-0.93559	-1.03207
C	4.34923	-0.57571	-1.83164
C	3.39603	-0.86427	0.47412
C	2.63973	-2.36381	-1.40738
H	5.16256	-1.27136	-1.57227
H	4.17006	-0.65441	-2.91693
H	4.68581	0.44895	-1.60179
H	3.81634	0.11769	0.73763
H	4.13606	-1.63780	0.73687
H	2.48455	-1.01856	1.06935
H	1.70852	-2.62824	-0.88681
H	3.42157	-3.08860	-1.12614
H	2.46509	-2.44310	-2.49319
C	-1.90244	-2.38342	0.95655
C	-0.66693	-2.84476	0.38841
C	-1.65916	-1.94992	2.30148
H	-2.86182	-2.35768	0.44680
C	0.35105	-2.72832	1.40974
H	-0.53220	-3.25587	-0.60859
C	-0.26362	-2.17345	2.56444
H	-2.39516	-1.56550	3.00230
H	1.39664	-3.00466	1.31190
H	0.25237	-1.91179	3.48634
C	0.66071	0.86239	2.29305
C	1.45831	1.79266	1.74256
C	2.81727	2.18938	2.23642
C	3.35097	1.37966	3.41710
H	3.51763	2.13415	1.38131
H	-0.43439	0.84139	2.01190
H	0.94638	0.33687	3.20274
H	1.10659	2.31510	0.84784
H	2.77975	3.26574	2.49465
H	3.42490	0.31035	3.15700
H	4.35204	1.73352	3.70805
H	2.68897	1.47351	4.29407

67			
n11 | iu110t-iuf19 | Energy: -907439.2168114			
Ru	-0.66876	-0.98186	1.13543
P	-1.87782	0.48808	-0.34807
C	-0.23047	0.68294	-1.11916
N	0.41906	1.22258	-2.18175
C	1.67895	0.65991	-2.20751
C	1.76268	-0.24149	-1.16020
N	0.56345	-0.19694	-0.49044
C	-0.09371	2.22009	-3.11252
H	-1.13874	1.98656	-3.35963
H	0.50818	2.18912	-4.03060
H	-0.03936	3.22927	-2.67447
H	2.40713	0.94101	-2.96136
C	-2.68417	2.14989	-0.02551
C	-3.23176	2.85225	-1.27491
C	-1.73777	3.07288	0.75021
C	-2.92508	-0.27950	-1.69552
C	-2.28073	-1.55932	-2.23631
C	-4.34802	-0.52273	-1.17453
H	-3.53269	1.88344	0.63055
H	-2.96658	0.46735	-2.50624
H	-3.97267	2.24411	-1.81405
H	-2.41892	3.11580	-1.97034
H	-3.72409	3.79139	-0.97196
H	-0.84902	3.31785	0.14269
H	-2.25553	4.01756	0.98324
H	-1.39910	2.62690	1.69579
H	-2.27547	-2.34880	-1.47177
H	-2.86065	-1.92220	-3.10086
H	-1.24075	-1.39170	-2.55983
H	-4.83786	0.41040	-0.85365
H	-4.96294	-0.97279	-1.97141
H	-4.34297	-1.21751	-0.31835
C	2.87089	-1.21256	-0.82976
C	4.12187	-0.88538	-1.65791
C	3.21288	-1.14823	0.66922
C	2.38065	-2.63054	-1.19329
H	4.92611	-1.59517	-1.40858
H	3.91917	-0.97054	-2.73855
H	4.48348	0.13430	-1.44471
H	3.71669	-0.20111	0.91177
H	3.89566	-1.97354	0.92941
H	2.30465	-1.22611	1.28532
H	1.46428	-2.87852	-0.64036
H	3.15792	-3.37114	-0.94234
H	2.16588	-2.70203	-2.27243
C	-2.08175	-2.60052	1.22042
C	-0.83944	-3.06575	0.66458
C	-1.84714	-2.15700	2.56450
H	-3.03861	-2.58532	0.70551
C	0.17099	-2.93988	1.69165
H	-0.69746	-3.48639	-0.32743
C	-0.45220	-2.37605	2.83720
H	-2.58770	-1.76868	3.25847
H	1.21846	-3.21196	1.60175
H	0.05817	-2.10501	3.75933
C	0.27730	0.70782	2.69507
C	1.10669	1.54778	2.04891
C	2.53193	1.83265	2.40896
C	3.10478	0.99601	3.55143
H	3.14179	1.71746	1.49391
H	-0.80919	0.70611	2.46233
H	0.59811	0.17094	3.58649
H	0.72361	2.08597	1.17762
H	2.59954	2.91148	2.65177
H	3.06238	-0.07884	3.30930
H	4.15563	1.26536	3.73922
H	2.54013	1.15986	4.48424

67			
n12 | iu110z-iuf19a | Energy: -907455.9935469			
Ru	-0.17635	-0.40726	1.02280
P	-1.48846	0.89032	-0.50706
C	0.07948	0.98390	-1.42594
N	0.61338	1.42442	-2.59003
C	1.87243	0.87220	-2.68214
C	2.07461	0.07920	-1.56471
N	0.93960	0.17681	-0.78817
C	-0.00635	2.33613	-3.54314
H	-1.06029	2.05678	-3.68407
H	0.51871	2.25457	-4.50410
H	0.05066	3.37498	-3.18168
H	2.52216	1.08389	-3.52454
C	-2.22057	2.60880	-0.27555
C	-3.05821	3.09937	-1.46640
C	-1.13800	3.64288	0.07146
C	-2.66022	0.02137	-1.68114
C	-2.02463	-1.23154	-2.29258
C	-3.98920	-0.27220	-0.97181
H	-2.88781	2.48906	0.59711
H	-2.84815	0.74246	-2.49328
H	-3.91180	2.44402	-1.68976
H	-2.44167	3.19414	-2.37519
H	-3.45535	4.10031	-1.23036
H	-0.35895	3.67817	-0.70939
H	-1.60287	4.64068	0.13024
H	-0.65330	3.44009	1.03427
H	-1.79757	-1.98479	-1.52633
H	-2.72779	-1.67791	-3.01490
H	-1.08806	-0.99509	-2.82278
H	-4.46625	0.64585	-0.59224
H	-4.68873	-0.75126	-1.67660
H	-3.84570	-0.95344	-0.11816
C	3.25524	-0.82078	-1.27849
C	4.39625	-0.50727	-2.25924
C	3.75007	-0.62304	0.16192
C	2.81959	-2.28747	-1.47596
H	5.25951	-1.15301	-2.03527
H	4.09309	-0.69953	-3.30188
H	4.71861	0.54324	-2.17112
H	4.18378	0.38163	0.28840
H	4.53120	-1.36626	0.39053
H	2.92509	-0.73825	0.87851
H	2.03207	-2.56090	-0.76159
H	3.68162	-2.95508	-1.31312
H	2.44008	-2.45082	-2.49815
C	-1.49887	-2.25966	1.06888
C	-0.21823	-2.60560	0.57008
C	-1.34214	-1.72431	2.38409
H	-2.43454	-2.34307	0.52485
C	0.75728	-2.33981	1.60580
H	-0.01218	-3.00745	-0.41839
C	0.05415	-1.81549	2.72253
H	-2.13813	-1.37384	3.03536
H	1.82342	-2.53855	1.55158
H	0.49476	-1.50840	3.66416
C	-0.38262	1.19564	2.51986
C	0.84849	1.39817	1.87489
C	2.20441	1.33288	2.55119
C	2.44899	0.22753	3.57454
H	2.98360	1.29390	1.77764
H	-1.25326	1.80977	2.28214
H	-0.39356	0.76901	3.52582
H	0.85777	2.10879	1.04427
H	2.33389	2.31240	3.05262
H	2.49307	-0.75913	3.08907
H	3.40817	0.39469	4.08966
H	1.66009	0.20348	4.34505

n13-15

67
n13 | iu111t-iuf71 | Energy: -907455.2132828

Ru	-0.14682	-0.39082	1.00434
P	-1.47475	0.88285	-0.52025
C	0.05567	0.92906	-1.49639
N	0.53968	1.35801	-2.68475
C	1.80869	0.83640	-2.80568
C	2.06434	0.07385	-1.67852
N	0.95047	0.15600	-0.86643
C	-0.13287	2.23541	-3.63236
H	-1.21595	2.18079	-3.45771
H	0.08571	1.90201	-4.65677
H	0.20369	3.27674	-3.50594
H	2.42697	1.04391	-3.67251
C	-2.09608	2.63865	-0.25316
C	-3.15844	3.10738	-1.25568
C	-0.91515	3.62101	-0.21395
C	-2.73310	0.04137	-1.61969
C	-2.10057	-1.11761	-2.40013
C	-3.94485	-0.38148	-0.77708
H	-2.56060	2.60105	0.74796
H	-3.06223	0.80442	-2.34286
H	-4.05298	2.46730	-1.25426
H	-2.75702	3.14309	-2.28238
H	-3.47278	4.12995	-0.98911
H	-0.44396	3.69856	-1.20765
H	-1.28274	4.62175	0.06629
H	-0.14134	3.32578	0.50822
H	-1.59341	-1.83188	-1.73539
H	-2.88528	-1.65655	-2.95627
H	-1.35457	-0.75175	-3.12327
H	-4.40385	0.47900	-0.26208
H	-4.71120	-0.83455	-1.42738
H	-3.66225	-1.12058	-0.01137
C	3.28226	-0.78287	-1.41847
C	4.44659	-0.31697	-2.30816
C	3.69508	-0.69169	0.05563
C	2.94406	-2.24580	-1.77139
H	5.33570	-0.93236	-2.09965
H	4.20529	-0.43026	-3.37812
H	4.69926	0.73774	-2.11154
H	4.02554	0.33041	0.29989
H	4.53076	-1.38262	0.25148
H	2.85216	-0.95031	0.71296
H	2.12787	-2.62081	-1.13790
H	3.82893	-2.88283	-1.60793
H	2.63794	-2.33527	-2.82654
C	-1.32519	-2.33116	0.88220
C	0.04971	-2.64655	0.76666
C	-1.52638	-1.66614	2.14207
H	-2.09112	-2.55582	0.14761
C	0.72991	-2.21730	1.95710
H	0.51007	-3.11889	-0.09652
C	-0.25817	-1.63192	2.80938
H	-2.47358	-1.32344	2.55012
H	1.78191	-2.35844	2.18615
H	-0.07799	-1.21154	3.79279
C	-0.26043	1.32998	2.38650
C	1.05605	1.28360	1.90097
C	2.28070	1.05240	2.76959
C	2.13094	0.22899	4.04949
H	3.09604	0.63760	2.16268
H	-0.96824	2.07119	2.02037
H	-0.46707	0.98352	3.40103
H	1.28681	1.91822	1.03877
H	2.61713	2.06934	3.05376
H	2.04977	-0.84708	3.83904
H	3.01872	0.37075	4.68597
H	1.25210	0.53745	4.64028

67
n14 | iu112a-iuf73a | Energy: -907456.1741692

Ru	-0.19818	-0.43905	0.99531
P	-1.57176	0.82271	-0.49226
C	-0.06771	0.87423	-1.50912
N	0.39573	1.30519	-2.70413
C	1.66640	0.78945	-2.84453
C	1.94196	0.03120	-1.71920
N	0.83965	0.10736	-0.89350
C	-0.30966	2.15187	-3.65555
H	-1.36025	2.22926	-3.34426
H	-0.25991	1.70404	-4.65905
H	0.13559	3.15874	-3.68086
H	2.26986	0.99739	-3.72187
C	-2.15986	2.58811	-0.19912
C	-3.35209	3.02295	-1.05943
C	-0.98595	3.56981	-0.35574
C	-2.85706	-0.01748	-1.56770
C	-2.21205	-1.06738	-2.48161
C	-3.96916	-0.60692	-0.68923
H	-2.48017	2.58194	0.85693
H	-3.29094	0.77381	-2.19821
H	-4.22930	2.37268	-0.92148
H	-3.09322	3.03330	-2.13220
H	-3.64162	4.04918	-0.77919
H	-0.71961	3.68148	-1.41889
H	-1.28268	4.56069	0.02533
H	-0.08266	3.24780	0.18490
H	-1.58430	-1.76893	-1.91242
H	-3.00128	-1.64229	-2.99365
H	-1.57498	-0.59886	-3.24774
H	-4.39075	0.14047	0.00438
H	-4.78835	-0.97654	-1.32763
H	-3.59145	-1.45334	-0.09538
C	3.15536	-0.83148	-1.46611
C	4.35713	-0.29452	-2.26020
C	3.49343	-0.84947	0.02975
C	2.83531	-2.26372	-1.94671
H	5.23530	-0.93298	-2.07493
H	4.15977	-0.30557	-3.34500
H	4.60425	0.73577	-1.95629
H	3.73646	0.16239	0.39011
H	4.36347	-1.50190	0.20558
H	2.64178	-1.22167	0.61528
H	1.93281	-2.65450	-1.45112
H	3.68034	-2.93510	-1.72053
H	2.65887	-2.27803	-3.03471
C	-1.07554	-2.46455	0.72467
C	0.31079	-2.63398	1.03240
C	-1.68617	-1.80313	1.85386
H	-1.58610	-2.83984	-0.15605
C	0.57163	-2.08693	2.31862
H	1.05641	-3.07323	0.37498
C	-0.67154	-1.57328	2.82702
H	-2.73634	-1.54665	1.96389
H	1.53246	-2.06033	2.82313
H	-0.81860	-1.09226	3.78945
C	-0.11671	1.37208	2.29862
C	1.19821	1.09309	1.90657
C	2.28954	0.64877	2.87094
C	1.85325	0.39027	4.31439
H	2.82709	-0.22602	2.47739
H	-0.67170	2.18961	1.84833
H	-0.43720	1.11687	3.30988
H	1.57936	1.62524	1.02938
H	3.03646	1.46482	2.87923
H	1.14447	-0.44769	4.39384
H	2.72978	0.14306	4.93428
H	1.37081	1.28049	4.75033

67
n15 | iu112t-iuf73 | Energy: -907455.4225447

Ru	-0.22089	-0.52947	0.93810
P	-1.58199	0.75713	-0.54529
C	-0.08310	0.77850	-1.57056
N	0.38672	1.22154	-2.75872
C	1.67880	0.75520	-2.87136
C	1.96298	0.01598	-1.73562
N	0.84096	0.04998	-0.93304
C	-0.32413	2.05476	-3.71793
H	-1.39042	2.06194	-3.45444
H	-0.20312	1.64031	-4.72943
H	0.06219	3.08597	-3.69569
H	2.28995	0.98056	-3.73897
C	-2.11088	2.53969	-0.25023
C	-3.23844	3.04060	-1.16028
C	-0.88673	3.46715	-0.33163
C	-2.91378	-0.03830	-1.59109
C	-2.33786	-1.15375	-2.47262
C	-4.05546	-0.51527	-0.68234
H	-2.48493	2.53204	0.78820
H	-3.30057	0.75543	-2.24916
H	-4.15387	2.43730	-1.06530
H	-2.93185	3.04317	-2.22013
H	-3.48629	4.07921	-0.88552
H	-0.55723	3.57458	-1.37776
H	-1.15739	4.46747	0.04391
H	-0.03134	3.09766	0.25426
H	-1.77200	-1.89192	-1.88537
H	-3.16138	-1.67686	-2.98627
H	-1.65709	-0.74800	-3.23750
H	-4.46548	0.30889	-0.07426
H	-4.87515	-0.92341	-1.29621
H	-3.71235	-1.30521	0.00376
C	3.21955	-0.76950	-1.44223
C	4.40071	-0.17889	-2.22924
C	3.52521	-0.73257	0.05966
C	3.00103	-2.23120	-1.88616
H	5.31394	-0.75304	-2.00696
H	4.22792	-0.23494	-3.31688
H	4.57432	0.87392	-1.95286
H	3.69090	0.29932	0.40658
H	4.43136	-1.32301	0.26921
H	2.68447	-1.15071	0.62831
H	2.14804	-2.67832	-1.35282
H	3.90098	-2.82870	-1.66496
H	2.80104	-2.28691	-2.96870
C	-1.32248	-2.48723	0.74369
C	0.06679	-2.77696	0.73621
C	-1.63257	-1.83027	1.99083
H	-2.03030	-2.74281	-0.03750
C	0.64285	-2.32398	1.96480
H	0.60966	-3.23146	-0.08871
C	-0.41843	-1.75508	2.74296
H	-2.61514	-1.51253	2.32967
H	1.68112	-2.42494	2.26653
H	-0.32152	-1.33094	3.73698
C	-0.20536	1.22492	2.29797
C	1.11994	1.00252	1.89610
C	2.22559	0.55165	2.84982
C	1.86560	0.58238	4.33832
H	2.60928	-0.44323	2.58395
H	-0.78475	2.04391	1.88122
H	-0.51655	0.92517	3.30027
H	1.48089	1.58537	1.04315
H	3.07514	1.23791	2.68624
H	1.07761	-0.14257	4.59597
H	2.75047	0.33408	4.94615
H	1.51021	1.58152	4.63993

n16-18

67			
n16 | iu210a-iuf21a | Energy: -907457.1422657			
Ru	-0.65110	-0.58592	-0.36828
P	-0.32221	1.77022	-0.31728
C	1.36006	1.31371	0.19816
N	2.56890	1.84989	0.47837
C	3.41075	0.79766	0.76818
C	2.67945	-0.37342	0.65783
N	1.39756	-0.02101	0.28781
C	2.90820	3.26563	0.48281
H	2.05251	3.83104	0.08982
H	3.78537	3.44283	-0.15731
H	3.12760	3.60436	1.50735
H	4.45055	0.95884	1.03231
C	-1.03752	2.90095	1.00779
C	-0.95833	4.40050	0.70063
C	-0.38823	2.58153	2.36398
C	-0.14220	2.79670	-1.87380
C	1.07424	2.36191	-2.70162
C	-1.45268	2.75807	-2.67230
H	-2.10221	2.61173	1.04591
H	0.02790	3.83032	-1.53571
H	-1.49551	4.66924	-0.22175
H	0.08777	4.73915	0.60638
H	-1.41375	4.96200	1.53315
H	0.65648	2.93374	2.38177
H	-0.93731	3.10070	3.16638
H	-0.38457	1.50461	2.58882
H	1.06705	1.28275	-2.91372
H	1.07352	2.90265	-3.66259
H	2.01718	2.58979	-2.18095
H	-2.31785	3.06019	-2.05765
H	-1.38688	3.44988	-3.52802
H	-1.64649	1.74723	-3.06249
C	3.14251	-1.77429	0.98690
C	4.67249	-1.85964	0.86013
C	2.74298	-2.08793	2.44527
C	2.49392	-2.79831	0.04500
H	5.00379	-2.88273	1.09771
H	5.00098	-1.61468	-0.16320
H	5.17268	-1.17547	1.56536
H	3.22833	-1.38281	3.13985
H	3.06202	-3.11052	2.70735
H	1.65468	-2.02003	2.58145
H	1.39890	-2.74605	0.11053
H	2.82016	-3.81256	0.32492
H	2.79459	-2.61400	-0.99970
C	-2.04815	-0.80360	-2.04509
C	-0.71298	-0.82242	-2.59528
C	-2.17694	-1.94164	-1.19511
H	-2.83302	-0.08682	-2.27105
C	-0.04350	-1.95909	-2.06156
H	-0.31131	-0.12932	-3.32616
C	-0.93302	-2.65860	-1.19182
H	-3.07033	-2.21013	-0.63967
H	0.99492	-2.22222	-2.24357
H	-0.71575	-3.57061	-0.64413
C	-1.98248	-0.42343	1.40884
C	-0.85585	-1.16019	1.79620
C	-0.86113	-2.63539	2.16786
C	-2.16907	-3.39823	1.95252
H	-0.02950	-3.15564	1.66545
H	-2.09343	0.61684	1.70670
H	-2.92359	-0.94172	1.21805
H	-0.04823	-0.60361	2.28100
H	-0.61467	-2.67570	3.24577
H	-2.42180	-3.50914	0.88844
H	-2.08678	-4.41104	2.37792
H	-3.01140	-2.89139	2.45164

67			
n17 | iu210t-iuf21 | Energy: -907436.4734906			
Ru	-1.87455	-0.79248	-0.64825
P	-0.68441	1.26401	-0.45898
C	0.93339	0.87304	0.29158
N	2.01730	1.65983	0.59237
C	3.05785	0.80544	0.87818
C	2.57629	-0.48229	0.73503
N	1.25465	-0.41793	0.36835
C	2.10599	3.11182	0.64219
H	1.77907	3.55369	-0.30989
H	3.15340	3.39051	0.81749
H	1.48813	3.51333	1.45962
H	4.03472	1.18578	1.16099
C	-1.56018	2.59580	0.56089
C	-1.26637	4.05253	0.17131
C	-1.32871	2.38476	2.06562
C	-0.16746	2.14320	-2.03805
C	0.89650	1.33690	-2.79296
C	-1.35071	2.51989	-2.94169
H	-2.62337	2.39409	0.34221
H	0.29238	3.07938	-1.68412
H	-1.48331	4.26332	-0.88503
H	-0.22062	4.32691	0.36983
H	-1.90252	4.71392	0.78286
H	-0.25512	2.42393	2.31393
H	-1.83763	3.18547	2.62732
H	-1.72450	1.42515	2.42445
H	0.52341	0.33555	-3.06130
H	1.16572	1.86475	-3.72313
H	1.80961	1.20312	-2.19268
H	-2.20621	2.92602	-2.37864
H	-1.02673	3.28993	-3.66098
H	-1.70057	1.65655	-3.52351
C	3.30621	-1.78720	0.96737
C	4.81579	-1.58564	0.75554
C	3.06484	-2.24985	2.41943
C	2.78969	-2.86015	-0.00584
H	5.34630	-2.53665	0.92326
H	5.02901	-1.24242	-0.27014
H	5.22320	-0.84606	1.46528
H	3.45180	-1.50649	3.13581
H	3.57741	-3.20951	2.60088
H	1.98991	-2.39055	2.61792
H	1.71113	-3.02912	0.13489
H	3.32179	-3.80877	0.17202
H	2.95760	-2.55477	-1.05202
C	-3.20880	-0.13756	-2.21448
C	-2.11860	-0.84842	-2.83199
C	-3.90905	-1.06232	-1.36569
H	-3.48651	0.89707	-2.38827
C	-2.14743	-2.18475	-2.32476
H	-1.40936	-0.45697	-3.55280
C	-3.26694	-2.34068	-1.44659
H	-4.78137	-0.81977	-0.76377
H	-1.40979	-2.95424	-2.54889
H	-3.56367	-3.25298	-0.93812
C	-2.87386	-0.86853	1.41899
C	-1.52298	-1.11561	1.55482
C	-0.87416	-2.46455	1.34280
C	-1.76476	-3.67611	1.61482
H	-0.46042	-2.51779	0.30157
H	-3.28057	0.10600	1.69789
H	-3.58778	-1.68697	1.32580
H	-0.86684	-0.33880	1.94283
H	0.04450	-2.49144	1.94770
H	-2.66036	-3.67054	0.97572
H	-1.21417	-4.60928	1.41739
H	-2.09720	-3.68450	2.66560

67			
n18 | iu220a-iuf23a | Energy: -907440.2225899			
Ru	-1.59239	-0.66059	-0.35713
P	-0.15362	1.24581	-0.32061
C	1.50465	0.95812	0.41729
N	2.54307	1.82986	0.66779
C	3.61436	1.06298	1.07149
C	3.20211	-0.25246	1.04321
N	1.89510	-0.29464	0.62939
C	2.57822	3.28415	0.63164
H	2.07791	3.66478	-0.26696
H	3.62844	3.60491	0.60887
H	2.09316	3.71295	1.52274
H	4.56060	1.52113	1.34215
C	-0.98799	2.64874	0.63547
C	-0.69673	4.10011	0.22140
C	-0.75037	2.47276	2.14310
C	0.34569	1.98271	-1.97976
C	1.23374	0.99546	-2.74776
C	-0.81058	2.49312	-2.85246
H	-2.05145	2.44232	0.42593
H	0.95705	2.85517	-1.69938
H	-0.72803	4.26240	-0.86444
H	0.27743	4.44179	0.59373
H	-1.46121	4.75075	0.67849
H	0.31618	2.60695	2.38824
H	-1.32535	3.23201	2.69873
H	-1.05619	1.48246	2.50748
H	0.67946	0.07127	-2.98014
H	1.55740	1.45179	-3.69809
H	2.12916	0.71566	-2.17166
H	-1.58044	3.03288	-2.28070
H	-0.40700	3.18829	-3.60691
H	-1.29834	1.67477	-3.39744
C	3.96314	-1.50563	1.40669
C	5.43608	-1.16876	1.67867
C	3.33760	-2.12175	2.67435
C	3.86744	-2.51647	0.24876
H	5.98852	-2.08517	1.94011
H	5.91017	-0.72231	0.78874
H	5.53245	-0.46211	2.52012
H	3.40329	-1.42205	3.52399
H	3.86737	-3.05043	2.94445
H	2.27494	-2.36535	2.50920
H	2.81472	-2.76073	0.03153
H	4.39624	-3.44609	0.51647
H	4.32224	-2.10677	-0.66835
C	-2.98148	0.31677	-1.76061
C	-2.16063	-0.61621	-2.49607
C	-3.74693	-0.42322	-0.81328
H	-3.03312	1.38871	-1.91707
C	-2.43886	-1.92018	-1.98279
H	-1.48310	-0.38838	-3.31133
C	-3.41674	-1.81735	-0.95033
H	-4.45589	0.00017	-0.10615
H	-1.95044	-2.83846	-2.30344
H	-3.83948	-2.64057	-0.38158
C	-2.25019	-0.85992	1.80719
C	-0.88885	-1.09912	1.66496
C	-0.35071	-2.24185	0.88308
C	-1.04797	-3.59573	0.95530
H	-0.24875	-1.88349	-0.27982
H	-2.57498	0.03786	2.33608
H	-2.98299	-1.66365	1.73067
H	-0.15768	-0.40111	2.06846
H	0.73426	-2.29992	1.02618
H	-2.14147	-3.49952	0.90554
H	-0.72155	-4.24540	0.12841
H	-0.78526	-4.09181	1.90370

n19-21

67
n19 | iu220t-iuf23 | Energy: -907438.3845456

Ru	-2.03003	-0.83370	-0.50396
P	-0.64424	1.09363	-0.45216
C	1.02932	0.79205	0.24967
N	2.07735	1.65805	0.48378
C	3.14204	0.88641	0.89788
C	2.71567	-0.42443	0.89460
N	1.40786	-0.45992	0.48452
C	2.13694	3.11067	0.40761
H	1.70132	3.47311	-0.53212
H	3.19182	3.41421	0.43989
H	1.60807	3.57418	1.25461
H	4.09432	1.33915	1.15613
C	-1.44599	2.47880	0.56129
C	-1.21245	3.92507	0.09889
C	-1.09162	2.33314	2.04978
C	-0.19193	1.87350	-2.10439
C	0.74284	0.94626	-2.89158
C	-1.37891	2.33348	-2.96423
H	-2.51848	2.25097	0.43709
H	0.36969	2.77520	-1.81480
H	-1.46879	4.08871	-0.95618
H	-0.17351	4.24415	0.25262
H	-1.85033	4.59069	0.70457
H	-0.01354	2.48834	2.21644
H	-1.63928	3.09235	2.63241
H	-1.35161	1.34566	2.45474
H	0.24502	-0.01074	-3.11870
H	1.02002	1.42544	-3.84534
H	1.66457	0.72200	-2.33304
H	-2.18228	2.80544	-2.37913
H	-1.02085	3.07432	-3.69777
H	-1.81250	1.50086	-3.53276
C	3.46124	-1.68144	1.27542
C	4.92663	-1.35168	1.59189
C	2.79385	-2.30109	2.51954
C	3.39457	-2.68594	0.10967
H	5.46728	-2.27102	1.86726
H	5.42927	-0.90589	0.71733
H	5.00067	-0.64679	2.43707
H	2.83674	-1.60658	3.37497
H	3.31042	-3.23395	2.80046
H	1.73581	-2.53727	2.31816
H	2.34700	-2.92260	-0.13927
H	3.90968	-3.62021	0.38791
H	3.87876	-2.27423	-0.79136
C	-3.48774	0.05769	-1.96414
C	-2.57655	-0.82941	-2.64825
C	-4.24083	-0.71648	-1.04334
H	-3.59759	1.12260	-2.13665
C	-2.79403	-2.14583	-2.13348
H	-1.88785	-0.56715	-3.44367
C	-3.80989	-2.08294	-1.13470
H	-4.99770	-0.33066	-0.36453
H	-2.25313	-3.03888	-2.43765
H	-4.20111	-2.92001	-0.56434
C	-2.74806	-0.85552	1.61351
C	-1.39322	-1.21074	1.55152
C	-0.92141	-2.34236	0.77855
C	-1.63228	-3.68121	0.76771
H	-0.66225	-1.75320	-0.60151
H	-3.01455	0.08181	2.10523
H	-3.53258	-1.61352	1.57997
H	-0.63106	-0.53074	1.92803
H	0.16911	-2.41348	0.80421
H	-2.70926	-3.58072	0.95975
H	-1.49448	-4.20068	-0.19285
H	-1.19596	-4.31695	1.55723

67
n20 | iu221a-iuf25b | Energy: -907444.9858197

Ru	-1.50242	-0.66747	-0.38381
P	-0.22576	1.32200	-0.24017
C	1.46273	0.96523	0.39841
N	2.52770	1.82166	0.57014
C	3.59319	1.04948	0.98135
C	3.14110	-0.25190	1.05211
N	1.82155	-0.28153	0.68231
C	2.62182	3.24881	0.30300
H	2.62268	3.45083	-0.77987
H	3.56157	3.62122	0.73213
H	1.78939	3.78115	0.77858
H	4.56136	1.49485	1.18859
C	-1.00018	2.63006	0.89576
C	-0.97667	4.08301	0.39754
C	-0.42847	2.52563	2.31834
C	0.17566	2.20724	-1.84892
C	1.20372	1.41088	-2.66322
C	-1.03900	2.57870	-2.71133
H	-2.05399	2.30887	0.92254
H	0.64045	3.14477	-1.50662
H	-1.47783	4.20694	-0.57182
H	0.04205	4.48595	0.30211
H	-1.50873	4.71087	1.13174
H	0.63272	2.81975	2.34460
H	-0.98772	3.20176	2.98613
H	-0.49871	1.50724	2.72688
H	0.81130	0.41399	-2.92317
H	1.42340	1.94802	-3.60088
H	2.14691	1.26752	-2.11428
H	-1.89320	2.94673	-2.12414
H	-0.74703	3.37580	-3.41431
H	-1.37589	1.72304	-3.31170
C	3.87039	-1.50785	1.46532
C	5.32854	-1.18266	1.81625
C	3.16309	-2.11461	2.69305
C	3.82657	-2.51912	0.30367
H	5.85638	-2.10194	2.11565
H	5.85749	-0.75101	0.94991
H	5.38455	-0.46780	2.65444
H	3.19010	-1.41656	3.54649
H	3.66300	-3.05089	2.99189
H	2.10929	-2.33845	2.45928
H	2.78327	-2.74353	0.02726
H	4.32249	-3.45757	0.60231
H	4.34239	-2.11829	-0.58481
C	-3.01178	0.10937	-1.90574
C	-2.00570	-0.71280	-2.52470
C	-3.74563	-0.69985	-1.00197
H	-3.18890	1.16122	-2.10054
C	-2.13563	-2.03913	-1.99063
H	-1.30457	-0.40398	-3.29346
C	-3.20122	-2.02097	-1.03727
H	-4.55992	-0.36162	-0.36543
H	-1.53664	-2.90210	-2.26874
H	-3.55162	-2.86863	-0.45847
C	-2.24784	-0.46865	1.70575
C	-0.94894	-1.02643	1.71460
C	-0.68248	-2.24090	1.03500
C	-1.53744	-3.47992	1.14125
H	-0.00743	-0.99297	-0.79934
H	-2.39317	0.52459	2.13240
H	-3.12368	-1.12016	1.72475
H	-0.09658	-0.43108	2.03340
H	0.38173	-2.42087	0.87119
H	-2.57184	-3.25341	1.43772
H	-1.55179	-4.05743	0.20359
H	-1.09852	-4.13245	1.91772

67
n21 | iu221t-iuf25 | Energy: -907439.8204504

Ru	-1.91668	-0.88239	-0.52885
P	-0.64112	1.12989	-0.36912
C	1.09386	0.69142	0.04592
N	2.19480	1.50764	0.13303
C	3.24519	0.71375	0.54402
C	2.74351	-0.56152	0.70543
N	1.40582	-0.55076	0.39338
C	2.31769	2.92073	-0.19207
H	2.55438	3.06707	-1.25819
H	3.12137	3.35635	0.41776
H	1.38233	3.43935	0.04450
H	4.24096	1.12423	0.68196
C	-1.14182	2.35317	1.01656
C	-1.36458	3.81025	0.58574
C	-0.18780	2.29120	2.22257
C	-0.47233	2.19576	-1.91183
C	0.56139	1.64044	-2.90203
C	-1.82791	2.47801	-2.57927
H	-2.11653	1.97241	1.34710
H	-0.08540	3.15222	-1.53155
H	-2.09042	3.90753	-0.23343
H	-0.43125	4.30693	0.27614
H	-1.75545	4.37167	1.45068
H	0.76188	2.80304	2.00815
H	-0.66035	2.80110	3.07833
H	0.06057	1.26176	2.52366
H	0.32616	0.61779	-3.23041
H	0.58966	2.28547	-3.79618
H	1.57016	1.60782	-2.46704
H	-2.62080	2.70276	-1.84934
H	-1.72778	3.34632	-3.25080
H	-2.16770	1.62895	-3.18676
C	3.44163	-1.82449	1.14891
C	4.91919	-1.53545	1.44672
C	2.75015	-2.36039	2.41755
C	3.33183	-2.87717	0.02889
H	5.42411	-2.45958	1.76969
H	5.43765	-1.15827	0.54918
H	5.02272	-0.78917	2.25232
H	2.82212	-1.63138	3.24200
H	3.22868	-3.30025	2.73903
H	1.68423	-2.55958	2.21817
H	2.27373	-3.07815	-0.20572
H	3.80752	-3.81890	0.34952
H	3.83384	-2.52679	-0.88848
C	-3.28140	-0.72929	-2.30794
C	-1.94264	-0.93467	-2.77063
C	-3.65405	-1.90170	-1.56543
H	-3.91019	0.13071	-2.51889
C	-1.48898	-2.20678	-2.30764
H	-1.37303	-0.25635	-3.39194
C	-2.55560	-2.80662	-1.57232
H	-4.61258	-2.07354	-1.08284
H	-0.51086	-2.64229	-2.49250
H	-2.52436	-3.77589	-1.08624
C	-3.37863	-0.23936	1.00936
C	-2.18774	-0.69185	1.63097
C	-1.74299	-2.02159	1.42801
C	-2.65074	-3.22656	1.51642
H	-0.39911	-1.26249	-0.24623
H	-3.65537	0.81317	1.08175
H	-4.22000	-0.92392	0.89638
H	-1.50695	0.01817	2.09464
H	-0.71006	-2.20651	1.73369
H	-3.65412	-3.03640	1.10907
H	-2.21821	-4.09865	1.00429
H	-2.76163	-3.49836	2.58218

n22-24

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n22 | iu230a-iug21b | Energy: -907446.5663843

Ru	-1.44424	-0.71371	-0.00892
P	-0.21118	1.31504	-0.04332
C	1.55970	0.92224	0.24483
N	2.67699	1.72771	0.15287
C	3.76067	0.93092	0.44612
C	3.27443	-0.33610	0.69403
N	1.91050	-0.32114	0.55922
C	2.81147	3.15298	-0.11689
H	1.96479	3.51283	-0.70811
H	3.73455	3.31742	-0.69108
H	2.86836	3.72728	0.82167
H	4.76852	1.33495	0.44747
C	-0.73908	2.53989	1.27832
C	-0.34010	4.00377	1.05875
C	-0.26175	2.03582	2.64713
C	-0.24524	2.29400	-1.64766
C	0.58368	1.64707	-2.76338
C	-1.68191	2.57319	-2.10069
H	-1.83947	2.49857	1.23367
H	0.21382	3.26137	-1.39657
H	-0.71762	4.40653	0.10651
H	0.74921	4.14104	1.09721
H	-0.77615	4.60931	1.87065
H	0.83572	2.11223	2.72043
H	-0.70515	2.65259	3.44583
H	-0.53329	0.98253	2.82040
H	0.09378	0.74316	-3.15293
H	0.67676	2.35716	-3.60152
H	1.59736	1.37786	-2.42601
H	-2.25294	3.12814	-1.33862
H	-1.66323	3.18407	-3.01821
H	-2.21479	1.63418	-2.31663
C	4.02760	-1.60265	1.02699
C	5.51270	-1.28935	1.25754
C	3.42507	-2.23399	2.29569
C	3.89009	-2.58970	-0.14932
H	6.05705	-2.21487	1.50329
H	5.97221	-0.85500	0.35358
H	5.64240	-0.58120	2.09287
H	3.53223	-1.55634	3.15898
H	3.94276	-3.17951	2.52708
H	2.35243	-2.44230	2.15210
H	2.82983	-2.81808	-0.34464
H	4.41134	-3.53274	0.08506
H	4.32883	-2.16789	-1.06910
C	-2.25374	-2.20593	-1.50054
C	-1.37798	-1.30042	-2.17677
C	-1.48160	-2.92365	-0.52861
H	-3.31355	-2.34111	-1.69830
C	-0.06906	-1.45773	-1.60279
H	-1.64794	-0.63271	-2.98981
C	-0.13790	-2.45807	-0.58992
H	-1.85474	-3.68494	0.14869
H	0.83006	-0.91520	-1.87250
H	0.68740	-2.75407	0.04893
C	-3.31260	0.46679	0.00823
C	-2.95352	0.09762	1.33110
C	-2.87300	-1.27184	1.67763
C	-3.93219	-2.27980	1.29732
H	-0.50195	-0.68667	1.27117
H	-3.28157	1.52333	-0.25471
H	-4.04008	-0.12602	-0.54914
H	-2.55246	0.83275	2.02479
H	-2.36506	-1.48618	2.62127
H	-4.37127	-2.08429	0.30942
H	-3.55498	-3.31229	1.32244
H	-4.74354	-2.21577	2.04533

67
n23 | iu230t-iug21 | Energy: -907436.6360093

Ru	-1.37184	-0.57369	-0.43645
P	-0.35707	1.54230	-0.38600
C	1.40139	1.11384	0.02208
N	2.58736	1.76488	0.10090
C	3.53079	0.86126	0.56324
C	2.88692	-0.34258	0.75370
N	1.56854	-0.14789	0.40945
C	2.84099	3.17356	-0.17675
H	2.24590	3.49034	-1.04282
H	3.90686	3.30210	-0.40845
H	2.58079	3.79345	0.69567
H	4.56869	1.14910	0.70276
C	-0.79489	2.80455	0.96240
C	-0.61686	4.28082	0.58628
C	-0.01596	2.49587	2.25393
C	-0.23458	2.56398	-1.95390
C	0.67088	1.92594	-3.01351
C	-1.64270	2.86473	-2.48459
H	-1.86954	2.62656	1.13693
H	0.22242	3.51691	-1.64604
H	-1.22576	4.57458	-0.28060
H	0.43650	4.51752	0.36730
H	-0.92484	4.90462	1.44201
H	1.03607	2.80755	2.14849
H	-0.45427	3.05878	3.09410
H	-0.01293	1.42638	2.51549
H	0.25491	0.98530	-3.39802
H	0.77411	2.61754	-3.86626
H	1.67879	1.71556	-2.61942
H	-2.26290	3.37868	-1.73252
H	-1.57429	3.51568	-3.37181
H	-2.16664	1.93977	-2.76803
C	3.40458	-1.68325	1.20729
C	4.87904	-1.56384	1.61529
C	2.56302	-2.16960	2.40325
C	3.26239	-2.68643	0.04463
H	5.25501	-2.54501	1.94458
H	5.49907	-1.22874	0.76702
H	5.00300	-0.85076	2.44713
H	2.63872	-1.46799	3.25038
H	2.92280	-3.15717	2.73440
H	1.50161	-2.26431	2.12008
H	2.20851	-2.76817	-0.26917
H	3.60831	-3.68283	0.36461
H	3.86200	-2.37010	-0.82476
C	-2.60730	-1.54384	-2.13844
C	-1.53681	-0.80645	-2.70158
C	-2.06313	-2.54985	-1.28209
H	-3.66477	-1.34553	-2.29675
C	-0.30115	-1.36217	-2.20413
H	-1.63433	0.01519	-3.40278
C	-0.63249	-2.45050	-1.33824
H	-2.62950	-3.28377	-0.71926
H	0.70160	-1.03937	-2.46978
H	0.07508	-3.09356	-0.82179
C	-3.26456	-0.08319	0.61717
C	-2.20078	-0.15476	1.54489
C	-1.38703	-1.31233	1.68229
C	-1.93906	-2.71398	1.82751
H	0.30183	-0.67588	0.24047
H	-3.75272	0.88302	0.47248
H	-3.88607	-0.95848	0.41408
H	-1.85975	0.76702	2.00592
H	-0.46741	-1.14518	2.25274
H	-2.93964	-2.80494	1.38122
H	-1.28075	-3.46961	1.36957
H	-2.02419	-2.95715	2.90205

67
n24 | iu230z-iug21a | Energy: -907447.5490014

Ru	-1.51175	-0.57705	-0.36162
P	-0.43004	1.44621	-0.26617
C	1.37881	1.03021	0.14627
N	2.57053	1.66135	0.21945
C	3.53704	0.77206	0.67371
C	2.92660	-0.43863	0.87851
N	1.60837	-0.23189	0.54000
C	2.83714	3.06829	-0.06969
H	2.18376	3.40389	-0.88231
H	3.88522	3.16771	-0.38236
H	2.66102	3.68047	0.82755
H	4.57135	1.07377	0.80203
C	-0.78988	2.73234	1.08686
C	-0.51308	4.19997	0.74330
C	-0.09125	2.34378	2.40049
C	-0.22482	2.48694	-1.82092
C	0.66664	1.83743	-2.88479
C	-1.61898	2.82858	-2.36365
H	-1.87942	2.62349	1.21911
H	0.25077	3.42586	-1.50036
H	-1.07839	4.53839	-0.13735
H	0.55671	4.38471	0.56021
H	-0.81463	4.82845	1.59823
H	0.99096	2.55003	2.33913
H	-0.49940	2.94237	3.23138
H	-0.21586	1.27891	2.65146
H	0.20762	0.93278	-3.30394
H	0.81814	2.54823	-3.71438
H	1.65873	1.56455	-2.48680
H	-2.22982	3.35860	-1.61453
H	-1.52367	3.47861	-3.24937
H	-2.16228	1.91483	-2.64791
C	3.43313	-1.78189	1.33037
C	4.89925	-1.65733	1.76544
C	2.56722	-2.27360	2.50836
C	3.31348	-2.77467	0.15489
H	5.27133	-2.64026	2.09277
H	5.53264	-1.31463	0.93043
H	5.00467	-0.95137	2.60549
H	2.62533	-1.57716	3.36060
H	2.92490	-3.26147	2.83876
H	1.50876	-2.37909	2.21362
H	2.26687	-2.86724	-0.18155
H	3.65790	-3.77055	0.47623
H	3.92746	-2.45011	-0.70077
C	-2.62433	-1.62404	-2.03939
C	-1.56848	-0.87302	-2.61336
C	-2.06246	-2.59512	-1.14627
H	-3.68417	-1.47005	-2.22620
C	-0.32460	-1.37909	-2.07493
H	-1.67826	-0.07771	-3.34313
C	-0.63344	-2.44975	-1.18655
H	-2.61314	-3.33781	-0.57867
H	0.67163	-1.03552	-2.34100
H	0.08373	-3.06405	-0.64714
C	-3.44106	-0.28820	0.70424
C	-2.35893	-0.17618	1.60290
C	-1.37632	-1.20192	1.76868
C	-1.73904	-2.65653	2.00288
H	0.80937	-0.89210	0.55009
H	-4.06164	0.59535	0.54120
H	-3.93878	-1.24813	0.54560
H	-2.15318	0.80674	2.02003
H	-0.50641	-0.88037	2.35628
H	-2.71593	-2.89989	1.56095
H	-0.99233	-3.34869	1.57863
H	-1.80200	-2.85884	3.08764

n25-26

67
n25 | iu310t-iuf29 | Energy: -907446.0474654

Ru	-1.83576	-0.82757	-0.65131
P	-0.78731	1.18320	-0.39204
C	1.04144	0.80666	-0.11654
N	2.23061	1.42609	-0.28063
C	3.24402	0.60308	0.19482
C	2.66726	-0.54451	0.67455
N	1.31578	-0.37745	0.45787
C	2.48065	2.71138	-0.93745
H	1.76963	3.46171	-0.57712
H	2.38329	2.60374	-2.02716
H	3.50088	3.02954	-0.68716
H	4.28566	0.90203	0.14671
C	-1.08586	2.32479	1.09444
C	-0.48160	3.73095	1.02917
C	-0.64271	1.63267	2.39145
C	-0.73452	2.39705	-1.82575
C	-0.12658	1.81767	-3.10567
C	-2.17133	2.88240	-2.06351
H	-2.18438	2.42883	1.09504
H	-0.12034	3.25056	-1.50577
H	-0.79754	4.29868	0.14201
H	0.61973	3.69047	1.06494
H	-0.80584	4.29767	1.91826
H	0.45882	1.58490	2.44300
H	-0.99162	2.21464	3.26025
H	-1.03355	0.61058	2.48284
H	-0.77931	1.04964	-3.54005
H	-0.01149	2.62255	-3.85070
H	0.86470	1.36519	-2.93576
H	-2.58771	3.38514	-1.17494
H	-2.19110	3.59961	-2.90069
H	-2.82351	2.02899	-2.31353
C	3.24517	-1.75363	1.36166
C	4.77347	-1.73880	1.21608
C	2.85890	-1.69701	2.85546
C	2.66556	-3.03510	0.73312
H	5.19949	-2.61473	1.72883
H	5.07229	-1.77818	0.15580
H	5.20682	-0.83472	1.67506
H	3.27195	-0.79486	3.33481
H	3.25975	-2.58347	3.37278
H	1.76302	-1.69197	2.98217
H	1.57421	-3.09489	0.88377
H	3.11430	-3.91508	1.21940
H	2.87927	-3.08506	-0.34708
C	-2.62784	-2.26242	-2.25211
C	-1.83196	-1.24310	-2.86405
C	-1.81285	-3.00218	-1.35836
H	-3.69002	-2.42254	-2.42013
C	-0.50378	-1.37121	-2.32752
H	-2.16392	-0.54666	-3.62758
C	-0.48334	-2.46043	-1.39734
H	-2.14120	-3.83539	-0.74653
H	0.35531	-0.77283	-2.61532
H	0.39305	-2.86528	-0.90105
C	-3.93089	-0.30905	-0.15443
C	-3.13941	-0.31834	1.01995
C	-2.40507	-1.46463	1.43182
C	-3.03043	-2.84475	1.49914
H	0.53848	-1.04255	0.60176
H	-4.36345	0.64251	-0.47057
H	-4.49835	-1.19665	-0.44321
H	-2.92839	0.63230	1.50393
H	-1.69482	-1.28220	2.24537
H	-3.76304	-3.00155	0.69331
H	-2.27452	-3.64394	1.43776
H	-3.55820	-2.96245	2.46373

67
n26 | iu310z-iuf29b | Energy: -907446.5194466

Ru	-1.43778	-0.66564	-0.44018
P	-0.37537	1.32977	-0.13476
C	1.45881	0.97089	0.07096
N	2.63113	1.59908	-0.16526
C	3.67297	0.81870	0.32080
C	3.13278	-0.31083	0.87882
N	1.77207	-0.17609	0.69807
C	2.83395	2.86928	-0.86821
H	2.28380	3.67197	-0.36302
H	2.49162	2.78209	-1.90785
H	3.90732	3.09679	-0.85239
H	4.70708	1.13039	0.22144
C	-0.61053	2.42356	1.39611
C	0.17837	3.73653	1.40771
C	-0.31542	1.62259	2.67020
C	-0.39946	2.59569	-1.52441
C	0.02096	2.00019	-2.86957
C	-1.82404	3.16281	-1.60557
H	-1.68653	2.66541	1.36180
H	0.29159	3.40765	-1.25748
H	-0.03917	4.37907	0.54173
H	1.26279	3.53843	1.45224
H	-0.08039	4.30551	2.31643
H	0.76436	1.40833	2.75057
H	-0.60350	2.21332	3.55527
H	-0.85732	0.66824	2.69747
H	-0.69316	1.22659	-3.18599
H	0.03219	2.79303	-3.63593
H	1.02413	1.54281	-2.83535
H	-2.12738	3.66062	-0.67037
H	-1.88289	3.90395	-2.41954
H	-2.54153	2.35404	-1.82012
C	3.75398	-1.47318	1.60779
C	5.27770	-1.43161	1.42410
C	3.40177	-1.35294	3.10622
C	3.19075	-2.79622	1.05502
H	5.73565	-2.27231	1.96736
H	5.55236	-1.51583	0.35991
H	5.70068	-0.49717	1.82866
H	3.80562	-0.42008	3.53163
H	3.83474	-2.20452	3.65525
H	2.30939	-1.36550	3.26004
H	2.10465	-2.87458	1.23308
H	3.67076	-3.64130	1.57227
H	3.38201	-2.89369	-0.02608
C	-2.10683	-2.30424	-1.85432
C	-1.42363	-1.27188	-2.58647
C	-1.18815	-2.88603	-0.94138
H	-3.14948	-2.58722	-1.97241
C	-0.07967	-1.22988	-2.09633
H	-1.83880	-0.67255	-3.39135
C	0.07550	-2.23401	-1.07799
H	-1.41640	-3.68189	-0.23969
H	0.70848	-0.58062	-2.46478
H	1.00245	-2.51888	-0.59141
C	-3.52779	0.03244	-0.25742
C	-2.92077	-0.02451	1.02498
C	-2.37205	-1.22519	1.54256
C	-3.11860	-2.54414	1.48455
H	1.01662	-0.84704	0.89807
H	-3.83007	1.01225	-0.63161
H	-4.13244	-0.80359	-0.61516
H	-2.69024	0.91025	1.53364
H	-1.77403	-1.10918	2.45146
H	-3.66213	-2.67052	0.53643
H	-2.44281	-3.40375	1.61312
H	-3.85792	-2.58285	2.30575

67
n27 | iu330t-iuf33 | Energy: -907437.6119811

Ru	-1.86977	-0.99306	-0.25242
P	-0.70820	1.00732	-0.12860
C	1.14266	0.79884	0.18646
N	2.19834	1.62370	0.38155
C	3.36528	0.87529	0.44955
C	3.03488	-0.44134	0.27742
N	1.66539	-0.43684	0.12366
C	2.21740	3.07765	0.53512
H	1.32258	3.51367	0.08795
H	3.11045	3.46511	0.02563
H	2.25764	3.34085	1.60247
H	4.32871	1.34555	0.61271
C	-1.28285	2.11741	1.28516
C	-0.91557	3.60729	1.31212
C	-0.95638	1.42991	2.61735
C	-0.52805	2.12972	-1.64434
C	0.03786	1.29459	-2.79973
C	-1.83677	2.81925	-2.05232
H	-2.37224	2.05714	1.13807
H	0.19874	2.91577	-1.38379
H	-0.89312	4.06654	0.31166
H	0.05363	3.77507	1.80272
H	-1.66899	4.14939	1.90754
H	0.13276	1.43916	2.80544
H	-1.44355	1.96761	3.44772
H	-1.30425	0.38460	2.61738
H	-0.64167	0.45725	-3.02916
H	0.14649	1.92267	-3.69957
H	1.02821	0.87204	-2.55757
H	-2.31213	3.35589	-1.21633
H	-1.62073	3.55383	-2.84593
H	-2.55821	2.09630	-2.45831
C	3.86475	-1.69577	0.20940
C	5.32039	-1.35783	0.56153
C	3.30774	-2.73371	1.20373
C	3.79195	-2.26254	-1.22429
H	5.93180	-2.27142	0.50714
H	5.74062	-0.62485	-0.14688
H	5.39742	-0.95150	1.58331
H	3.32167	-2.34419	2.23467
H	3.92662	-3.64377	1.16574
H	2.27506	-3.02327	0.94781
H	2.75522	-2.51583	-1.50379
H	4.39127	-3.18480	-1.28485
H	4.18532	-1.53904	-1.95636
C	-2.57174	-3.10761	-0.24186
C	-1.60507	-2.98560	-1.29318
C	-1.90361	-2.85914	1.00339
H	-3.61306	-3.38462	-0.36288
C	-0.35564	-2.65540	-0.71196
H	-1.79192	-3.12069	-2.35517
C	-0.54365	-2.57115	0.72908
H	-2.35992	-2.87519	1.98907
H	0.57527	-2.58634	-1.27286
H	0.21770	-2.38581	1.48308
C	-3.41512	-0.41582	-1.71600
C	-3.55184	0.35478	-0.53331
C	-3.71055	-0.24576	0.75040
C	-4.76173	-1.30323	1.02435
H	1.06214	-1.23216	-0.06391
H	-3.16736	0.10424	-2.64332
H	-4.00182	-1.32877	-1.84568
H	-3.32530	1.41956	-0.58672
H	-3.56268	0.43733	1.59340
H	-5.02800	-1.85470	0.11135
H	-4.44406	-2.02914	1.78977
H	-5.68042	-0.81449	1.39622

n28-30

67
n28 | iu330z-iuf33a | Energy: -907437.8923272

Ru	-1.47727	-0.74600	-0.09046
P	-0.32803	1.25722	-0.02744
C	1.49203	0.99769	0.36265
N	2.52364	1.77136	0.76471
C	3.70292	1.04039	0.70378
C	3.39865	-0.20992	0.23584
N	2.03465	-0.18756	0.04252
C	2.46817	3.16532	1.19600
H	1.84789	3.74173	0.50024
H	3.49033	3.56502	1.19359
H	2.04671	3.23281	2.20857
H	4.65217	1.47242	1.00066
C	-0.98621	2.45456	1.27351
C	-0.69587	3.96352	1.19838
C	-0.72586	1.87868	2.67133
C	-0.01449	2.32888	-1.56267
C	0.68838	1.48953	-2.63697
C	-1.29540	2.95818	-2.12693
H	-2.06150	2.33670	1.06821
H	0.65961	3.14076	-1.23573
H	-0.57415	4.33271	0.16927
H	0.19261	4.24414	1.77917
H	-1.54521	4.50781	1.64371
H	0.34793	1.92701	2.92779
H	-1.27684	2.46096	3.42838
H	-1.04993	0.82696	2.72784
H	0.07903	0.60380	-2.88463
H	0.82149	2.09068	-3.55169
H	1.68390	1.14341	-2.31357
H	-1.87561	3.50302	-1.36613
H	-1.02367	3.67339	-2.92110
H	-1.94262	2.19084	-2.57673
C	4.23603	-1.42829	-0.04580
C	5.71104	-1.10568	0.22961
C	3.76756	-2.57947	0.86876
C	4.05209	-1.83119	-1.52332
H	6.32596	-1.99493	0.02324
H	6.06555	-0.28553	-0.41625
H	5.86424	-0.82168	1.28384
H	3.88862	-2.31254	1.93115
H	4.37015	-3.47844	0.66362
H	2.70953	-2.83253	0.68949
H	2.99799	-2.06852	-1.74918
H	4.65077	-2.73076	-1.73600
H	4.37908	-1.02376	-2.19824
C	-2.17411	-2.84210	0.24777
C	-1.23020	-2.88695	-0.82158
C	-1.48784	-2.38727	1.42870
H	-3.21480	-3.13839	0.18778
C	0.03161	-2.46636	-0.32573
H	-1.43831	-3.18830	-1.84507
C	-0.13446	-2.14242	1.08111
H	-1.92760	-2.25318	2.41327
H	0.96011	-2.54325	-0.89062
H	0.64657	-1.81597	1.76320
C	-2.89229	-0.31341	-1.72816
C	-3.12960	0.55821	-0.63474
C	-3.40159	0.07221	0.67736
C	-4.47776	-0.95723	0.95761
H	1.44547	-0.92636	-0.34331
H	-2.56729	0.12668	-2.67323
H	-3.46694	-1.23864	-1.82367
H	-2.89501	1.61561	-0.75664
H	-3.32275	0.82505	1.46874
H	-4.67614	-1.58520	0.07702
H	-4.22453	-1.61349	1.80588
H	-5.41821	-0.43635	1.21359

67
n29 | iu340t-iuf35 | Energy: -907437.2166815

Ru	-1.80567	-1.03479	-0.05208
P	-0.73335	1.00020	-0.01939
C	1.09514	0.72245	0.32661
N	2.14143	1.46486	0.74841
C	3.31556	0.74097	0.59190
C	2.99145	-0.47431	0.04820
N	1.62224	-0.43690	-0.09929
C	2.09892	2.81896	1.29391
H	1.48932	3.46054	0.64683
H	3.12544	3.20533	1.33172
H	1.67147	2.80555	2.30623
H	4.27616	1.15132	0.88355
C	-1.40368	2.13640	1.32799
C	-1.07704	3.63900	1.35287
C	-1.19311	1.48310	2.69965
C	-0.41512	2.17373	-1.48523
C	0.23929	1.40494	-2.63963
C	-1.64492	2.95688	-1.97890
H	-2.47486	2.03989	1.07910
H	0.30932	2.90522	-1.08623
H	-0.93900	4.07499	0.35277
H	-0.18517	3.85441	1.95636
H	-1.91496	4.17303	1.83108
H	-0.12340	1.48664	2.97864
H	-1.74185	2.04480	3.47345
H	-1.55073	0.44241	2.69553
H	-0.41564	0.58286	-2.97172
H	0.40577	2.08408	-3.49238
H	1.21297	0.97317	-2.35686
H	-2.31805	3.27031	-1.16629
H	-1.30450	3.86501	-2.50338
H	-2.22541	2.36424	-2.70238
C	3.81967	-1.67987	-0.30955
C	5.30565	-1.29331	-0.30787
C	3.56649	-2.78224	0.74178
C	3.40833	-2.18680	-1.70560
H	5.91396	-2.17478	-0.56217
H	5.51206	-0.50353	-1.04851
H	5.62245	-0.94058	0.68769
H	3.87490	-2.44514	1.74457
H	4.15002	-3.67944	0.47995
H	2.50188	-3.06513	0.78202
H	2.34723	-2.49030	-1.73242
H	4.01216	-3.06976	-1.96644
H	3.56963	-1.41295	-2.47366
C	-2.53781	-2.97848	0.84296
C	-1.59545	-3.31197	-0.16364
C	-1.86870	-2.19986	1.85234
H	-3.58065	-3.27252	0.85321
C	-0.32845	-2.76332	0.19461
H	-1.80492	-3.88052	-1.06647
C	-0.51066	-2.05781	1.44582
H	-2.30900	-1.82269	2.77127
H	0.60819	-2.99483	-0.30737
H	0.26682	-1.54751	2.00930
C	-2.80720	-1.00110	-2.02831
C	-3.30423	0.04323	-1.21126
C	-3.87722	-0.19821	0.06994
C	-4.98115	-1.21145	0.29086
H	1.00160	-1.15125	-0.49585
H	-2.27519	-0.72592	-2.94141
H	-3.32898	-1.96109	-2.06483
H	-3.05175	1.06791	-1.46960
H	-4.00045	0.70018	0.68454
H	-4.90242	-2.05870	-0.40666
H	-4.98579	-1.60465	1.32021
H	-5.95902	-0.72487	0.11952

67
n30 | iu410a-iuf37a | Energy: -907445.3921698

Ru	-1.42731	-0.73190	0.01510
P	-0.47485	1.35832	0.15668
C	1.40003	1.09173	0.06310
N	2.52330	1.83685	0.14151
C	3.63216	1.02025	-0.04612
C	3.17889	-0.25723	-0.25450
N	1.80690	-0.16303	-0.18005
C	2.59529	3.27237	0.40344
H	1.80028	3.78479	-0.15121
H	3.57144	3.63958	0.06063
H	2.48355	3.47152	1.47941
H	4.64179	1.41669	-0.01867
C	-0.67611	2.19562	1.85803
C	-0.70788	3.72847	1.87523
C	0.34171	1.67058	2.87974
C	-0.62665	2.79936	-1.06326
C	0.20358	2.63152	-2.34484
C	-2.11091	3.07772	-1.34581
H	-1.67494	1.83262	2.14587
H	-0.22952	3.67645	-0.53178
H	-1.48782	4.14025	1.21811
H	0.25975	4.16508	1.58105
H	-0.92149	4.06558	2.90340
H	1.35872	2.02961	2.65052
H	0.07816	2.04183	3.88409
H	0.37091	0.57441	2.92014
H	-0.04739	1.72009	-2.90779
H	0.01849	3.49262	-3.00908
H	1.28404	2.60002	-2.13052
H	-2.69359	3.16852	-0.41456
H	-2.20565	4.02577	-1.90111
H	-2.56995	2.28311	-1.95080
C	3.87450	-1.56538	-0.51765
C	5.39273	-1.34505	-0.53560
C	3.49551	-2.56022	0.59930
C	3.40097	-2.11571	-1.87899
H	5.90177	-2.30211	-0.72697
H	5.68085	-0.63889	-1.33176
H	5.74838	-0.95517	0.43245
H	3.82127	-2.19119	1.58545
H	3.98223	-3.53003	0.40986
H	2.40498	-2.72822	0.63020
H	2.30937	-2.27811	-1.88722
H	3.88950	-3.08352	-2.07420
H	3.65788	-1.42238	-2.69621
C	-2.78950	-1.68645	1.52425
C	-2.19052	-2.71180	0.71166
C	-1.75397	-1.01776	2.22713
H	-3.84995	-1.45595	1.58155
C	-0.77759	-2.67931	0.94027
H	-2.71831	-3.41333	0.07484
C	-0.49649	-1.63255	1.86108
H	-1.88364	-0.20630	2.93690
H	-0.04487	-3.33940	0.48116
H	0.48505	-1.38333	2.25517
C	-0.86407	-1.39559	-2.01167
C	-1.83165	-0.35556	-2.08377
C	-3.09996	-0.43707	-1.45284
C	-4.00641	-1.64405	-1.57726
H	1.08421	-0.89493	-0.30205
H	0.11298	-1.19361	-2.46168
H	-1.17745	-2.44264	-2.05389
H	-1.50315	0.61682	-2.43918
H	-3.63857	0.51233	-1.38561
H	-3.43556	-2.55890	-1.79328
H	-4.60673	-1.81434	-0.66930
H	-4.71188	-1.48380	-2.41282

n31-33

67			
n31 | iu410t-iuf37 | Energy: -907434.2842419			
Ru	-1.62125	-1.04283	0.11087
P	-0.76364	1.14952	0.25686
C	1.06545	0.85383	0.18518
N	2.19109	1.60310	0.28574
C	3.27223	0.76438	0.06551
C	2.76989	-0.49563	-0.17997
N	1.39911	-0.40093	-0.10269
C	2.27958	3.02552	0.59245
H	1.44091	3.55381	0.12103
H	3.22209	3.41684	0.18631
H	2.25354	3.19527	1.68022
H	4.29243	1.13531	0.10088
C	-1.08341	1.97812	1.93521
C	-1.13651	3.51058	1.94209
C	-0.08995	1.47347	2.99144
C	-0.95798	2.55529	-0.99200
C	-0.07475	2.40953	-2.23990
C	-2.43526	2.78686	-1.33929
H	-2.08790	1.60177	2.18652
H	-0.60328	3.44494	-0.45079
H	-1.90011	3.90837	1.25728
H	-0.16345	3.95408	1.67643
H	-1.38648	3.85113	2.96070
H	0.92163	1.86414	2.79607
H	-0.40105	1.82872	3.98782
H	-0.02449	0.37840	3.02294
H	-0.29586	1.50314	-2.82350
H	-0.24601	3.27680	-2.89964
H	0.99537	2.38373	-1.98283
H	-3.07506	2.80322	-0.44148
H	-2.54353	3.75724	-1.85133
H	-2.81553	2.00847	-2.01643
C	3.46145	-1.80053	-0.47939
C	4.98184	-1.59494	-0.50003
C	3.08286	-2.82178	0.61225
C	2.98099	-2.31969	-1.84899
H	5.48412	-2.55067	-0.71637
H	5.27264	-0.87124	-1.27962
H	5.34575	-1.22973	0.47483
H	3.42019	-2.48099	1.60516
H	3.55656	-3.79325	0.39664
H	1.99002	-2.96725	0.64381
H	1.88886	-2.47138	-1.84612
H	3.46428	-3.28465	-2.07255
H	3.23455	-1.60742	-2.65142
C	-3.08053	-1.96074	1.62075
C	-2.46462	-2.99113	0.83426
C	-2.06319	-1.27742	2.33183
H	-4.14001	-1.71927	1.63912
C	-1.05603	-2.95469	1.09022
H	-2.97932	-3.69643	0.19000
C	-0.79952	-1.88774	2.00353
H	-2.21021	-0.44285	3.01078
H	-0.30862	-3.61609	0.65965
H	0.17617	-1.61385	2.39418
C	-1.19584	-1.79062	-1.92576
C	-2.05530	-0.66655	-1.99297
C	-3.31108	-0.65227	-1.33156
C	-4.29774	-1.79745	-1.42099
H	0.15515	-1.01966	-0.18769
H	-0.19557	-1.69276	-2.35240
H	-1.60791	-2.80248	-1.92602
H	-1.64951	0.27121	-2.36203
H	-3.78246	0.32947	-1.24902
H	-3.79701	-2.75730	-1.61107
H	-4.91081	-1.89609	-0.51186
H	-4.98801	-1.60794	-2.26289

67			
n32 | iu410z-iuf37b | Energy: -907447.1735750			
Ru	-1.46975	-0.73453	-1.01673
P	-0.28665	1.19851	-0.31582
C	1.52329	0.88997	-0.36953
N	2.55422	1.46509	-1.07841
C	3.71179	0.84638	-0.65023
C	3.34862	-0.08433	0.29920
N	1.98631	-0.04129	0.45734
C	2.56633	2.56521	-2.03669
H	1.75101	2.46223	-2.76041
H	3.52026	2.53344	-2.58011
H	2.48566	3.53792	-1.52517
H	4.67654	1.12184	-1.06417
C	-0.52986	1.70081	1.47855
C	0.51585	2.73771	1.90982
C	-0.55182	0.50198	2.43035
C	-0.57562	2.80805	-1.25448
C	-0.83075	2.58351	-2.75193
C	-1.67666	3.68700	-0.63363
H	-1.52802	2.16927	1.47732
H	0.36761	3.35914	-1.13537
H	0.55894	3.60276	1.22877
H	1.51388	2.27368	1.95070
H	0.26892	3.11124	2.91738
H	0.43497	0.01635	2.44993
H	-0.79203	0.85383	3.44730
H	-1.30756	-0.23809	2.12647
H	-1.84453	2.19475	-2.93087
H	-0.74027	3.54431	-3.28472
H	-0.13035	1.86539	-3.20452
H	-1.39506	4.05647	0.36225
H	-1.83546	4.56244	-1.28465
H	-2.64266	3.16738	-0.53949
C	4.20454	-1.05252	1.07956
C	5.68212	-0.87252	0.70581
C	4.01222	-0.79186	2.58563
C	3.75761	-2.49048	0.75109
H	6.30257	-1.57960	1.27878
H	5.84629	-1.06553	-0.36777
H	6.02654	0.14967	0.93581
H	4.34114	0.22650	2.85180
H	4.60384	-1.51431	3.17184
H	2.95119	-0.89951	2.86383
H	2.69500	-2.63409	1.00555
H	4.35527	-3.21334	1.33058
H	3.89355	-2.70809	-0.32192
C	-1.88903	-2.97175	-1.03434
C	-0.81213	-2.63650	-1.92381
C	-1.48090	-2.66185	0.29479
H	-2.84543	-3.39819	-1.32599
C	0.25187	-2.09567	-1.13078
H	-0.80510	-2.77820	-3.00129
C	-0.17469	-2.10777	0.24171
H	-2.08334	-2.78577	1.18977
H	1.21869	-1.74817	-1.48069
H	0.41946	-1.73602	1.06800
C	-3.28222	-0.48183	-2.28590
C	-3.28524	0.46316	-1.23885
C	-3.27288	0.01913	0.11276
C	-4.18038	-1.07613	0.63013
H	-0.91635	-0.01515	-2.32111
H	-3.14015	-0.13014	-3.30830
H	-3.81867	-1.42471	-2.17754
H	-3.08173	1.50555	-1.46814
H	-3.06453	0.79671	0.85218
H	-4.31183	-1.89244	-0.09405
H	-3.80452	-1.50000	1.57311
H	-5.17584	-0.64357	0.83831

67			
n33 | iu420t-iuf39 | Energy: -907434.2394879			
Ru	-1.77502	-1.03115	0.07885
P	-0.67729	1.07779	0.20386
C	1.12329	0.71649	0.10822
N	2.20672	1.56159	0.18660
C	3.33242	0.77931	0.03671
C	2.89774	-0.51836	-0.13654
N	1.52684	-0.53528	-0.09140
C	2.24300	2.99916	0.41216
H	1.54050	3.51284	-0.25773
H	3.25736	3.35875	0.19372
H	1.99847	3.24275	1.45724
H	4.32677	1.21462	0.06456
C	-0.97279	1.94448	1.87540
C	-0.99137	3.48024	1.86460
C	0.01193	1.43814	2.93903
C	-0.91858	2.47416	-1.03971
C	-0.16084	2.25260	-2.35603
C	-2.40495	2.81996	-1.23196
H	-1.98738	1.60669	2.13772
H	-0.45910	3.34313	-0.54808
H	-1.75823	3.89109	1.19330
H	-0.01844	3.90561	1.57883
H	-1.21724	3.83116	2.88539
H	1.04106	1.75288	2.70451
H	-0.25905	1.86420	3.91933
H	0.01641	0.34522	3.03222
H	-0.48464	1.35048	-2.89827
H	-0.32759	3.11669	-3.02106
H	0.92189	2.15558	-2.18024
H	-2.94116	2.87805	-0.27119
H	-2.48845	3.80312	-1.72394
H	-2.93362	2.09252	-1.86404
C	3.69430	-1.78352	-0.34958
C	5.19732	-1.47410	-0.32783
C	3.35222	-2.78418	0.77136
C	3.30932	-2.39651	-1.70997
H	5.77367	-2.40008	-0.48192
H	5.46733	-0.76610	-1.12938
H	5.49841	-1.04011	0.64045
H	3.63335	-2.37930	1.75807
H	3.89724	-3.72964	0.61380
H	2.27046	-2.99761	0.77598
H	2.22812	-2.60971	-1.74246
H	3.85859	-3.33948	-1.86828
H	3.55517	-1.70650	-2.53445
C	-3.19113	-1.87546	1.66056
C	-2.63215	-2.95914	0.90263
C	-2.13264	-1.18012	2.30095
H	-4.24419	-1.61053	1.71293
C	-1.21781	-2.92992	1.09479
H	-3.18656	-3.68381	0.31513
C	-0.89398	-1.82830	1.94322
H	-2.24001	-0.32398	2.95902
H	-0.49482	-3.60461	0.64203
H	0.10944	-1.55499	2.25232
C	-1.44287	-1.61880	-2.04272
C	-2.39462	-0.54227	-1.95209
C	-3.59975	-0.63663	-1.23078
C	-4.52405	-1.83035	-1.30149
H	-0.46963	-1.42210	-0.81268
H	-0.56003	-1.42578	-2.66025
H	-1.79097	-2.65407	-2.08381
H	-2.06619	0.43205	-2.29365
H	-4.10049	0.32033	-1.05673
H	-3.98285	-2.75420	-1.55009
H	-5.08341	-1.98774	-0.36717
H	-5.26548	-1.64721	-2.10000

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67			
n34 | iu430a-iuf41a | Energy: -907438.0551910			
Ru	-1.42059	-0.77297	0.01224
P	-0.33977	1.37859	0.13354
C	1.44702	0.97049	0.02300
N	2.56345	1.77274	0.07338
C	3.65324	0.94827	-0.11032
C	3.16330	-0.33102	-0.27645
N	1.79455	-0.29641	-0.19275
C	2.65488	3.20554	0.31299
H	1.96555	3.75163	-0.34536
H	3.68006	3.53034	0.09075
H	2.42604	3.44532	1.36264
H	4.66443	1.34388	-0.10554
C	-0.61537	2.27993	1.79193
C	-0.57157	3.81585	1.74632
C	0.34299	1.77193	2.88011
C	-0.55533	2.76234	-1.13042
C	0.14936	2.46901	-2.46200
C	-2.02979	3.17177	-1.29462
H	-1.64345	1.98475	2.05715
H	-0.04147	3.62073	-0.67513
H	-1.30828	4.24715	1.05547
H	0.42393	4.19129	1.46783
H	-0.79689	4.19762	2.75591
H	1.39408	1.94022	2.59563
H	0.15127	2.32453	3.81481
H	0.22121	0.70441	3.09625
H	-0.25077	1.57984	-2.97293
H	0.01743	3.32833	-3.14091
H	1.22883	2.30736	-2.31490
H	-2.54726	3.25721	-0.32602
H	-2.08065	4.15468	-1.79164
H	-2.60321	2.46519	-1.91257
C	3.90236	-1.62561	-0.51828
C	5.41623	-1.37615	-0.54924
C	3.56074	-2.61520	0.61255
C	3.44575	-2.21999	-1.86486
H	5.94994	-2.32365	-0.72477
H	5.68541	-0.67691	-1.35866
H	5.76798	-0.95711	0.40844
H	3.89213	-2.22513	1.58945
H	4.06034	-3.58184	0.43444
H	2.47197	-2.78393	0.65613
H	2.35640	-2.39105	-1.85919
H	3.95174	-3.18319	-2.04416
H	3.68832	-1.53786	-2.69683
C	-2.76734	-1.68389	1.49859
C	-2.08841	-2.74117	0.80477
C	-1.79254	-0.87906	2.16573
H	-3.84016	-1.50761	1.50354
C	-0.68643	-2.57240	1.04809
H	-2.54957	-3.52653	0.21541
C	-0.49106	-1.44667	1.89363
H	-2.00202	-0.01852	2.79340
H	0.11456	-3.16997	0.61736
H	0.47606	-1.08211	2.21994
C	-0.93355	-1.19140	-2.27965
C	-2.06278	-0.26070	-1.99413
C	-3.26161	-0.64371	-1.39975
C	-3.93155	-1.98493	-1.55976
H	-0.21200	-1.27658	-1.34540
H	-0.22099	-0.77473	-3.00542
H	-1.22405	-2.21566	-2.53955
H	-1.91943	0.77929	-2.25580
H	-3.93845	0.18235	-1.15941
H	-3.21901	-2.77691	-1.82944
H	-4.47181	-2.29292	-0.65141
H	-4.67945	-1.90326	-2.36927

67			
n35 | iu430t-iuf41 | Energy: -907436.3721918			
Ru	-1.69576	-0.98694	0.23378
P	-0.69532	1.22024	0.33515
C	1.07749	0.79297	0.20703
N	2.20954	1.56789	0.22794
C	3.27517	0.71819	0.01722
C	2.75181	-0.55054	-0.13569
N	1.38601	-0.48314	-0.01620
C	2.31813	3.00119	0.45586
H	1.59244	3.54066	-0.16854
H	3.33007	3.32483	0.17808
H	2.14171	3.24720	1.51456
H	4.29560	1.08878	-0.00288
C	-0.96398	2.11952	1.98948
C	-0.91802	3.65389	1.93722
C	0.00331	1.60759	3.06657
C	-0.93296	2.58410	-0.94432
C	-0.18355	2.31269	-2.25679
C	-2.42537	2.89952	-1.13609
H	-1.99025	1.82453	2.26381
H	-0.47434	3.47572	-0.49268
H	-1.66353	4.08031	1.25148
H	0.07610	4.02296	1.64270
H	-1.12987	4.04362	2.94666
H	1.04954	1.81486	2.78961
H	-0.20621	2.12570	4.01702
H	-0.08790	0.52997	3.24503
H	-0.50224	1.38610	-2.75719
H	-0.36324	3.14763	-2.95485
H	0.90143	2.23358	-2.08570
H	-2.92506	3.09946	-0.17432
H	-2.53307	3.79881	-1.76507
H	-2.97317	2.08161	-1.62823
C	3.45294	-1.86248	-0.39435
C	4.96949	-1.64668	-0.48537
C	3.13334	-2.83496	0.75775
C	2.93117	-2.45744	-1.71690
H	5.47524	-2.60705	-0.67307
H	5.22233	-0.95955	-1.31021
H	5.36682	-1.22854	0.45470
H	3.51004	-2.44431	1.71781
H	3.60454	-3.81385	0.56951
H	2.04361	-2.97905	0.84396
H	1.83981	-2.60706	-1.66737
H	3.41039	-3.43195	-1.90788
H	3.15351	-1.78667	-2.56355
C	-3.10997	-1.84189	1.62709
C	-2.43010	-2.93296	0.98236
C	-2.13663	-1.06894	2.34978
H	-4.17772	-1.63960	1.59303
C	-1.03984	-2.79102	1.27624
H	-2.88117	-3.70725	0.37173
C	-0.84786	-1.67042	2.14076
H	-2.34898	-0.19390	2.95684
H	-0.23733	-3.40272	0.86765
H	0.11313	-1.33302	2.51207
C	-1.15940	-1.54218	-2.33008
C	-2.23200	-0.58424	-1.87372
C	-3.45331	-0.93576	-1.32211
C	-4.15061	-2.26143	-1.47501
H	-0.32221	-1.59781	-1.58125
H	-0.66943	-1.17175	-3.24575
H	-1.53258	-2.56195	-2.48989
H	-2.07211	0.45958	-2.11514
H	-4.11431	-0.09730	-1.07822
H	-3.45575	-3.07800	-1.71380
H	-4.72212	-2.53730	-0.57525
H	-4.87743	-2.17406	-2.30302

67			
n36 | iu430z-iuf41b | Energy: -907458.9270282			
Ru	-0.64715	-0.75590	0.07228
P	-0.51675	1.63348	0.27406
C	1.25008	1.34308	-0.03874
N	2.44305	1.97893	-0.09775
C	3.40399	1.00283	-0.25813
C	2.76147	-0.22331	-0.28390
N	1.41012	0.01942	-0.15412
C	2.67074	3.41335	0.00941
H	1.69774	3.92167	0.03623
H	3.24101	3.76971	-0.86152
H	3.22767	3.64354	0.93102
H	4.45646	1.25104	-0.34607
C	-0.64358	2.29594	2.03594
C	-0.65340	3.82215	2.17214
C	0.47378	1.67779	2.88985
C	-1.07502	3.02871	-0.85022
C	-0.33757	3.07221	-2.19662
C	-2.60215	2.97903	-1.00309
H	-1.61662	1.90769	2.38318
H	-0.81182	3.94949	-0.30769
H	-1.51768	4.28426	1.67129
H	0.26943	4.26776	1.76284
H	-0.70300	4.08752	3.24126
H	1.44686	2.12487	2.62672
H	0.28189	1.88151	3.95586
H	0.55416	0.59117	2.74562
H	-0.54562	2.19763	-2.83051
H	-0.66692	3.96754	-2.75012
H	0.75348	3.13652	-2.06209
H	-3.11019	3.00634	-0.02393
H	-2.94686	3.84865	-1.58637
H	-2.91952	2.06405	-1.52708
C	3.38206	-1.59749	-0.35459
C	4.85392	-1.48619	-0.77848
C	3.30092	-2.24501	1.04379
C	2.61008	-2.47059	-1.35398
H	5.29881	-2.49211	-0.83080
H	4.94651	-1.01415	-1.77042
H	5.43723	-0.89768	-0.05075
H	3.84352	-1.64114	1.78975
H	3.75023	-3.25149	1.01561
H	2.25268	-2.34122	1.36324
H	1.56494	-2.56195	-1.03357
H	3.06136	-3.47491	-1.39696
H	2.62877	-2.03398	-2.36601
C	-2.43527	-1.50430	1.13290
C	-1.81297	-2.58518	0.43096
C	-1.50106	-1.05924	2.13162
H	-3.44381	-1.13180	0.97766
C	-0.49310	-2.77674	0.94918
H	-2.25931	-3.15642	-0.37515
C	-0.31548	-1.82827	2.01954
H	-1.66108	-0.24622	2.83458
H	0.22001	-3.53256	0.63259
H	0.58310	-1.70158	2.61845
C	-0.68541	-2.72089	-2.53174
C	-0.51263	-1.27757	-2.11310
C	-1.58554	-0.38766	-1.95011
C	-3.04683	-0.75241	-2.06556
H	-0.01717	-3.41118	-1.99590
H	-0.44253	-2.80696	-3.60634
H	-1.71892	-3.07112	-2.40608
H	0.44434	-0.83702	-2.40569
H	-1.38949	0.65140	-2.19838
H	-3.26447	-1.77284	-1.72343
H	-3.67260	-0.05997	-1.48014
H	-3.36739	-0.67952	-3.12166

n37-39

67			
n37 | iu431t-iuf81 | Energy: -907458.8533397			
Ru	0.04388	-0.34266	1.09414
P	-1.31516	1.13168	-0.23508
C	-0.46032	0.31086	-1.61294
N	-0.33487	0.33777	-2.96007
C	0.69370	-0.52379	-3.27881
C	1.18378	-1.05416	-2.09718
N	0.43552	-0.52138	-1.06855
C	-1.12541	1.13174	-3.89084
H	-1.89996	1.66568	-3.32450
H	-1.60637	0.47611	-4.63233
H	-0.48386	1.86153	-4.40855
H	0.99103	-0.69687	-4.30772
C	-0.72221	2.92452	-0.26054
C	-1.59206	3.90212	-1.05823
C	0.73353	2.96929	-0.74946
C	-3.14738	1.20397	-0.63804
C	-3.69240	-0.01283	-1.40064
C	-3.93378	1.48966	0.64858
H	-0.75325	3.21757	0.80306
H	-3.24110	2.07346	-1.30656
H	-2.61056	3.99013	-0.65067
H	-1.66176	3.60463	-2.11870
H	-1.12981	4.90269	-1.02543
H	0.77707	2.77657	-1.83437
H	1.15587	3.97015	-0.56352
H	1.36349	2.21975	-0.25060
H	-3.82966	-0.88918	-0.75028
H	-4.68340	0.24460	-1.81026
H	-3.04138	-0.30695	-2.23933
H	-3.57723	2.40354	1.15372
H	-5.00160	1.62860	0.41245
H	-3.84311	0.64794	1.35392
C	2.36606	-1.97488	-1.91115
C	2.78953	-2.56051	-3.26629
C	3.53438	-1.15914	-1.31942
C	2.00938	-3.10807	-0.93784
H	3.65006	-3.23256	-3.12391
H	1.96955	-3.13954	-3.72211
H	3.09462	-1.76647	-3.96809
H	3.81424	-0.32813	-1.98769
H	4.41350	-1.81073	-1.18471
H	3.25515	-0.74573	-0.33902
H	1.73256	-2.68762	0.03722
H	2.87958	-3.77131	-0.80731
H	1.16487	-3.70879	-1.31339
C	0.19082	0.49728	3.12874
C	0.76719	-0.81014	3.11290
C	0.99668	1.32159	2.26529
H	-0.65833	0.81925	3.72506
C	1.88727	-0.81465	2.21762
H	0.40905	-1.66456	3.67574
C	2.02968	0.52472	1.71202
H	0.82989	2.37367	2.05147
H	2.54153	-1.65610	2.00802
H	2.77649	0.86299	0.99797
C	-0.16378	-3.52136	1.79820
C	-0.74684	-2.44484	0.91145
C	-1.81164	-1.61256	1.28817
C	-2.46132	-1.59796	2.65204
H	-0.43970	-3.39237	2.85343
H	0.93249	-3.58792	1.72966
H	-0.56667	-4.49812	1.47464
H	-0.64762	-2.64834	-0.15732
H	-2.47987	-1.31045	0.48634
H	-3.27130	-2.35020	2.69042
H	-1.75638	-1.82833	3.46220
H	-2.90965	-0.61524	2.86769

67			
n38 | iu431z-iuf81a | Energy: -907460.7106172			
Ru	0.13132	-0.28030	1.09204
P	-1.20940	1.22200	-0.18774
C	-0.47501	0.33428	-1.59522
N	-0.40989	0.31122	-2.94644
C	0.68646	-0.45872	-3.27779
C	1.28358	-0.87671	-2.09953
N	0.52765	-0.37751	-1.06261
C	-1.31539	0.98032	-3.87165
H	-2.12741	1.44192	-3.29382
H	-1.74196	0.25006	-4.57565
H	-0.77760	1.75945	-4.43378
H	0.94996	-0.65419	-4.31206
C	-0.46337	2.95147	-0.32545
C	-1.27180	3.93197	-1.18351
C	0.98058	2.85401	-0.84195
C	-3.04488	1.48096	-0.41110
C	-3.83858	0.22703	-0.79430
C	-3.59476	2.13707	0.86502
H	-0.44986	3.31403	0.71745
H	-3.12217	2.20240	-1.24059
H	-2.27340	4.12876	-0.77350
H	-1.38163	3.55687	-2.21583
H	-0.73473	4.89351	-1.23633
H	0.98480	2.60462	-1.91606
H	1.48151	3.82757	-0.71640
H	1.56067	2.08264	-0.31709
H	-3.92741	-0.46718	0.05250
H	-4.85721	0.52980	-1.08851
H	-3.38253	-0.31078	-1.64174
H	-3.06986	3.07555	1.10894
H	-4.66355	2.37120	0.73215
H	-3.49921	1.45239	1.72449
C	2.60105	-1.59599	-1.92328
C	3.00419	-2.28167	-3.23748
C	3.66014	-0.53250	-1.55874
C	2.52600	-2.64019	-0.79776
H	3.97064	-2.79281	-3.10535
H	2.25379	-3.03036	-3.54014
H	3.12155	-1.54839	-4.05263
H	3.77002	0.20389	-2.37162
H	4.63628	-1.01609	-1.38852
H	3.36830	0.00465	-0.64300
H	2.20807	-2.17603	0.14725
H	3.52024	-3.09352	-0.65733
H	1.81387	-3.44288	-1.04852
C	0.12198	0.78333	3.00041
C	0.40280	-0.59029	3.24169
C	1.20763	1.31962	2.20695
H	-0.73894	1.33267	3.37332
C	1.65589	-0.91468	2.60328
H	-0.21550	-1.26799	3.82118
C	2.14581	0.27249	1.98737
H	1.31023	2.34687	1.87098
H	2.14932	-1.88141	2.61438
H	3.06054	0.35176	1.40538
C	0.00752	-3.45762	1.79975
C	-0.42073	-2.44073	0.77158
C	-1.60202	-1.68551	0.83466
C	-2.58431	-1.72931	1.98162
H	-0.25902	-3.17473	2.82701
H	1.09152	-3.64376	1.75500
H	-0.49790	-4.41654	1.58159
H	-0.05178	-2.65847	-0.23138
H	-2.04771	-1.46101	-0.13543
H	-3.36186	-2.49185	1.78724
H	-2.09760	-1.98682	2.93249
H	-3.09435	-0.76204	2.11525

67			
n39 | iu510t-iuf43 | Energy: -907436.0851313			
Ru	0.67093	0.27548	1.44629
P	-0.98635	1.43464	0.13816
C	-0.19257	0.50346	-1.21820
N	-0.22247	0.29345	-2.55377
C	0.82794	-0.55644	-2.85005
C	1.48511	-0.84256	-1.66791
N	0.82311	-0.17499	-0.66251
C	-1.16964	0.86319	-3.50344
H	-2.01248	1.29129	-2.94469
H	-1.54208	0.07345	-4.17217
H	-0.68824	1.65276	-4.10168
H	1.01177	-0.89766	-3.86365
C	-0.63906	3.24832	-0.17817
C	-1.59279	3.91431	-1.17568
C	0.82521	3.41138	-0.60794
C	-2.83286	1.21548	-0.00966
C	-3.20157	-0.25529	-0.22854
C	-3.50001	1.80514	1.24085
H	-0.77425	3.71391	0.81485
H	-3.14368	1.80000	-0.89159
H	-2.63852	3.89588	-0.83288
H	-1.53767	3.42458	-2.16297
H	-1.30150	4.96909	-1.31168
H	0.98049	2.98501	-1.61372
H	1.08458	4.48171	-0.64631
H	1.51159	2.90036	0.08278
H	-2.88069	-0.88212	0.61643
H	-4.29607	-0.34536	-0.32832
H	-2.73679	-0.66097	-1.14220
H	-3.25655	2.87257	1.37500
H	-4.59544	1.71449	1.15769
H	-3.17891	1.26078	2.14560
C	2.70220	-1.69687	-1.42085
C	3.12245	-2.40101	-2.71824
C	3.84828	-0.78726	-0.93302
C	2.37488	-2.74593	-0.34084
H	4.01345	-3.02062	-2.53172
H	2.31897	-3.05739	-3.09186
H	3.37569	-1.66923	-3.50348
H	4.12334	-0.05632	-1.71134
H	4.73615	-1.39710	-0.69799
H	3.54658	-0.23806	-0.02967
H	2.02659	-2.26069	0.58484
H	3.27517	-3.33969	-0.11334
H	1.58796	-3.43297	-0.69321
C	0.77038	0.92800	3.53189
C	1.50285	-0.29755	3.38784
C	1.38515	1.88729	2.65867
H	-0.08374	1.09628	4.18197
C	2.57499	-0.10837	2.46315
H	1.25015	-1.24147	3.86810
C	2.49081	1.25055	1.98778
H	1.07102	2.91954	2.51994
H	3.30730	-0.85364	2.16675
H	3.15919	1.72234	1.27065
C	-1.89778	-4.57529	1.53218
C	-1.07103	-3.37804	1.16185
C	-1.04103	-2.19983	1.79659
C	-1.78745	-1.75427	3.01659
H	-2.52776	-4.40093	2.41667
H	-1.24516	-5.44260	1.73830
H	-2.55212	-4.86625	0.69081
H	-0.42587	-3.49016	0.28399
H	-0.34645	-1.45966	1.33583
H	-2.36690	-0.83801	2.80773
H	-2.47907	-2.52945	3.37707
H	-1.09121	-1.50513	3.83560

n40-42

67			
n40 | iu510z-iuf43b | Energy: -907441.7079299			
Ru	0.47322	0.11956	1.21167
P	-1.22731	1.15989	-0.12977
C	-0.45694	0.15768	-1.44534
N	-0.55428	-0.19369	-2.74779
C	0.54280	-0.98669	-3.03096
C	1.29210	-1.09661	-1.87295
N	0.64101	-0.37767	-0.89727
C	-1.58836	0.22446	-3.68542
H	-2.43273	0.63617	-3.11636
H	-1.93245	-0.64295	-4.26753
H	-1.19925	0.99345	-4.37131
H	0.69589	-1.41134	-4.01769
C	-0.83178	2.93839	-0.60018
C	-1.81002	3.55831	-1.60468
C	0.60958	3.02615	-1.12072
C	-3.08695	1.04530	-0.22492
C	-3.58729	-0.39902	-0.24345
C	-3.67863	1.84189	0.94747
H	-0.90245	3.48528	0.35704
H	-3.37187	1.53581	-1.17023
H	-2.83459	3.62671	-1.20978
H	-1.83304	2.97626	-2.54236
H	-1.47696	4.57899	-1.85600
H	0.68632	2.55327	-2.11435
H	0.90237	4.08367	-1.22252
H	1.32031	2.51870	-0.45414
H	-3.34860	-0.91176	0.69825
H	-4.68266	-0.40213	-0.37129
H	-3.13952	-0.97650	-1.06652
H	-3.35339	2.89529	0.94052
H	-4.77930	1.82592	0.88958
H	-3.38154	1.39274	1.91082
C	2.58223	-1.83914	-1.62887
C	3.01363	-2.57264	-2.90614
C	3.66796	-0.82381	-1.22158
C	2.38175	-2.85490	-0.48756
H	3.95644	-3.11141	-2.72373
H	2.25342	-3.30828	-3.21776
H	3.18003	-1.86376	-3.73428
H	3.83620	-0.08608	-2.02351
H	4.61654	-1.35015	-1.02587
H	3.36699	-0.28922	-0.30917
H	2.04348	-2.34439	0.42802
H	3.33471	-3.36589	-0.27403
H	1.63488	-3.61691	-0.76327
C	0.54473	1.09519	3.17212
C	1.27117	-0.13236	3.23723
C	1.18932	1.91202	2.17214
H	-0.31839	1.36538	3.77427
C	2.36657	-0.09154	2.30831
H	1.01060	-0.98235	3.86589
C	2.30651	1.18439	1.64689
H	0.89244	2.91504	1.87580
H	3.11360	-0.86568	2.15604
H	2.98707	1.53829	0.87583
C	-2.46302	-3.51293	-0.06094
C	-1.22931	-2.71418	0.22869
C	-0.94755	-2.03626	1.35450
C	-1.78827	-1.92114	2.59481
H	-3.23508	-3.40949	0.71447
H	-2.20495	-4.58361	-0.15330
H	-2.90174	-3.21374	-1.02891
H	-0.46753	-2.71032	-0.55618
H	0.14098	-1.74770	1.45092
H	-2.10662	-0.87693	2.75532
H	-2.68359	-2.55909	2.54940
H	-1.20669	-2.21602	3.48460

67			
n41 | ju110a-juf51b | Energy: -907438.9384922			
Ru	-0.49238	-0.81012	0.96203
P	-1.67749	0.67032	-0.50615
C	-0.01778	0.88907	-1.24633
N	0.67959	1.49324	-2.24161
C	1.94214	0.93535	-2.23916
C	1.98116	-0.02452	-1.24240
N	0.74965	-0.02581	-0.63686
C	0.21197	2.54984	-3.12997
H	-0.83458	2.35902	-3.40468
H	0.82852	2.54702	-4.03892
H	0.28750	3.53427	-2.64133
H	2.70485	1.26342	-2.93772
C	-2.53143	2.29419	-0.13656
C	-2.99953	3.07139	-1.37350
C	-1.68315	3.18031	0.78023
C	-2.69944	-0.06953	-1.88934
C	-2.05533	-1.34851	-2.43247
C	-4.13889	-0.30584	-1.41253
H	-3.42070	1.95783	0.42748
H	-2.71038	0.68979	-2.68971
H	-3.67599	2.48538	-2.01288
H	-2.14074	3.40384	-1.97851
H	-3.54271	3.97428	-1.04811
H	-0.79856	3.55996	0.24077
H	-2.27672	4.05200	1.10032
H	-1.34178	2.64677	1.67954
H	-2.09602	-2.15406	-1.68597
H	-2.60628	-1.68199	-3.32719
H	-1.00026	-1.19378	-2.70972
H	-4.63533	0.62963	-1.11003
H	-4.72943	-0.75552	-2.22781
H	-4.16426	-0.99942	-0.55543
C	3.08659	-0.99130	-0.89112
C	4.36829	-0.61859	-1.64997
C	3.36195	-0.97352	0.62426
C	2.63227	-2.40349	-1.31754
H	5.17037	-1.32758	-1.39192
H	4.21424	-0.66320	-2.74099
H	4.70721	0.39594	-1.38167
H	3.80311	-0.01476	0.93235
H	4.07395	-1.77662	0.87525
H	2.43331	-1.12395	1.19272
H	1.69229	-2.67607	-0.81643
H	3.40466	-3.14299	-1.04889
H	2.47069	-2.44734	-2.40735
C	-1.93127	-2.43016	1.01124
C	-0.69020	-2.89774	0.46131
C	-1.70592	-2.00377	2.36155
H	-2.88216	-2.39529	0.48618
C	0.31291	-2.79235	1.49743
H	-0.54269	-3.30435	-0.53566
C	-0.31577	-2.23587	2.64483
H	-2.45012	-1.61701	3.05239
H	1.35697	-3.07894	1.41423
H	0.18627	-1.98063	3.57645
C	0.72113	0.79158	2.34174
C	1.35578	1.82762	1.77038
C	2.75524	2.27675	2.06217
C	3.49394	2.72971	0.79359
H	3.30684	1.47677	2.58382
H	-0.40048	0.71023	2.22292
H	1.19466	0.20203	3.12778
H	0.82481	2.40610	1.00882
H	2.70354	3.13235	2.76288
H	2.96429	3.57522	0.32069
H	4.51678	3.06095	1.03270
H	3.55250	1.91538	0.05380

67			
n42 | ju110t-juf51 | Energy: -907438.7008794			
Ru	-0.67486	-1.08153	1.27912
P	-1.85996	0.40637	-0.19204
C	-0.20029	0.62619	-0.93347
N	0.45753	1.15530	-1.99635
C	1.70559	0.56814	-2.02721
C	1.77331	-0.33918	-0.98370
N	0.57643	-0.27649	-0.31451
C	-0.03502	2.16865	-2.92082
H	-1.10924	2.01356	-3.08966
H	0.49863	2.06751	-3.87563
H	0.12822	3.18053	-2.51702
H	2.44218	0.84639	-2.77383
C	-2.74856	2.01780	0.15604
C	-3.15226	2.81553	-1.09014
C	-1.97524	2.89792	1.14180
C	-2.85256	-0.34417	-1.59392
C	-2.19289	-1.62323	-2.11847
C	-4.30251	-0.58229	-1.15206
H	-3.66555	1.65675	0.65721
H	-2.84697	0.41041	-2.39896
H	-3.76996	2.23124	-1.78816
H	-2.26234	3.18365	-1.62582
H	-3.73826	3.69714	-0.78097
H	-1.06978	3.30992	0.66452
H	-2.60558	3.74918	1.44626
H	-1.67749	2.34904	2.04762
H	-2.25636	-2.42932	-1.37445
H	-2.71785	-1.95595	-3.02901
H	-1.13007	-1.46969	-2.36514
H	-4.81174	0.35480	-0.87717
H	-4.86887	-1.04718	-1.97599
H	-4.34702	-1.26368	-0.28578
C	2.87622	-1.31144	-0.63903
C	4.14483	-0.96706	-1.43282
C	3.18438	-1.26539	0.86930
C	2.40038	-2.72680	-1.02971
H	4.94618	-1.67724	-1.17556
H	3.96798	-1.03620	-2.51912
H	4.49679	0.05062	-1.19531
H	3.66697	-0.31514	1.13915
H	3.87325	-2.08589	1.12810
H	2.26316	-1.36897	1.46180
H	1.47293	-2.98468	-0.49977
H	3.17456	-3.46755	-0.76971
H	2.20981	-2.78680	-2.11405
C	-2.10663	-2.68758	1.31245
C	-0.85914	-3.15617	0.77153
C	-1.89260	-2.27069	2.66837
H	-3.05347	-2.65178	0.78005
C	0.13367	-3.05850	1.81811
H	-0.70339	-3.56056	-0.22509
C	-0.50547	-2.50738	2.96193
H	-2.64200	-1.88751	3.35570
H	1.17884	-3.34355	1.74322
H	-0.01107	-2.25719	3.89871
C	0.38512	0.53575	2.84725
C	1.03552	1.51956	2.20023
C	2.48121	1.87615	2.35983
C	3.11788	2.36333	1.05084
H	3.03548	1.02416	2.78671
H	-0.72349	0.48261	2.79526
H	0.89510	-0.08092	3.58879
H	0.47385	2.13605	1.49355
H	2.54068	2.69292	3.10548
H	2.59014	3.25748	0.67534
H	4.17404	2.63419	1.20654
H	3.06763	1.58885	0.26964

n43-45

67			
n43 | ju110z-juf51a | Energy: -907458.4871189			
Ru	-0.19453	-0.44174	0.93435
P	-1.55367	0.80568	-0.59577
C	-0.04797	0.78864	-1.61145
N	0.42047	1.14852	-2.82834
C	1.71869	0.68994	-2.90306
C	2.00653	0.03821	-1.71650
N	0.88281	0.12104	-0.92001
C	-0.28887	1.92221	-3.83781
H	-1.36919	1.77033	-3.70773
H	0.00711	1.57326	-4.83699
H	-0.05755	2.99507	-3.74046
H	2.33017	0.85785	-3.78323
C	-2.06343	2.60419	-0.38873
C	-3.07643	3.10615	-1.42521
C	-0.81196	3.49787	-0.37831
C	-2.88522	-0.00738	-1.62300
C	-2.36422	-1.28028	-2.29988
C	-4.12498	-0.25936	-0.75336
H	-2.53689	2.63625	0.60815
H	-3.14914	0.72236	-2.40574
H	-4.01765	2.53740	-1.40671
H	-2.66052	3.06049	-2.44554
H	-3.31386	4.16154	-1.21200
H	-0.36805	3.54466	-1.38654
H	-1.09447	4.52144	-0.08291
H	-0.03604	3.14023	0.31407
H	-2.01364	-2.01678	-1.56246
H	-3.17624	-1.74084	-2.88637
H	-1.52610	-1.06207	-2.98119
H	-4.50905	0.67173	-0.30502
H	-4.92865	-0.69659	-1.36840
H	-3.90101	-0.96052	0.06647
C	3.26612	-0.70808	-1.35155
C	4.40014	-0.32848	-2.31518
C	3.66388	-0.36829	0.09085
C	2.99146	-2.22276	-1.46182
H	5.31654	-0.87166	-2.03627
H	4.15161	-0.60060	-3.35460
H	4.61128	0.75267	-2.27302
H	3.86415	0.70934	0.20822
H	4.57045	-0.92738	0.37307
H	2.84732	-0.64209	0.76885
H	2.17189	-2.52022	-0.79119
H	3.89525	-2.78807	-1.18007
H	2.71637	-2.49692	-2.49364
C	-1.48686	-2.30855	1.03042
C	-0.20541	-2.64916	0.52628
C	-1.33109	-1.73961	2.33527
H	-2.42774	-2.42305	0.50050
C	0.77299	-2.32873	1.54133
H	0.00316	-3.07394	-0.45278
C	0.06770	-1.78945	2.65692
H	-2.12917	-1.39139	2.98535
H	1.84300	-2.50550	1.48300
H	0.51681	-1.44595	3.58347
C	-0.32642	1.29590	2.29970
C	1.02190	1.12773	1.94321
C	2.05656	0.71107	2.97443
C	2.98904	1.88838	3.29418
H	2.66349	-0.14250	2.63809
H	-0.93547	2.09402	1.88245
H	-0.64587	0.95641	3.28954
H	1.42190	1.74464	1.13038
H	1.53872	0.39342	3.89474
H	2.41555	2.75739	3.65860
H	3.72460	1.60986	4.06626
H	3.54268	2.20082	2.39164

67			
n44 | ju210t-juf11 | Energy: -907437.7749892			
Ru	-1.98688	-0.42697	-0.68898
P	-0.68759	1.30669	0.35792
C	1.00478	0.74348	-0.03345
N	2.22010	1.37878	-0.04379
C	3.16537	0.41579	-0.33190
C	2.49017	-0.78138	-0.46890
N	1.14902	-0.55633	-0.28351
C	2.50455	2.79922	0.10936
H	1.87119	3.22696	0.89585
H	2.32681	3.34273	-0.83224
H	3.55672	2.91864	0.40146
H	4.21794	0.66821	-0.41754
C	-0.70355	1.51543	2.24037
C	-0.30663	2.89087	2.78972
C	0.17386	0.42424	2.87061
C	-0.85875	3.05613	-0.28539
C	-0.42815	3.23244	-1.74689
C	-2.29172	3.55145	-0.04627
H	-1.76014	1.33798	2.50748
H	-0.17843	3.65191	0.34125
H	0.75112	3.11736	2.57957
H	-0.41970	2.87891	3.88679
H	-0.92838	3.70868	2.39794
H	1.23893	0.66813	2.72472
H	-0.02353	0.36022	3.95323
H	0.00721	-0.56243	2.41888
H	-1.18876	2.85290	-2.44226
H	-0.29870	4.30678	-1.95829
H	0.52334	2.72211	-1.96566
H	-2.57669	3.49312	1.01647
H	-2.38244	4.60303	-0.36497
H	-3.01497	2.95131	-0.62086
C	3.02122	-2.16727	-0.74594
C	4.53381	-2.11694	-0.99926
C	2.72612	-3.06316	0.47401
C	2.30382	-2.74734	-1.97997
H	4.91626	-3.13096	-1.19624
H	4.76830	-1.48492	-1.87217
H	5.06805	-1.71577	-0.12171
H	3.24122	-2.68357	1.37207
H	3.07334	-4.09189	0.28069
H	1.64318	-3.08937	0.67955
H	1.21770	-2.79941	-1.79738
H	2.67177	-3.76571	-2.18684
H	2.48311	-2.12239	-2.87100
C	-2.70338	0.68225	-2.39995
C	-1.37730	0.19462	-2.69991
C	-3.55817	-0.45953	-2.21895
H	-3.02583	1.71823	-2.38477
C	-1.42284	-1.22529	-2.62906
H	-0.49482	0.79105	-2.90247
C	-2.77602	-1.64422	-2.35720
H	-4.61806	-0.41462	-1.98106
H	-0.55844	-1.88078	-2.71851
H	-3.12586	-2.66927	-2.26558
C	-3.70484	-1.00338	0.70762
C	-2.48863	-1.26727	1.30831
C	-1.64308	-2.46835	0.95866
C	-1.02396	-3.18056	2.17203
H	-0.78516	-2.13053	0.30565
H	-4.30969	-0.15871	1.04499
H	-4.21509	-1.77482	0.12729
H	-2.15566	-0.65506	2.14541
H	-2.23583	-3.17425	0.35843
H	-0.39632	-2.50206	2.76876
H	-1.82044	-3.57478	2.82399
H	-0.39458	-4.02039	1.83978

67			
n45 | ju220a-juf13b | Energy: -907439.2651046			
Ru	-1.60114	-0.40649	-0.39675
P	-0.21632	1.26188	0.62638
C	1.49437	0.68776	0.31128
N	2.68984	1.36662	0.28447
C	3.66125	0.44192	-0.03433
C	3.02571	-0.77532	-0.17621
N	1.68164	-0.60307	0.04277
C	2.94687	2.78985	0.46221
H	2.38346	3.17469	1.32037
H	2.66801	3.35851	-0.43832
H	4.01878	2.92862	0.65676
H	4.70224	0.73302	-0.13638
C	-0.31470	1.59704	2.49900
C	0.06969	3.00233	2.98542
C	0.51535	0.56465	3.27355
C	-0.31332	2.99421	-0.09345
C	0.17274	3.11492	-1.54406
C	-1.72821	3.56114	0.08618
H	-1.38612	1.44931	2.72231
H	0.37171	3.58271	0.53306
H	1.14848	3.18840	2.86442
H	-0.14216	3.06219	4.06606
H	-0.48614	3.81112	2.49287
H	1.58811	0.69814	3.05755
H	0.36104	0.70717	4.35589
H	0.25576	-0.47030	3.02462
H	-0.59159	2.78904	-2.26129
H	0.39120	4.17345	-1.76252
H	1.08863	2.53100	-1.72783
H	-2.04835	3.55333	1.13966
H	-1.75945	4.60407	-0.27046
H	-2.46448	2.97672	-0.48483
C	3.60704	-2.12731	-0.51699
C	5.09598	-1.99185	-0.86441
C	3.44239	-3.06673	0.69333
C	2.84344	-2.71436	-1.71987
H	5.51433	-2.97939	-1.11570
H	5.24216	-1.32471	-1.73037
H	5.66596	-1.58878	-0.01045
H	3.98697	-2.67584	1.56898
H	3.84062	-4.06671	0.45294
H	2.37912	-3.16662	0.96052
H	1.77049	-2.80611	-1.48219
H	3.23630	-3.71486	-1.96501
H	2.95267	-2.06855	-2.60753
C	-2.23929	0.74813	-2.15559
C	-0.94724	0.15418	-2.42504
C	-3.17575	-0.31857	-1.97257
H	-2.48339	1.80392	-2.17937
C	-1.10143	-1.25525	-2.35636
H	-0.01973	0.67828	-2.62584
C	-2.48474	-1.56096	-2.08115
H	-4.23165	-0.19296	-1.74531
H	-0.29242	-1.97658	-2.45511
H	-2.91742	-2.55359	-1.98333
C	-3.32219	-0.80488	1.01908
C	-2.10261	-1.14252	1.59538
C	-1.26024	-2.25150	1.06541
C	-0.20717	-2.86081	1.99797
H	-0.55209	-1.80421	0.20508
H	-3.87875	0.04519	1.41890
H	-3.89460	-1.53931	0.44830
H	-1.72732	-0.57490	2.44412
H	-1.87392	-3.02395	0.58368
H	0.63286	-2.17259	2.15747
H	-0.66212	-3.12430	2.96624
H	0.20396	-3.77504	1.54486

n46-48

67
n46 | ju220t-juf13 | Energy: -907437.0492557

Ru	-2.13469	-0.47148	-0.57825
P	-0.70928	1.15325	0.39648
C	1.00944	0.59991	0.07076
N	2.19244	1.30293	0.05031
C	3.18842	0.39063	-0.22635
C	2.58137	-0.84264	-0.34905
N	1.23051	-0.69178	-0.16065
C	2.42723	2.73336	0.20349
H	1.87794	3.12287	1.06882
H	2.12080	3.28496	-0.69818
H	3.50076	2.89151	0.37207
H	4.22471	0.70143	-0.31755
C	-0.78117	1.46194	2.27385
C	-0.40659	2.86727	2.76727
C	0.08151	0.43371	3.01994
C	-0.82230	2.88738	-0.31322
C	-0.35119	3.00394	-1.76967
C	-2.23788	3.44740	-0.11908
H	-1.84561	1.29748	2.51644
H	-0.13417	3.47938	0.30636
H	0.66731	3.06794	2.62895
H	-0.60018	2.91481	3.85194
H	-0.98132	3.67271	2.29115
H	1.14869	0.60676	2.80556
H	-0.07480	0.54242	4.10587
H	-0.14297	-0.60342	2.74253
H	-1.11969	2.66938	-2.47793
H	-0.14051	4.06224	-1.99664
H	0.56515	2.42298	-1.96024
H	-2.54230	3.44695	0.93913
H	-2.28043	4.48695	-0.48421
H	-2.97872	2.85275	-0.67327
C	3.19882	-2.19182	-0.63270
C	4.68699	-2.03211	-0.97332
C	3.04860	-3.08484	0.61462
C	2.46124	-2.84671	-1.81610
H	5.13190	-3.01791	-1.18234
H	4.82398	-1.39576	-1.86359
H	5.23960	-1.58211	-0.13140
H	3.57779	-2.64514	1.47644
H	3.47263	-4.08372	0.41774
H	1.98621	-3.20032	0.87925
H	1.38799	-2.95205	-1.58655
H	2.87986	-3.84723	-2.01409
H	2.56601	-2.23700	-2.72941
C	-2.81206	0.68461	-2.38326
C	-1.54769	0.03494	-2.64776
C	-3.78342	-0.33403	-2.16413
H	-3.01154	1.74929	-2.42058
C	-1.76247	-1.37041	-2.57069
H	-0.60625	0.52040	-2.88196
C	-3.14591	-1.60533	-2.25926
H	-4.82956	-0.16331	-1.92063
H	-0.99523	-2.13048	-2.69960
H	-3.62187	-2.57521	-2.13560
C	-3.79826	-0.64041	0.89200
C	-2.62726	-1.20716	1.42188
C	-1.92223	-2.28255	0.75861
C	-0.75638	-2.98079	1.44071
H	-0.97233	-1.56013	-0.18191
H	-4.20234	0.24924	1.37948
H	-4.51874	-1.25742	0.35016
H	-2.13579	-0.72520	2.26406
H	-2.55288	-2.97460	0.19062
H	0.02378	-2.27583	1.75433
H	-1.12927	-3.53736	2.31726
H	-0.28641	-3.69744	0.75108

67
n47 | ju220z-juf13a | Energy: -907451.3467389

Ru	-1.57658	-0.47656	-0.24867
P	-0.13763	1.16953	0.63005
C	1.58551	0.74581	0.17269
N	2.70613	1.54901	0.08165
C	3.75440	0.71542	-0.24189
C	3.24595	-0.56488	-0.32415
N	1.89996	-0.52377	-0.06739
C	2.85959	2.99473	0.21636
H	2.43367	3.34781	1.16385
H	2.38065	3.52420	-0.62025
H	3.93332	3.22394	0.21181
H	4.75568	1.10879	-0.38783
C	-0.13174	1.28130	2.50252
C	0.65553	2.47145	3.06277
C	0.40172	-0.02780	3.09961
C	-0.37101	2.93317	0.04245
C	-0.13420	3.08146	-1.46454
C	-1.74005	3.49600	0.43839
H	-1.19599	1.40716	2.76705
H	0.39810	3.50809	0.57529
H	1.72840	2.36278	2.83574
H	0.55486	2.48353	4.16054
H	0.29880	3.44099	2.68361
H	1.46972	-0.14939	2.85701
H	0.29436	-0.00159	4.19633
H	-0.12618	-0.91059	2.71219
H	-0.95916	2.63163	-2.03558
H	-0.09406	4.15199	-1.72499
H	0.80809	2.61230	-1.78919
H	-1.94114	3.38772	1.51659
H	-1.77566	4.57052	0.19474
H	-2.54331	2.99361	-0.12200
C	3.96879	-1.86300	-0.59850
C	5.39737	-1.57909	-1.08413
C	4.01815	-2.68432	0.70573
C	3.20556	-2.66602	-1.66740
H	5.92339	-2.52767	-1.27607
H	5.39029	-0.99194	-2.01776
H	5.97112	-1.02275	-0.32384
H	4.58355	-2.14650	1.48492
H	4.51119	-3.65402	0.52369
H	2.99811	-2.87186	1.07923
H	2.19979	-2.92657	-1.30051
H	3.74389	-3.60204	-1.88835
H	3.10692	-2.08999	-2.60297
C	-2.09939	0.21513	-2.33780
C	-0.70358	-0.11023	-2.28278
C	-2.82807	-0.98091	-2.05048
H	-2.52745	1.18766	-2.56368
C	-0.57056	-1.50045	-1.98762
H	0.12481	0.57257	-2.43907
C	-1.88112	-2.04128	-1.84696
H	-3.91063	-1.07660	-2.00698
H	0.37227	-2.01923	-1.84664
H	-2.12005	-3.07462	-1.60820
C	-3.27473	0.44305	0.81320
C	-2.74688	-0.62044	1.59451
C	-2.72725	-1.92084	1.05107
C	-2.06204	-3.07902	1.74044
H	-0.41656	-1.17289	0.58056
H	-3.19749	1.45398	1.20987
H	-4.14353	0.25945	0.17571
H	-2.18947	-0.42043	2.50867
H	-3.54085	-2.18201	0.36718
H	-1.24808	-2.74100	2.39972
H	-2.80271	-3.62916	2.34917
H	-1.64247	-3.78946	1.01092

67
n48 | ju230t-jug21 | Energy: -907438.4404567

Ru	-1.54058	-0.36816	-0.24917
P	-0.35493	1.42895	0.64041
C	1.40794	0.94054	0.34309
N	2.62576	1.52451	0.42370
C	3.56490	0.59601	0.00771
C	2.88574	-0.55378	-0.33492
N	1.54926	-0.30737	-0.10066
C	2.92731	2.86442	0.91422
H	2.95805	2.87556	2.01497
H	2.15982	3.56550	0.56202
H	3.90440	3.17334	0.51940
H	4.62369	0.83595	-0.02056
C	-0.40362	1.81325	2.49453
C	-0.18574	3.28092	2.88350
C	0.59476	0.91688	3.24632
C	-0.50844	3.10782	-0.18305
C	0.07551	3.13958	-1.59982
C	-1.97908	3.54566	-0.15223
H	-1.42996	1.53416	2.78577
H	0.07132	3.80355	0.44271
H	0.81622	3.63242	2.58973
H	-0.25932	3.37192	3.98006
H	-0.93359	3.95311	2.43915
H	1.62713	1.26201	3.07041
H	0.39918	0.97064	4.32973
H	0.54378	-0.13794	2.93679
H	-0.50785	2.52072	-2.29462
H	0.05158	4.17516	-1.97808
H	1.12122	2.79100	-1.62484
H	-2.37671	3.57998	0.87506
H	-2.07710	4.55303	-0.58942
H	-2.60608	2.84763	-0.72757
C	3.38969	-1.82592	-0.96910
C	4.91201	-1.92710	-0.79706
C	2.70189	-3.04227	-0.32939
C	3.03883	-1.78272	-2.47243
H	5.27786	-2.85010	-1.27330
H	5.42455	-1.07579	-1.27554
H	5.18935	-1.95262	0.26953
H	2.88890	-3.08533	0.75586
H	3.08452	-3.96727	-0.78940
H	1.61423	-2.99884	-0.49271
H	1.94949	-1.68602	-2.61639
H	3.37187	-2.71292	-2.96153
H	3.53306	-0.93084	-2.96764
C	-2.19445	0.49186	-2.23999
C	-0.89178	-0.12064	-2.33839
C	-3.13168	-0.53132	-1.92835
H	-2.42897	1.53614	-2.41846
C	-1.04028	-1.51867	-2.07622
H	0.03614	0.38059	-2.59871
C	-2.43213	-1.76379	-1.80741
H	-4.19564	-0.38497	-1.75716
H	-0.25000	-2.26378	-2.10865
H	-2.87554	-2.72634	-1.56573
C	-3.13533	-0.24776	1.26291
C	-2.04052	-0.97190	1.80817
C	-1.53823	-2.12568	1.17714
C	-0.30440	-2.81983	1.69132
H	0.27879	-0.74733	-0.13984
H	-3.40021	0.70536	1.72677
H	-3.97182	-0.79254	0.81687
H	-1.44665	-0.53193	2.60654
H	-2.25767	-2.77318	0.66782
H	0.46377	-2.09857	2.01283
H	-0.55701	-3.46596	2.55254
H	0.14013	-3.46484	0.92026

n49-51

67
n49 | ju230z-jug21a | Energy: -907448.9794155

Ru	-1.66866	-0.35972	-0.33422
P	-0.39136	1.27174	0.62941
C	1.42368	0.79998	0.36118
N	2.63669	1.37807	0.48542
C	3.61727	0.48359	0.07848
C	2.99386	-0.67772	-0.30326
N	1.65062	-0.43632	-0.11017
C	2.90750	2.72328	0.98864
H	2.73678	2.76039	2.07415
H	2.25478	3.44584	0.48308
H	3.95579	2.96803	0.77447
H	4.66854	0.75186	0.08548
C	-0.41195	1.59938	2.50523
C	-0.22308	3.05254	2.95827
C	0.58062	0.68784	3.24296
C	-0.40743	3.00345	-0.11576
C	0.22953	3.07408	-1.50815
C	-1.85128	3.52458	-0.12067
H	-1.43699	1.29528	2.77515
H	0.18008	3.63716	0.56532
H	0.78106	3.43200	2.71080
H	-0.33081	3.09820	4.05504
H	-0.96466	3.73457	2.51950
H	1.61859	1.01975	3.07032
H	0.39127	0.73299	4.32808
H	0.50861	-0.36348	2.92801
H	-0.33297	2.48411	-2.24326
H	0.23366	4.12144	-1.85397
H	1.27189	2.71331	-1.50998
H	-2.29563	3.51759	0.88738
H	-1.86900	4.56147	-0.49578
H	-2.49023	2.90138	-0.76276
C	3.53096	-1.99744	-0.79456
C	4.93729	-1.78884	-1.37613
C	3.60009	-2.97708	0.39712
C	2.59158	-2.56641	-1.87480
H	5.33779	-2.75417	-1.72236
H	4.91614	-1.09255	-2.23019
H	5.62761	-1.39392	-0.61224
H	4.28550	-2.60023	1.17329
H	3.97100	-3.95439	0.04787
H	2.60570	-3.12391	0.84733
H	1.58714	-2.77080	-1.46596
H	2.99723	-3.52013	-2.24586
H	2.49291	-1.87356	-2.72676
C	-2.17568	0.62742	-2.31639
C	-0.93790	-0.11125	-2.43458
C	-3.20746	-0.29851	-2.01314
H	-2.30512	1.69208	-2.47895
C	-1.22302	-1.48716	-2.20678
H	0.03044	0.30700	-2.69813
C	-2.63294	-1.60328	-1.92473
H	-4.25153	-0.04936	-1.84028
H	-0.51259	-2.30779	-2.26903
H	-3.17037	-2.52443	-1.71430
C	-3.23380	-0.51505	1.19876
C	-2.06167	-1.18023	1.65335
C	-1.44847	-2.20980	0.90241
C	-0.15103	-2.84273	1.34306
H	0.83332	-1.03563	-0.31522
H	-3.57478	0.35334	1.76776
H	-4.02935	-1.08935	0.71488
H	-1.49930	-0.75706	2.48529
H	-2.10676	-2.88649	0.34894
H	0.51241	-2.11886	1.84283
H	-0.33157	-3.67610	2.04758
H	0.39640	-3.26715	0.48414

67
n50 | ju250t | Energy: -907444.8263759

Ru	-1.93003	-1.09699	-0.31197
P	-0.98163	0.95657	-0.03478
C	0.86204	0.81614	-0.39674
N	1.84777	1.61049	-0.87172
C	3.06405	0.94713	-0.75964
C	2.82791	-0.28251	-0.20358
N	1.46586	-0.31568	0.00101
C	1.72528	2.94742	-1.46076
H	1.33163	3.65564	-0.72087
H	1.06011	2.91260	-2.33296
H	2.72620	3.26872	-1.77537
H	3.98866	1.40468	-1.09409
C	-0.81709	1.81125	1.65293
C	-0.36780	3.27529	1.61022
C	0.11735	1.00192	2.56485
C	-1.47530	2.34651	-1.19462
C	-1.43291	1.84355	-2.64043
C	-2.87613	2.85089	-0.82393
H	-1.83997	1.76091	2.06097
H	-0.76794	3.17602	-1.05918
H	0.66409	3.35144	1.22694
H	-0.35931	3.68573	2.63407
H	-1.02422	3.91029	0.99810
H	1.17110	1.18801	2.29507
H	-0.01858	1.31490	3.61282
H	-0.07661	-0.07861	2.50202
H	-2.14115	1.00869	-2.76330
H	-1.71244	2.65358	-3.33455
H	-0.43278	1.47180	-2.92526
H	-2.94360	3.16424	0.23028
H	-3.13284	3.71920	-1.45292
H	-3.62878	2.07130	-1.00420
C	3.73377	-1.44678	0.10310
C	5.18507	-0.95120	0.18912
C	3.31491	-2.08744	1.43976
C	3.60589	-2.48369	-1.03428
H	5.85096	-1.80210	0.40008
H	5.50756	-0.50077	-0.76434
H	5.30438	-0.20676	0.99293
H	3.37273	-1.36112	2.26676
H	3.98610	-2.92999	1.66674
H	2.28700	-2.48847	1.39449
H	2.56749	-2.83717	-1.14304
H	4.24381	-3.35404	-0.81106
H	3.92763	-2.05157	-1.99551
C	-1.90335	-1.84151	-2.41615
C	-0.56358	-1.72903	-1.93296
C	-2.55687	-2.84416	-1.61816
H	-2.33282	-1.30273	-3.25554
C	-0.37959	-2.66963	-0.85203
H	0.20279	-1.08029	-2.35026
C	-1.62718	-3.34208	-0.66912
H	-3.59313	-3.15801	-1.71287
H	0.55383	-2.93784	-0.36375
H	-1.83425	-4.09568	0.08699
C	-4.06898	-0.56300	-0.20286
C	-3.50631	-0.48090	1.09762
C	-2.86366	-1.59045	1.68758
C	-2.24028	-1.49629	3.05731
H	0.89622	-1.07776	0.38003
H	-4.46873	0.34460	-0.65433
H	-4.59008	-1.47820	-0.49379
H	-3.38944	0.49858	1.56894
H	-3.26084	-2.57949	1.43533
H	-2.01495	-0.45240	3.32335
H	-2.93189	-1.89430	3.82298
H	-1.30712	-2.07941	3.12851

67
n51 | ju310a-juf25b | Energy: -907445.2475037

Ru	-1.66466	-0.31187	-0.51403
P	-0.33536	1.16747	0.60255
C	1.44420	0.99009	0.02512
N	2.52081	1.78992	-0.14689
C	3.61981	1.01221	-0.49452
C	3.21827	-0.29585	-0.53609
N	1.87996	-0.25944	-0.20887
C	2.59675	3.24668	-0.00404
H	2.41216	3.53203	1.04027
H	1.86114	3.72745	-0.66097
H	3.60727	3.56025	-0.29498
H	4.58783	1.45977	-0.69027
C	0.00994	0.97146	2.45531
C	0.89205	2.06638	3.06332
C	0.59362	-0.41884	2.73748
C	-0.62437	3.01561	0.42363
C	-0.82223	3.35492	-1.05677
C	-1.81800	3.46557	1.28059
H	-1.00070	1.02598	2.89497
H	0.26131	3.53429	0.81277
H	1.89720	2.05069	2.60598
H	1.02517	1.88250	4.14268
H	0.46365	3.07268	2.94429
H	1.65714	-0.45826	2.44590
H	0.53685	-0.63897	3.81596
H	0.04497	-1.20297	2.19369
H	-1.68850	2.80525	-1.45801
H	-0.99138	4.43764	-1.18146
H	0.05310	3.06765	-1.66598
H	-1.67510	3.22465	2.34566
H	-1.92915	4.55933	1.19500
H	-2.75944	3.00981	0.94712
C	3.93430	-1.57102	-0.89396
C	5.44679	-1.31068	-0.93293
C	3.61060	-2.64937	0.15837
C	3.44748	-2.03637	-2.28347
H	5.97207	-2.24004	-1.20138
H	5.69842	-0.54981	-1.69029
H	5.81767	-0.97328	0.04864
H	3.93599	-2.33576	1.16356
H	4.13132	-3.58364	-0.10287
H	2.52943	-2.87105	0.19350
H	2.35909	-2.21073	-2.29262
H	3.94782	-2.98117	-2.54991
H	3.68581	-1.28532	-3.05383
C	-1.69398	-0.39783	-2.74069
C	-0.37165	-0.68167	-2.29522
C	-2.55117	-1.44201	-2.23947
H	-1.99531	0.44266	-3.35961
C	-0.39636	-1.91724	-1.53890
H	0.51263	-0.09523	-2.53218
C	-1.74849	-2.36383	-1.51000
H	-3.62476	-1.51787	-2.39112
H	0.45389	-2.49814	-1.18654
H	-2.10811	-3.25310	-0.99779
C	-3.54820	0.80017	-0.34875
C	-3.21378	0.26897	0.92860
C	-3.00161	-1.11553	1.10954
C	-2.58186	-1.67654	2.44429
H	1.22629	-1.04186	-0.15612
H	-3.58511	1.88321	-0.47239
H	-4.25386	0.25288	-0.97870
H	-2.91433	0.94644	1.73361
H	-3.61169	-1.79169	0.50077
H	-2.04732	-0.92550	3.04578
H	-3.46568	-2.00494	3.02244
H	-1.92326	-2.55300	2.32971

n52-54

67
n52 | ju310t-juf25 | Energy: -907438.2163919

Ru	-1.98088	-0.82391	-0.34899
P	-0.64549	0.82101	0.58823
C	1.19374	0.58842	0.21232
N	2.35545	1.20828	0.53153
C	3.40282	0.61019	-0.15569
C	2.88452	-0.38984	-0.93243
N	1.53222	-0.36483	-0.67091
C	2.59420	2.33294	1.43587
H	1.66621	2.87860	1.61061
H	3.33132	2.99939	0.96662
H	2.98742	1.96528	2.39509
H	4.42495	0.95149	-0.03373
C	-0.73519	0.90133	2.46701
C	-0.09698	2.05935	3.24102
C	-0.32306	-0.45808	3.04318
C	-0.74398	2.62619	0.02487
C	-0.59696	2.68100	-1.50036
C	-2.01663	3.34081	0.49997
H	-1.82595	1.00353	2.57216
H	0.11420	3.14574	0.47955
H	0.97400	1.88423	3.41756
H	-0.57451	2.12972	4.23269
H	-0.22614	3.03339	2.74311
H	0.76704	-0.60727	2.93843
H	-0.56705	-0.50436	4.11746
H	-0.84245	-1.27787	2.52395
H	-1.39384	2.09415	-1.98420
H	-0.66146	3.72578	-1.84751
H	0.37262	2.27133	-1.83199
H	-2.18257	3.22733	1.58304
H	-1.92254	4.41836	0.28497
H	-2.90686	2.97527	-0.03003
C	3.51339	-1.34314	-1.91351
C	5.04121	-1.21259	-1.83699
C	3.08868	-2.78476	-1.57007
C	3.03052	-0.98393	-3.33478
H	5.50452	-1.90434	-2.55694
H	5.36576	-0.19000	-2.09133
H	5.41089	-1.46417	-0.82948
H	3.40605	-3.05931	-0.55086
H	3.55759	-3.48256	-2.28135
H	1.99654	-2.91393	-1.64677
H	1.93312	-1.05848	-3.41891
H	3.47317	-1.68427	-4.06077
H	3.33103	0.04072	-3.60657
C	-2.14059	-1.99945	-2.28305
C	-0.76949	-1.98264	-1.91659
C	-2.87058	-2.65909	-1.24957
H	-2.55765	-1.57396	-3.19196
C	-0.64252	-2.65228	-0.63097
H	0.02877	-1.65209	-2.57959
C	-1.93600	-3.06786	-0.23131
H	-3.94185	-2.84167	-1.24701
H	0.27987	-2.84846	-0.08932
H	-2.17738	-3.60436	0.68270
C	-3.61904	0.49089	-0.94978
C	-3.62976	0.36973	0.47277
C	-3.71828	-0.88927	1.10155
C	-3.67115	-1.07790	2.59585
H	0.80273	-0.92574	-1.10682
H	-3.44730	1.48004	-1.37756
H	-4.28995	-0.14310	-1.53765
H	-3.37571	1.23285	1.09133
H	-4.31373	-1.65008	0.59044
H	-3.17960	-0.24480	3.11758
H	-4.69801	-1.15983	2.99775
H	-3.14342	-2.00714	2.86614

67
n53 | ju410a-juf35a | Energy: -907446.1303343

Ru	-1.37936	-0.83842	0.01058
P	-0.52180	1.28927	0.09602
C	1.36660	1.06286	0.08055
N	2.46235	1.84991	0.14237
C	3.60038	1.07215	-0.03366
C	3.19484	-0.22606	-0.20796
N	1.82053	-0.18085	-0.13207
C	2.47497	3.30403	0.27529
H	2.16643	3.77061	-0.67231
H	3.49473	3.62203	0.52793
H	1.79296	3.60534	1.07814
H	4.59449	1.50630	-0.01398
C	-0.82377	2.18080	1.75526
C	-1.00095	3.70441	1.71097
C	0.20521	1.78210	2.82201
C	-0.57926	2.68308	-1.18644
C	0.24031	2.36711	-2.44734
C	-2.02242	3.07485	-1.54113
H	-1.79283	1.74153	2.03759
H	-0.11270	3.54297	-0.68176
H	-1.78379	4.01839	1.00676
H	-0.07369	4.23426	1.44148
H	-1.29277	4.05289	2.71589
H	1.19879	2.20834	2.60538
H	-0.11485	2.17008	3.80347
H	0.31598	0.69263	2.90745
H	-0.09415	1.44067	-2.93886
H	0.12472	3.19012	-3.17278
H	1.31537	2.25921	-2.23085
H	-2.68631	3.09893	-0.66308
H	-2.02491	4.07765	-1.99936
H	-2.46044	2.37724	-2.26888
C	3.93870	-1.51547	-0.42731
C	5.44565	-1.23431	-0.49037
C	3.62644	-2.47180	0.74275
C	3.45924	-2.14732	-1.75048
H	5.99022	-2.17742	-0.65076
H	5.68682	-0.55309	-1.32299
H	5.80526	-0.78740	0.45126
H	3.95838	-2.04406	1.70273
H	4.14878	-3.42896	0.58640
H	2.54482	-2.68152	0.80806
H	2.37491	-2.35228	-1.72722
H	3.98195	-3.10341	-1.91178
H	3.67093	-1.48369	-2.60450
C	-1.71859	-1.12517	2.22689
C	-2.68093	-1.88488	1.51509
C	-0.40857	-1.63159	1.87992
H	-1.92598	-0.31951	2.92537
C	-1.98298	-2.86358	0.71819
H	-3.75853	-1.74732	1.55706
C	-0.58249	-2.71197	0.96841
H	0.54037	-1.29516	2.28945
H	-2.43910	-3.60754	0.07018
H	0.21063	-3.31521	0.53172
C	-0.77325	-1.38548	-2.02225
C	-1.91741	-0.52926	-2.08084
C	-3.11589	-0.84941	-1.41379
C	-4.27915	0.10368	-1.32756
H	1.12697	-0.93940	-0.25207
H	0.14247	-1.01705	-2.49565
H	-0.91461	-2.46876	-2.09625
H	-1.80095	0.48635	-2.45459
H	-3.38497	-1.90891	-1.35331
H	-3.94344	1.15046	-1.32664
H	-4.97063	-0.04088	-2.17927
H	-4.85843	-0.06776	-0.40572

67
n54 | ju410t-juf35 | Energy: -907434.4464029

Ru	-1.57362	-1.20926	0.12672
P	-0.80168	1.01204	0.21531
C	1.04069	0.76119	0.25051
N	2.13934	1.55325	0.35320
C	3.24989	0.75680	0.12297
C	2.79477	-0.52033	-0.12376
N	1.42273	-0.47904	-0.04017
C	2.18034	2.99105	0.59220
H	1.66191	3.52731	-0.21683
H	3.23053	3.30960	0.61677
H	1.71018	3.23442	1.55499
H	4.25521	1.16583	0.16186
C	-1.24400	1.93862	1.81030
C	-1.30176	3.46961	1.71680
C	-0.33512	1.50736	2.97060
C	-0.87682	2.34134	-1.12829
C	-0.00796	1.99317	-2.34689
C	-2.30717	2.72286	-1.53477
H	-2.26308	1.56908	2.01141
H	-0.42842	3.21930	-0.63844
H	-2.00757	3.82066	0.95093
H	-0.31473	3.90606	1.49859
H	-1.63172	3.87079	2.68948
H	0.70340	1.83807	2.80727
H	-0.69264	1.96956	3.90568
H	-0.31927	0.41971	3.11358
H	-0.30702	1.04506	-2.81981
H	-0.11046	2.78997	-3.10265
H	1.05757	1.90992	-2.08232
H	-2.98856	2.79791	-0.67253
H	-2.29087	3.70240	-2.04043
H	-2.73485	1.99714	-2.24122
C	3.53597	-1.79917	-0.41787
C	5.04151	-1.52119	-0.51997
C	3.26414	-2.80131	0.72220
C	3.01569	-2.38567	-1.74486
H	5.57972	-2.45752	-0.73493
H	5.25778	-0.80651	-1.33141
H	5.43393	-1.11152	0.42582
H	3.63336	-2.41220	1.68548
H	3.77330	-3.75606	0.51219
H	2.18287	-2.99657	0.81559
H	1.93270	-2.58427	-1.68501
H	3.53196	-3.33509	-1.96092
H	3.19860	-1.69047	-2.58092
C	-2.09268	-1.44826	2.33210
C	-2.98896	-2.25819	1.59398
C	-0.75347	-1.91245	2.06192
H	-2.36480	-0.62242	2.98340
C	-2.22412	-3.22829	0.85649
H	-4.06972	-2.14136	1.56132
C	-0.84467	-3.02740	1.17020
H	0.16688	-1.52275	2.48704
H	-2.62639	-3.99470	0.19867
H	-0.00756	-3.60651	0.78921
C	-1.09067	-1.82053	-1.92466
C	-2.17452	-0.89599	-1.96777
C	-3.36553	-1.16202	-1.26883
C	-4.49851	-0.18031	-1.14047
H	0.17700	-1.13641	-0.19037
H	-0.14898	-1.51990	-2.38910
H	-1.29996	-2.89375	-1.96096
H	-2.01017	0.10737	-2.35376
H	-3.65816	-2.21283	-1.18008
H	-4.14330	0.85845	-1.14175
H	-5.21306	-0.30528	-1.97567
H	-5.05942	-0.35037	-0.20733

n55-57

67
n55 | ju420a-juf37a | Energy: -907443.8561144

Ru	-1.37227	-0.98501	-0.38379
P	-0.35710	1.13801	-0.12948
C	1.45980	0.87078	0.01399
N	2.44446	1.81802	0.19828
C	3.64567	1.14335	0.19819
C	3.35289	-0.19265	0.01959
N	1.99320	-0.33901	-0.09404
C	2.34400	3.26564	0.31156
H	2.46856	3.75048	-0.67085
H	3.13082	3.62594	0.98968
H	1.37173	3.54133	0.73274
H	4.58582	1.67023	0.33014
C	-0.88481	1.96806	1.50235
C	-1.27946	3.45243	1.44310
C	0.14395	1.71098	2.61605
C	-0.34990	2.38640	-1.55502
C	0.18627	1.67235	-2.80605
C	-1.61737	3.18818	-1.88408
H	-1.78845	1.39405	1.75214
H	0.40604	3.11626	-1.23040
H	-2.26104	3.59243	0.96979
H	-0.55219	4.07886	0.90362
H	-1.35373	3.84153	2.47237
H	1.06838	2.28699	2.46404
H	-0.29411	2.02134	3.57916
H	0.42180	0.65053	2.69401
H	-0.54067	0.93478	-3.18222
H	0.35844	2.41696	-3.60052
H	1.13260	1.14467	-2.61026
H	-1.99986	3.75735	-1.02922
H	-1.35755	3.91205	-2.67454
H	-2.43433	2.56818	-2.27664
C	4.27941	-1.38385	-0.03417
C	5.73942	-0.92567	0.08340
C	3.93978	-2.33319	1.13185
C	4.07168	-2.12467	-1.36882
H	6.41103	-1.79777	0.04253
H	6.00857	-0.24653	-0.74287
H	5.91533	-0.40356	1.03903
H	4.09097	-1.83204	2.10270
H	4.58777	-3.22458	1.09503
H	2.88965	-2.66256	1.06993
H	3.01986	-2.43623	-1.47799
H	4.71199	-3.02150	-1.40616
H	4.32909	-1.47514	-2.22195
C	-1.60463	-1.73144	1.72184
C	-2.27897	-2.64867	0.84799
C	-0.21592	-1.75502	1.36954
H	-2.05673	-1.15575	2.52544
C	-1.30828	-3.23314	-0.02320
H	-3.34397	-2.86890	0.84952
C	-0.03643	-2.66924	0.28777
H	0.58885	-1.18865	1.82204
H	-1.50960	-3.95546	-0.81019
H	0.90758	-2.85491	-0.21366
C	-2.41574	-1.45439	-2.27718
C	-2.83708	-0.19147	-1.80393
C	-3.44395	-0.11160	-0.52616
C	-3.86653	1.19203	0.09426
H	-0.25214	-0.79311	-1.49974
H	-1.83117	-1.50744	-3.19598
H	-3.00914	-2.33987	-2.03786
H	-2.51608	0.70873	-2.32094
H	-4.04914	-0.97130	-0.22503
H	-3.21476	2.02204	-0.20732
H	-4.89787	1.43979	-0.21756
H	-3.86843	1.12995	1.19396

67
n56 | ju420t-juf37 | Energy: -907436.1802429

Ru	-1.76803	-1.16890	0.15186
P	-0.69337	0.94501	0.24448
C	1.11019	0.61079	0.08575
N	2.16334	1.49116	0.11979
C	3.31077	0.74848	-0.06754
C	2.91717	-0.56673	-0.20304
N	1.54823	-0.62877	-0.10398
C	2.13781	2.94248	0.21920
H	2.04332	3.40518	-0.77660
H	3.07049	3.28418	0.68928
H	1.29557	3.25850	0.84403
H	4.28993	1.21763	-0.08205
C	-0.90484	1.72297	1.97584
C	-1.29325	3.20746	2.00672
C	0.31339	1.46322	2.87795
C	-0.91850	2.37725	-0.96985
C	-0.13746	2.18574	-2.27954
C	-2.39399	2.69974	-1.24870
H	-1.75654	1.15720	2.37666
H	-0.47976	3.23647	-0.44241
H	-2.19445	3.42215	1.41485
H	-0.48385	3.86184	1.64528
H	-1.49784	3.49521	3.05154
H	1.14436	2.14044	2.62992
H	0.03276	1.64827	3.92819
H	0.69981	0.43650	2.79165
H	-0.49049	1.31563	-2.85461
H	-0.27914	3.07703	-2.91386
H	0.94022	2.05055	-2.11058
H	-3.03210	2.60371	-0.35641
H	-2.48016	3.73406	-1.61968
H	-2.80107	2.03974	-2.02841
C	3.74892	-1.80768	-0.42017
C	5.23740	-1.44149	-0.49439
C	3.50992	-2.78236	0.74939
C	3.31139	-2.47910	-1.73651
H	5.83970	-2.34985	-0.65381
H	5.43368	-0.74936	-1.33045
H	5.57554	-0.96657	0.44191
H	3.82764	-2.33334	1.70528
H	4.08396	-3.71032	0.59089
H	2.43985	-3.03811	0.82131
H	2.23941	-2.73413	-1.69994
H	3.88679	-3.40593	-1.89655
H	3.48364	-1.80852	-2.59504
C	-2.86129	-1.20289	2.12201
C	-3.43007	-2.22685	1.31290
C	-1.46920	-1.53497	2.31053
H	-3.39219	-0.36047	2.55676
C	-2.41521	-3.17871	0.98056
H	-4.46254	-2.25735	0.97241
C	-1.20382	-2.75269	1.61324
H	-0.75718	-0.98444	2.91466
H	-2.54398	-4.06884	0.36969
H	-0.23893	-3.25059	1.55824
C	-1.06318	-1.76198	-1.86059
C	-2.16499	-0.84396	-1.98436
C	-3.40927	-1.17972	-1.43575
C	-4.59359	-0.25605	-1.39665
H	-0.27535	-1.50719	-0.37605
H	-0.10421	-1.44658	-2.27928
H	-1.26052	-2.83401	-1.94758
H	-1.99549	0.16669	-2.34554
H	-3.65058	-2.24648	-1.38971
H	-4.29219	0.79536	-1.30904
H	-5.19493	-0.37592	-2.31679
H	-5.25163	-0.49975	-0.54733

67
n57 | ju420z-juf37b | Energy: -907441.9477703

Ru	-1.40595	-0.84163	0.02264
P	-0.30810	1.29075	0.14497
C	1.47794	0.92905	-0.05989
N	2.54583	1.79443	-0.06614
C	3.67990	1.02304	-0.20521
C	3.26222	-0.29099	-0.27022
N	1.89244	-0.32855	-0.17511
C	2.53971	3.24781	0.00046
H	2.41097	3.69261	-0.99940
H	3.49356	3.58824	0.42662
H	1.72575	3.58603	0.65213
H	4.66722	1.47338	-0.24215
C	-0.45469	2.03799	1.89855
C	-0.81842	3.52732	1.97296
C	0.80054	1.75775	2.74282
C	-0.59539	2.74343	-1.02568
C	0.11931	2.57896	-2.37592
C	-2.09043	3.04697	-1.21274
H	-1.29616	1.47540	2.32625
H	-0.14031	3.60214	-0.51130
H	-1.74298	3.76943	1.43070
H	-0.01467	4.17349	1.58487
H	-0.96673	3.79851	3.03164
H	1.62150	2.43516	2.46279
H	0.56897	1.93211	3.80672
H	1.17984	0.73145	2.62620
H	-0.28120	1.73930	-2.96405
H	-0.02557	3.49482	-2.97339
H	1.19940	2.41014	-2.25842
H	-2.65980	2.98486	-0.27246
H	-2.21093	4.06525	-1.61735
H	-2.55505	2.35308	-1.92804
C	4.07406	-1.55531	-0.42025
C	5.57095	-1.22211	-0.47867
C	3.79255	-2.47862	0.78089
C	3.64959	-2.27032	-1.71795
H	6.15797	-2.14781	-0.58755
H	5.79801	-0.56994	-1.33874
H	5.89964	-0.71428	0.44359
H	4.10039	-1.99921	1.72517
H	4.34936	-3.42386	0.67040
H	2.71591	-2.70892	0.84070
H	2.57185	-2.50200	-1.69350
H	4.20876	-3.21407	-1.83011
H	3.85239	-1.63764	-2.59833
C	-2.42877	-0.88031	1.94839
C	-2.96593	-1.94050	1.14633
C	-1.03111	-1.18143	2.16971
H	-2.99225	-0.05824	2.38119
C	-1.91718	-2.84890	0.81904
H	-3.99564	-2.00562	0.80340
C	-0.71420	-2.36420	1.45326
H	-0.33822	-0.60078	2.76651
H	-2.00541	-3.74273	0.20631
H	0.27734	-2.80422	1.37372
C	-0.56534	-1.28933	-2.16396
C	-1.79655	-0.44469	-2.07950
C	-3.00025	-0.96704	-1.62651
C	-4.26675	-0.16125	-1.54258
H	-0.00004	-1.36776	-1.13344
H	0.23076	-0.82029	-2.75804
H	-0.75324	-2.32307	-2.48118
H	-1.74978	0.58925	-2.40409
H	-3.12413	-2.05451	-1.64130
H	-4.05784	0.91505	-1.45919
H	-4.88139	-0.33214	-2.44515
H	-4.87627	-0.46407	-0.67590

n58-60

67
n58 | ju430t-juf39 | Energy: -907439.9019325

Ru	-1.71552	-1.12307	0.20184
P	-0.69500	1.06504	0.29585
C	1.07769	0.67055	0.09763
N	2.17324	1.49562	0.08119
C	3.27723	0.68401	-0.07006
C	2.81250	-0.61495	-0.13231
N	1.44252	-0.60293	-0.02196
C	2.20839	2.94841	0.14587
H	2.17572	3.39205	-0.86244
H	3.13229	3.26422	0.65055
H	1.35097	3.30998	0.72555
H	4.28020	1.09746	-0.11545
C	-0.85604	1.83104	2.03671
C	-1.19548	3.32671	2.08978
C	0.38923	1.54348	2.89319
C	-0.98564	2.49587	-0.89783
C	-0.25756	2.31391	-2.23806
C	-2.48434	2.77080	-1.09837
H	-1.71011	1.28181	2.46088
H	-0.54656	3.37044	-0.39537
H	-2.10725	3.57926	1.53068
H	-0.37298	3.95160	1.70525
H	-1.35375	3.61386	3.14273
H	1.21993	2.20667	2.60700
H	0.15514	1.73556	3.95348
H	0.75434	0.51038	2.79227
H	-0.62771	1.44511	-2.80274
H	-0.42454	3.20840	-2.86150
H	0.82614	2.18173	-2.10660
H	-3.04790	2.76451	-0.15217
H	-2.61701	3.76018	-1.56611
H	-2.94515	2.02675	-1.76459
C	3.57771	-1.90580	-0.29862
C	5.08509	-1.62523	-0.36413
C	3.27215	-2.83092	0.89495
C	3.11911	-2.59257	-1.60025
H	5.63791	-2.57008	-0.48631
H	5.32929	-0.97319	-1.21952
H	5.43780	-1.13852	0.56060
H	3.59278	-2.36915	1.84368
H	3.80178	-3.79042	0.77541
H	2.18994	-3.03361	0.95149
H	2.03446	-2.78840	-1.57056
H	3.64535	-3.55334	-1.72611
H	3.33614	-1.95790	-2.47564
C	-2.81894	-1.23097	2.04005
C	-3.21026	-2.35665	1.23023
C	-1.42055	-1.40054	2.36268
H	-3.48177	-0.45552	2.41628
C	-2.06277	-3.15678	0.97817
H	-4.20811	-2.52637	0.83461
C	-0.94892	-2.54463	1.66975
H	-0.82619	-0.75127	2.99347
H	-2.02266	-4.05622	0.36861
H	0.08608	-2.87727	1.63387
C	-0.87477	-1.59273	-2.35127
C	-2.08594	-0.77262	-1.95477
C	-3.25683	-1.34584	-1.49021
C	-4.54516	-0.58352	-1.32904
H	-0.09867	-1.63823	-1.54735
H	-0.35467	-1.12826	-3.20483
H	-1.15584	-2.62555	-2.60413
H	-2.09932	0.27860	-2.22678
H	-3.34274	-2.43598	-1.54223
H	-4.36257	0.49545	-1.21716
H	-5.18497	-0.74008	-2.21655
H	-5.11693	-0.93038	-0.45327

67
n59 | ju510a-jug43b | Energy: -907452.2037537

Ru	-1.16722	-0.98072	0.35185
P	-0.76960	1.40976	0.44627
C	0.93325	0.90111	0.04673
N	2.16985	1.39913	-0.19168
C	3.00191	0.31660	-0.39443
C	2.23721	-0.83075	-0.26722
N	0.94622	-0.43574	-0.00415
C	2.54997	2.80478	-0.21259
H	2.91376	3.08672	-1.21259
H	3.33924	2.99429	0.53076
H	1.66645	3.40860	0.03444
H	4.05869	0.44477	-0.60459
C	-0.71485	2.13625	2.19250
C	-0.59306	3.66150	2.28462
C	0.40391	1.45979	2.99634
C	-1.24318	2.85970	-0.65543
C	-0.65000	2.84398	-2.07040
C	-2.77340	2.98445	-0.66410
H	-1.68962	1.84261	2.61792
H	-0.82622	3.73967	-0.14414
H	-1.44745	4.18344	1.82786
H	0.33499	4.02201	1.80786
H	-0.55155	3.95188	3.34760
H	1.38964	1.81102	2.64795
H	0.30518	1.72056	4.06262
H	0.38458	0.36721	2.89640
H	-1.11796	2.09194	-2.71841
H	-0.82473	3.83121	-2.53002
H	0.43526	2.65953	-2.06275
H	-3.18364	3.07604	0.35600
H	-3.07395	3.88008	-1.23232
H	-3.23701	2.10379	-1.14000
C	2.69077	-2.27171	-0.28504
C	4.12399	-2.36428	-0.82934
C	2.66956	-2.79502	1.16741
C	1.75327	-3.12832	-1.15474
H	4.44627	-3.41720	-0.84487
H	4.18398	-1.96872	-1.85663
H	4.82960	-1.80516	-0.19256
H	3.35629	-2.20989	1.80112
H	2.98779	-3.85045	1.18986
H	1.65919	-2.72451	1.59429
H	0.70197	-2.97768	-0.86318
H	2.00914	-4.19341	-1.03369
H	1.86545	-2.87104	-2.22017
C	-2.94422	-1.66675	1.46501
C	-2.32045	-2.82834	0.88995
C	-1.98759	-1.09735	2.37584
H	-3.96618	-1.33682	1.30543
C	-0.99821	-2.94509	1.38562
H	-2.77067	-3.49800	0.16379
C	-0.78912	-1.86806	2.32317
H	-2.14638	-0.21725	2.99291
H	-0.28134	-3.71662	1.12115
H	0.11982	-1.69392	2.89154
C	-0.12556	-0.45025	-2.73389
C	-1.40373	-0.45779	-1.93757
C	-2.11656	-1.61071	-1.65841
C	-3.62782	-1.58852	-1.64503
H	0.56048	0.35724	-2.44430
H	-0.37740	-0.29806	-3.79964
H	0.40343	-1.40621	-2.63800
H	-2.00373	0.45279	-1.98104
H	-1.64000	-2.56827	-1.89468
H	-3.99878	-0.61565	-1.28579
H	-3.98977	-1.73306	-2.67949
H	-4.08014	-2.38117	-1.03197

67
n60 | ju510t-jug43 | Energy: -907440.7730224

Ru	-1.14054	-1.01632	0.54716
P	-0.86318	1.37222	0.51407
C	0.80239	0.91705	-0.08571
N	2.01351	1.42601	-0.41110
C	2.89408	0.36270	-0.46504
C	2.19077	-0.78505	-0.14874
N	0.88351	-0.41392	0.07018
C	2.33267	2.82495	-0.66522
H	2.82422	2.92374	-1.64480
H	2.99986	3.21364	0.11957
H	1.39886	3.40229	-0.66852
H	3.93487	0.50230	-0.73849
C	-0.53199	2.11154	2.21267
C	-0.08755	3.57868	2.18345
C	0.49035	1.24967	2.96469
C	-1.59214	2.78156	-0.46698
C	-1.71391	2.46042	-1.95601
C	-2.95765	3.13040	0.14534
H	-1.50862	2.03956	2.72423
H	-0.90744	3.63544	-0.33170
H	-0.84821	4.24413	1.74932
H	0.84882	3.69439	1.61147
H	0.10985	3.92022	3.21318
H	1.48767	1.34441	2.50279
H	0.56443	1.59216	4.00943
H	0.21688	0.18635	2.95245
H	-2.41684	1.62988	-2.11681
H	-2.09572	3.34671	-2.48953
H	-0.74486	2.17938	-2.39748
H	-2.87976	3.41590	1.20664
H	-3.40293	3.97654	-0.40303
H	-3.64798	2.27293	0.06428
C	2.69136	-2.20258	-0.00946
C	4.16719	-2.27881	-0.42524
C	2.55208	-2.62205	1.46795
C	1.85575	-3.15374	-0.88714
H	4.52722	-3.31437	-0.32304
H	4.30042	-1.97059	-1.47553
H	4.79449	-1.63620	0.21475
H	3.13705	-1.95447	2.12196
H	2.92083	-3.65252	1.59941
H	1.49873	-2.58284	1.77781
H	0.78212	-3.04189	-0.66736
H	2.15057	-4.19610	-0.68424
H	2.02186	-2.95550	-1.95806
C	-3.05766	-1.60131	1.42728
C	-2.48172	-2.74023	0.77919
C	-2.12563	-1.17936	2.43867
H	-4.02074	-1.15109	1.20332
C	-1.22093	-3.04993	1.38149
H	-2.91682	-3.26081	-0.07156
C	-0.99482	-2.06757	2.40984
H	-2.25462	-0.34171	3.12040
H	-0.56590	-3.87628	1.12011
H	-0.13031	-2.01372	3.06727
C	0.49427	-0.43420	-3.09338
C	-0.99479	-0.49663	-2.98304
C	-1.70480	-1.27217	-2.14562
C	-3.20988	-1.33378	-2.14973
H	0.86800	0.56678	-2.80816
H	0.80725	-0.60277	-4.13851
H	0.98092	-1.17596	-2.45093
H	-1.55588	0.13905	-3.67889
H	-1.15188	-2.00345	-1.52288
H	-3.62022	-0.73274	-2.97766
H	-3.56464	-2.37157	-2.27741
H	-3.63227	-0.95875	-1.20333

n61

67
n61 | ju510z-jug43a | Energy: -907441.0140927

Ru	-0.87222	-0.82939	0.34872
P	-0.61059	1.56298	0.30513
C	1.06060	1.12207	-0.28378
N	2.26484	1.64249	-0.61679
C	3.15778	0.58938	-0.65965
C	2.46749	-0.56344	-0.33149
N	1.15664	-0.20489	-0.11453
C	2.56732	3.04423	-0.87540
H	3.07584	3.14333	-1.84615
H	3.21343	3.44960	-0.08134
H	1.62485	3.60697	-0.90146
H	4.19706	0.73822	-0.93383
C	-0.29253	2.30491	2.00699
C	0.11590	3.78271	1.98564
C	0.75361	1.46642	2.75307
C	-1.34345	2.97281	-0.67409
C	-1.43056	2.69150	-2.17426
C	-2.72485	3.29316	-0.08204
H	-1.26530	2.20654	2.52135
H	-0.67333	3.83240	-0.50664
H	-0.66587	4.43354	1.56722
H	1.04232	3.92683	1.40372
H	0.31718	4.11924	3.01625
H	1.74857	1.59658	2.29488
H	0.81454	1.80028	3.80143
H	0.51326	0.39555	2.72934
H	-2.14435	1.88107	-2.37789
H	-1.78155	3.60034	-2.69091
H	-0.45533	2.40464	-2.59814
H	-2.67156	3.55445	0.98711
H	-3.16839	4.14729	-0.61931
H	-3.40402	2.43072	-0.19666
C	2.98324	-1.97502	-0.18671
C	4.46110	-2.03568	-0.59793
C	2.84434	-2.39427	1.29056
C	2.16061	-2.93605	-1.06605
H	4.83249	-3.06683	-0.49193
H	4.59391	-1.72887	-1.64869
H	5.07919	-1.38415	0.04202
H	3.41886	-1.71892	1.94587
H	3.22509	-3.42005	1.42450
H	1.78958	-2.36798	1.59687
H	1.08526	-2.83889	-0.84711
H	2.46949	-3.97469	-0.86491
H	2.32434	-2.73292	-2.13645
C	-2.77351	-1.40977	1.26590
C	-2.19987	-2.55428	0.62598
C	-1.83400	-0.97621	2.26708
H	-3.74063	-0.96617	1.04670
C	-0.92973	-2.84847	1.21861
H	-2.64105	-3.09092	-0.21205
C	-0.70201	-1.85703	2.23823
H	-1.95896	-0.13018	2.93901
H	-0.27272	-3.67412	0.96014
H	0.16803	-1.79240	2.88696
C	0.77821	-0.26576	-3.30244
C	-0.71245	-0.25152	-3.19530
C	-1.45464	-0.82374	-2.23512
C	-2.95923	-0.79992	-2.21756
H	1.19189	0.74357	-3.11679
H	1.09021	-0.55392	-4.32074
H	1.22931	-0.95495	-2.58097
H	-1.25033	0.27996	-3.99064
H	-0.91672	-1.51830	-1.52977
H	-3.35008	-0.38116	-3.15929
H	-3.37419	-1.81467	-2.09653
H	-3.33961	-0.19541	-1.37688

2.9.5.4. Ru(η³-allyl) without hydride

67			
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Ru	-0.53912	-0.24116	1.67634
P	-1.08381	0.37226	-0.56620
C	-2.26530	1.83636	-0.49494
C	-1.45830	3.11707	-0.24105
C	-3.29080	2.02077	-1.62336
C	-1.93210	-0.98673	-1.54823
C	-3.22562	-1.48708	-0.89934
C	-0.95156	-2.14578	-1.77143
C	0.31046	0.76284	-1.69517
N	1.54186	0.40725	-1.34100
C	2.36588	0.65359	-2.40864
C	1.60737	1.16357	-3.44093
N	0.30499	1.22099	-2.99384
C	3.84660	0.36644	-2.34321
C	4.05695	-1.13985	-2.09256
C	4.52176	0.76804	-3.66165
C	4.46026	1.16454	-1.17665
C	-0.79235	1.73972	-3.79552
C	-1.12105	0.20516	3.74467
C	-1.11588	-1.21644	3.59398
C	-2.11835	-1.56256	2.62500
C	-2.72627	-0.35706	2.18247
C	-2.10549	0.75163	2.85445
H	-2.82956	1.60497	0.42051
H	-2.14485	3.96299	-0.07100
H	-0.82670	3.36042	-1.11234
H	-0.80366	3.01234	0.63850
H	-2.86012	2.54049	-2.48824
H	-4.11356	2.65144	-1.24711
H	-3.72893	1.07115	-1.96588
H	-2.17699	-0.53379	-2.52362
H	-3.72256	-2.19823	-1.57948
H	-3.93657	-0.67296	-0.68620
H	-3.00352	-2.01859	0.03842
H	-0.02530	-1.81744	-2.26776
H	-0.68214	-2.60880	-0.80631
H	-1.42929	-2.91869	-2.39573
H	1.87153	1.49366	-4.44078
H	3.62296	-1.73968	-2.90984
H	5.13466	-1.36377	-2.02879
H	3.58347	-1.44651	-1.14522
H	4.10471	0.19957	-4.51000
H	4.39026	1.84470	-3.86129
H	5.60194	0.55915	-3.60883
H	5.53611	0.93882	-1.09072
H	4.34296	2.24890	-1.33927
H	3.96774	0.90030	-0.22648
H	-1.69940	1.14521	-3.63405
H	-1.00052	2.79232	-3.54645
H	-0.51128	1.67230	-4.85530
H	-0.46899	0.78030	4.39877
H	-0.46973	-1.91319	4.12269
H	-2.36675	-2.56597	2.28793
H	-3.51838	-0.28543	1.44438
H	-2.37098	1.80031	2.75280
C	1.15110	1.22176	1.63718
C	1.51894	-0.04296	2.13718
C	1.56295	-1.23051	1.26141
H	1.05909	2.03937	2.35674
H	1.37851	1.48671	0.60867
H	1.72465	-0.19008	3.20189
H	1.96173	-0.99859	0.26617
H	0.41531	-1.52336	0.88587
C	2.07436	-2.51372	1.90101
H	1.85949	-3.39011	1.27039
H	1.61752	-2.67311	2.89092
H	3.16696	-2.44536	2.03065

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Ru	-0.52874	-0.35945	1.63432
P	-1.17284	0.48679	-0.52447
C	-1.86114	2.26304	-0.51502
C	-0.75310	3.27502	-0.84765
C	-3.12709	2.53574	-1.34024
C	-2.42043	-0.48134	-1.55766
C	-3.71420	-0.82751	-0.80409
C	-1.79749	-1.71429	-2.22711
C	0.28355	0.49168	-1.64963
N	1.47031	0.07021	-1.22813
C	2.32571	0.12103	-2.30038
C	1.63110	0.57846	-3.40029
N	0.33854	0.81817	-2.98621
C	3.78317	-0.25263	-2.17060
C	3.89379	-1.67327	-1.58589
C	4.46750	-0.20278	-3.54351
C	4.46872	0.74718	-1.21763
C	-0.73295	1.22936	-3.88020
C	-0.40296	-1.86369	3.28733
C	-0.36575	-2.59196	2.05655
C	-1.56608	-2.32944	1.34969
C	-2.37184	-1.42195	2.14002
C	-1.64646	-1.15274	3.34274
H	-2.14261	2.38961	0.54050
H	-1.09967	4.29334	-0.60575
H	-0.49563	3.24671	-1.91778
H	0.17823	3.08341	-0.29104
H	-2.96743	2.44346	-2.42502
H	-3.44741	3.57343	-1.14769
H	-3.95911	1.87284	-1.06420
H	-2.68462	0.23265	-2.35145
H	-4.52154	-1.00245	-1.53379
H	-4.04063	-0.02420	-0.12565
H	-3.60327	-1.74766	-0.21511
H	-1.01086	-1.43899	-2.94485
H	-1.33949	-2.39891	-1.49736
H	-2.58217	-2.26853	-2.76907
H	1.93496	0.76026	-4.42657
H	3.43840	-2.41300	-2.26520
H	4.95366	-1.93918	-1.43892
H	3.37560	-1.73221	-0.61508
H	3.99419	-0.90758	-4.24740
H	4.41804	0.81137	-3.97446
H	5.52937	-0.47805	-3.44332
H	5.52819	0.47374	-1.07993
H	4.42253	1.77067	-1.62556
H	3.97584	0.74300	-0.23246
H	-1.36157	0.37073	-4.16570
H	-1.35378	1.99307	-3.39935
H	-0.28655	1.66224	-4.78555
H	0.37339	-1.85527	4.04827
H	0.45766	-3.20947	1.70393
H	-1.83887	-2.76111	0.39424
H	-3.37132	-1.07200	1.90647
H	-1.97460	-0.50183	4.15046
C	-0.44485	1.72981	2.40612
C	0.67354	0.95575	2.77209
C	1.63946	0.54723	1.73490
H	-1.18193	1.98131	3.17229
H	-0.35153	2.43990	1.58875
H	0.83029	0.61773	3.79928
H	1.87480	1.33976	1.01230
H	1.12211	-0.20790	0.91973
C	2.86347	-0.22370	2.20882
H	3.38013	-0.69412	1.35984
H	2.57418	-1.00941	2.92475
H	3.56800	0.46210	2.70690

67			
aufaa aug51.fchk			
Ru	-0.75862	-0.55997	2.13876
P	-1.36365	0.26720	-0.03220
C	-2.01598	2.06434	0.00480
C	-0.98127	3.05729	-0.55358
C	-3.37934	2.30768	-0.65811
C	-2.61166	-0.72344	-1.04863
C	-3.95941	-1.03297	-0.37797
C	-1.96444	-2.00847	-1.58464
C	0.05411	0.32426	-1.19962
N	1.28792	0.08439	-0.77837
C	2.12132	0.21129	-1.86192
C	1.36455	0.53789	-2.96696
N	0.05372	0.61763	-2.54608
C	3.61374	0.01680	-1.73712
C	3.89412	-1.37362	-1.13566
C	4.27874	0.12941	-3.11592
C	4.18644	1.09861	-0.80011
C	-1.06327	0.88078	-3.44118
C	-1.06328	-1.65961	4.07553
C	-1.05466	-2.61906	3.01879
C	-2.11920	-2.32029	2.12478
C	-2.80323	-1.14765	2.63381
C	-2.14476	-0.74847	3.83707
H	-2.12572	2.24816	1.08399
H	-1.28644	4.08182	-0.28379
H	-0.93013	2.99905	-1.65176
H	0.03687	2.88540	-0.17503
H	-3.37917	2.05300	-1.72994
H	-3.61915	3.38133	-0.57932
H	-4.19498	1.75176	-0.17697
H	-2.82476	-0.05965	-1.89730
H	-4.69438	-1.26969	-1.16468
H	-4.35976	-0.19361	0.20620
H	-3.89839	-1.91050	0.27792
H	-1.09668	-1.80027	-2.22851
H	-1.61871	-2.65288	-0.75986
H	-2.70651	-2.57468	-2.17207
H	1.63292	0.72014	-4.00297
H	3.51236	-2.17086	-1.79491
H	4.97975	-1.51619	-1.00594
H	3.40570	-1.47326	-0.15253
H	3.88811	-0.63607	-3.80705
H	4.10511	1.12448	-3.55904
H	5.36652	-0.01600	-3.02130
H	5.27492	0.96272	-0.68728
H	3.99973	2.10753	-1.20374
H	3.72452	1.03388	0.19909
H	-1.56111	-0.05611	-3.73865
H	-1.79085	1.54287	-2.95565
H	-0.68036	1.38443	-4.33913
H	-0.36817	-1.62354	4.91031
H	-0.33062	-3.42201	2.89507
H	-2.38140	-2.89998	1.24705
H	-3.69374	-0.68761	2.22121
H	-2.41651	0.10120	4.45952
C	-0.02842	1.51714	2.54352
C	0.79803	0.51988	3.09242
C	1.60314	-0.33163	2.19326
H	-0.64354	2.12093	3.21421
H	0.25938	1.98524	1.60484
H	0.85212	0.34931	4.16997
H	2.09437	0.22663	1.38790
H	0.86932	-0.94193	1.43319
C	2.48969	-1.37263	2.85975
H	2.88302	-2.08707	2.12047
H	1.93595	-1.93188	3.63053
H	3.34606	-0.87287	3.34153

67			
auf73b auf73b.fchk			
Ru	-0.54578	-0.32972	1.69838
P	-1.19345	0.50515	-0.46388
C	-1.88360	2.28063	-0.46274
C	-0.77656	3.29203	-0.80036
C	-3.14995	2.54810	-1.28906
C	-2.44141	-0.46933	-1.49058
C	-3.73382	-0.81281	-0.73343
C	-1.81840	-1.70493	-2.15504
C	0.26167	0.50569	-1.59070
N	1.44921	0.08726	-1.16832
C	2.30330	0.13278	-2.24185
C	1.60711	0.58384	-3.34338
N	0.31487	0.82498	-2.92911
C	3.76116	-0.23927	-2.11188
C	3.87348	-1.65608	-1.51829
C	4.44337	-0.19784	-3.48614
C	4.44759	0.76702	-1.16641
C	-0.75768	1.23146	-3.82401
C	-0.41455	-1.82682	3.35727
C	-0.37838	-2.56016	2.12944
C	-1.58040	-2.30249	1.42370
C	-2.38625	-1.39307	2.21167
C	-1.65915	-1.11773	3.41199
H	-2.16507	2.41192	0.59221
H	-1.12406	4.31121	-0.56347
H	-0.51905	3.25867	-1.87034
H	0.15497	3.10402	-0.24284
H	-2.99030	2.45076	-2.37338
H	-3.47133	3.58635	-1.10141
H	-3.98122	1.88563	-1.00971
H	-2.70743	0.24052	-2.28745
H	-4.54207	-0.99201	-1.46108
H	-4.05989	-0.00637	-0.05854
H	-3.62132	-1.72992	-0.14005
H	-1.03310	-1.43239	-2.87527
H	-1.35869	-2.38574	-1.42283
H	-2.60343	-2.26241	-2.69319
H	1.90964	0.76024	-4.37099
H	3.41740	-2.40038	-2.19214
H	4.93372	-1.92048	-1.37133
H	3.35686	-1.70911	-0.54631
H	3.96938	-0.90742	-4.18476
H	4.39268	0.81349	-3.92352
H	5.50555	-0.47186	-3.38581
H	5.50738	0.49496	-1.02839
H	4.40037	1.78780	-1.58094
H	3.95608	0.76907	-0.18055
H	-1.38872	0.37199	-4.10147
H	-1.37588	2.00040	-3.34804
H	-0.31219	1.65611	-4.73368
H	0.36318	-1.81391	4.11673
H	0.44541	-3.17777	1.77787
H	-1.85417	-2.73844	0.47049
H	-3.38672	-1.04573	1.97844
H	-1.98690	-0.46400	4.21760
C	-0.46541	1.76313	2.46075
C	0.65507	0.99308	2.82875
C	1.62062	0.58191	1.79223
H	-1.20205	2.01648	3.22673
H	-0.37462	2.46981	1.64015
H	0.81378	0.65991	3.85724
H	1.85333	1.37161	1.06569
H	1.10401	-0.17824	0.98129
C	2.84689	-0.18412	2.26829
H	3.36352	-0.65748	1.42094
H	2.56014	-0.96704	2.98829
H	3.55054	0.50555	2.76226

67			
auf73a auf73a.fchk			
Ru	-0.44406	-0.46576	1.36875
P	-1.65824	0.64023	-0.32015
C	-2.59525	2.23279	-0.05918
C	-3.26695	2.78615	-1.32086
C	-3.61071	2.05012	1.08216
C	-2.59888	-0.34078	-1.61137
C	-3.88392	-0.93281	-1.01593
C	-1.69918	-1.41533	-2.23734
C	-0.03676	0.87426	-1.10918
N	0.81259	0.06224	-0.45411
C	1.91843	-0.10837	-1.26277
C	1.71348	0.64817	-2.40600
N	0.48060	1.24686	-2.30424
C	3.10790	-1.01338	-1.00083
C	2.71240	-2.12934	-0.02718
C	3.54834	-1.65045	-2.33469
C	4.29983	-0.21060	-0.43957
C	-0.16110	2.08674	-3.30805
C	0.05079	-1.98519	2.95305
C	-0.12821	-2.69397	1.73445
C	-1.44710	-2.45486	1.25062
C	-2.11076	-1.58874	2.20044
C	-1.18522	-1.29110	3.24125
H	-1.81796	2.93637	0.27770
H	-3.72500	3.76250	-1.09184
H	-4.06971	2.11684	-1.67071
H	-2.55179	2.93348	-2.14498
H	-4.44443	1.39909	0.77377
H	-4.03698	3.02988	1.35264
H	-3.14386	1.61220	1.97783
H	-2.87890	0.38590	-2.39257
H	-4.41849	-1.50463	-1.79240
H	-4.56459	-0.15171	-0.64444
H	-3.65796	-1.61822	-0.18426
H	-0.87584	-0.97219	-2.81852
H	-1.25127	-2.06059	-1.46684
H	-2.29987	-2.04433	-2.91460
H	2.34616	0.80163	-3.27407
H	1.94726	-2.78053	-0.48119
H	3.59568	-2.74135	0.21443
H	2.29858	-1.71275	0.89954
H	2.71993	-2.20809	-2.80128
H	3.90565	-0.88847	-3.04683
H	4.38069	-2.34779	-2.14853
H	5.17641	-0.87373	-0.35164
H	4.56219	0.61984	-1.11544
H	4.08543	0.20071	0.55481
H	0.40918	2.01548	-4.24350
H	-1.18695	1.73089	-3.48400
H	-0.18863	3.13616	-2.97704
H	0.95099	-1.97395	3.56043
H	0.63063	-3.28498	1.23082
H	-1.88937	-2.89788	0.36428
H	-3.13848	-1.23797	2.14692
H	-1.38333	-0.66708	4.10969
C	-0.20812	1.64670	2.00627
C	0.79876	0.90867	2.64265
C	2.26646	1.07565	2.33688
H	-1.09877	1.95460	2.55633
H	0.08948	2.30397	1.18281
H	0.59860	0.58466	3.66852
H	2.56295	2.07432	2.71217
H	2.41968	1.09858	1.24848
C	3.14649	0.02447	3.01532
H	4.21413	0.20559	2.81372
H	2.90431	-0.99228	2.67024
H	3.00263	0.05345	4.10916

67			
muf73 auf73.fchk			
Ru	-0.66574	-0.53731	1.95104
P	-1.52267	0.37550	-0.11233
C	-2.18479	2.15732	-0.06168
C	-1.09458	3.16115	-0.47143
C	-3.48806	2.42800	-0.82593
C	-2.79202	-0.58486	-1.12286
C	-4.02686	-0.98763	-0.30231
C	-2.17055	-1.78728	-1.84742
C	-0.06324	0.36530	-1.20917
N	1.08503	-0.09923	-0.72959
C	1.98713	-0.08843	-1.76641
C	1.35539	0.38891	-2.89765
N	0.05663	0.68019	-2.53826
C	3.42080	-0.52108	-1.57295
C	3.44660	-1.92349	-0.93625
C	4.15272	-0.54743	-2.92170
C	4.11796	0.47671	-0.62633
C	-0.97977	1.12077	-3.45805
C	-0.32901	-2.07129	3.52934
C	-0.38087	-2.76915	2.28050
C	-1.64058	-2.53345	1.67850
C	-2.39181	-1.64803	2.54551
C	-1.57738	-1.38619	3.70008
H	-2.39936	2.29479	1.00867
H	-1.41369	4.17977	-0.19566
H	-0.92829	3.14043	-1.55968
H	-0.12372	2.95830	0.00679
H	-3.36573	2.34308	-1.91765
H	-3.80669	3.46283	-0.61700
H	-4.30420	1.75701	-0.52179
H	-3.11661	0.13747	-1.88707
H	-4.85738	-1.22517	-0.98696
H	-4.36659	-0.18863	0.37586
H	-3.83029	-1.88671	0.29813
H	-1.43661	-1.47700	-2.60476
H	-1.64939	-2.46586	-1.15591
H	-2.96783	-2.35833	-2.35206
H	1.71035	0.55180	-3.91075
H	2.96561	-2.66363	-1.59738
H	4.48909	-2.23668	-0.76105
H	2.91258	-1.91784	0.02805
H	3.67208	-1.25362	-3.61915
H	4.16381	0.45294	-3.38624
H	5.19723	-0.86501	-2.77527
H	5.16050	0.16355	-0.44938
H	4.12677	1.48998	-1.06128
H	3.59587	0.51832	0.34229
H	-1.43954	0.26204	-3.97438
H	-1.75256	1.66374	-2.90344
H	-0.53937	1.79802	-4.20348
H	0.50941	-2.06143	4.22014
H	0.43373	-3.34094	1.83967
H	-1.98143	-2.95443	0.74017
H	-3.41211	-1.30788	2.39959
H	-1.85954	-0.76362	4.54677
C	-0.57614	1.56126	2.71275
C	0.49494	0.79887	3.19410
C	1.76624	0.64590	2.40049
H	-1.41722	1.79065	3.37158
H	-0.40033	2.26657	1.90313
H	0.50254	0.46236	4.23402
H	2.12927	1.63801	2.07445
H	1.53297	0.14307	1.42173
C	2.85749	-0.14306	3.12108
H	3.73780	-0.27403	2.47324
H	2.49270	-1.14399	3.40502
H	3.17930	0.37812	4.03799

67			
auf69b auf69b.fchk			
Ru	-0.48154	-0.47433	1.68845
P	-1.11052	0.14674	-0.43049
C	-1.85419	1.86990	-0.60480
C	-0.89938	2.92109	-0.02957
C	-2.31281	2.23928	-2.01819
C	-2.35259	-0.94602	-1.32327
C	-3.74376	-0.88044	-0.67947
C	-1.81492	-2.37876	-1.38756
C	0.23453	0.27311	-1.76546
N	1.49023	0.59512	-1.39453
C	2.36627	0.63210	-2.45542
C	1.60204	0.32154	-3.54541
N	0.29950	0.10561	-3.11115
C	3.82846	0.93250	-2.26772
C	4.43751	-0.15253	-1.35385
C	4.52837	0.93013	-3.63301
C	3.97446	2.31384	-1.59716
C	-0.77106	-0.25679	-4.04490
C	-0.79661	-0.71830	3.87503
C	-1.13058	-1.95422	3.22758
C	-2.23229	-1.72141	2.35745
C	-2.57436	-0.31942	2.46633
C	-1.70746	0.28987	3.41687
H	-2.73444	1.80173	0.05867
H	-1.38445	3.91109	-0.04001
H	0.01815	2.99510	-0.64078
H	-0.61435	2.66886	1.00227
H	-1.45041	2.29377	-2.70560
H	-2.78426	3.23609	-2.00834
H	-3.04872	1.52645	-2.42235
H	-2.46428	-0.54504	-2.33652
H	-4.45057	-1.45024	-1.30535
H	-4.11806	0.15319	-0.60751
H	-3.75359	-1.32652	0.32193
H	-0.84513	-2.43067	-1.91308
H	-1.65526	-2.76873	-0.36968
H	-2.53076	-3.03143	-1.91494
H	1.86914	0.23109	-4.59220
H	4.34944	-1.14984	-1.81447
H	5.50469	0.06525	-1.18963
H	3.93955	-0.17759	-0.36924
H	4.43762	-0.05327	-4.12330
H	4.10466	1.70106	-4.29766
H	5.59914	1.14574	-3.49702
H	5.04263	2.53697	-1.44842
H	3.53403	3.10729	-2.22245
H	3.48736	2.33271	-0.60673
H	-1.59715	0.45994	-3.96475
H	-0.35547	-0.21741	-5.05969
H	-1.12656	-1.27442	-3.83549
H	0.00299	-0.57315	4.59802
H	-0.62191	-2.90441	3.36867
H	-2.74753	-2.47465	1.76930
H	-3.38955	0.17915	1.94850
H	-1.72620	1.33100	3.72849
C	1.23990	0.86407	1.77820
C	1.63864	-0.51324	1.89526
C	1.32951	-1.53750	0.94810
H	1.34143	1.45413	2.69453
H	1.40434	1.50321	0.90725
H	1.93645	-0.85310	2.89298
H	1.75919	0.72988	-0.42315
H	1.44712	-1.35610	-0.11922
C	1.57828	-2.98158	1.32499
H	0.85275	-3.64925	0.83133
H	1.48801	-3.12781	2.41344
H	2.59058	-3.30976	1.02228

67			
auf69a auf69a.fchk			
Ru	-0.54446	-0.32178	1.67602
P	-1.08567	0.24926	-0.57848
C	-2.26922	1.71266	-0.53612
C	-1.46492	2.99832	-0.29951
C	-3.28979	1.87756	-1.67196
C	-1.93031	-1.12940	-1.53599
C	-3.22596	-1.61725	-0.88183
C	-0.94831	-2.29204	-1.73264
C	0.30998	0.62101	-1.71221
N	1.54209	0.27849	-1.34774
C	2.36774	0.50656	-2.41818
C	1.60958	0.99155	-3.46267
N	0.30582	1.05221	-3.02014
C	3.84964	0.22794	-2.34319
C	4.06670	-1.27174	-2.06069
C	4.52618	0.60526	-3.66809
C	4.45649	1.05316	-1.19203
C	-0.79120	1.55031	-3.83528
C	-1.13155	0.16172	3.73452
C	-1.12306	-1.26242	3.61046
C	-2.12283	-1.62875	2.64615
C	-2.73248	-0.43307	2.18000
C	-2.11541	0.68932	2.83235
H	-2.83716	1.49528	0.38047
H	-2.15326	3.84612	-0.14693
H	-0.82934	3.22788	-1.17165
H	-0.81456	2.90886	0.58485
H	-2.85582	2.38495	-2.54255
H	-4.11565	2.51215	-1.30939
H	-3.72426	0.92182	-2.00195
H	-2.17223	-0.69659	-2.52119
H	-3.72058	-2.34143	-1.54980
H	-3.93759	-0.79913	-0.68701
H	-3.00727	-2.13059	0.06678
H	-0.02052	-1.97287	-2.23212
H	-0.68198	-2.73566	-0.75760
H	-1.42325	-3.07749	-2.34326
H	1.87482	1.30203	-4.46851
H	3.63751	-1.89063	-2.86621
H	5.14533	-1.48896	-1.98989
H	3.59260	-1.56085	-1.10816
H	4.11395	0.01727	-4.50541
H	4.39007	1.67688	-3.89042
H	5.60720	0.40268	-3.60832
H	5.53319	0.83455	-1.09881
H	4.33435	2.13331	-1.37752
H	3.96282	0.80632	-0.23778
H	-1.69868	0.96130	-3.65768
H	-0.99842	2.60940	-3.61439
H	-0.51046	1.45428	-4.89297
H	-0.48200	0.75038	4.37903
H	-0.47649	-1.94777	4.15339
H	-2.36837	-2.63883	2.32740
H	-3.52330	-0.37700	1.43920
H	-2.38304	1.73533	2.71063
C	1.14341	1.14320	1.61426
C	1.51234	-0.11185	2.13726
C	1.55990	-1.31463	1.28275
H	1.04842	1.97320	2.31911
H	1.37256	1.39034	0.58169
H	1.71604	-0.23989	3.20482
H	1.95986	-1.09965	0.28419
H	0.41318	-1.61656	0.91103
C	2.07264	-2.58535	1.94579
H	1.86026	-3.47321	1.33058
H	1.61454	-2.72784	2.93769
H	3.16491	-2.51272	2.07582

67			
muf69 auf69.fchk			
Ru	-0.78788	-0.29682	2.16808
P	-1.40289	0.20587	-0.03496
C	-2.54895	1.70342	-0.07382
C	-1.74516	3.00146	0.08077
C	-3.59601	1.81088	-1.19164
C	-2.25606	-1.13543	-1.03688
C	-3.52167	-1.62892	-0.32634
C	-1.28697	-2.29770	-1.28763
C	0.04303	0.54369	-1.16843
N	1.28090	0.16175	-0.80837
C	2.16806	0.39247	-1.83025
C	1.44153	0.94012	-2.85879
N	0.12524	1.01989	-2.44097
C	3.62864	0.05210	-1.69196
C	3.76236	-1.46190	-1.42632
C	4.37246	0.43012	-2.97926
C	4.20632	0.83212	-0.49303
C	-0.94946	1.55267	-3.27122
C	-1.20505	-0.15240	4.33442
C	-1.18071	-1.53603	3.96978
C	-2.23953	-1.78051	3.03706
C	-2.89959	-0.52869	2.81087
C	-2.27032	0.48145	3.60890
H	-3.08930	1.53201	0.87221
H	-2.43806	3.85407	0.17325
H	-1.10565	3.18229	-0.80049
H	-1.10487	2.97359	0.97389
H	-3.17058	2.20043	-2.12561
H	-4.37036	2.52791	-0.87127
H	-4.09677	0.85579	-1.40648
H	-2.54099	-0.68029	-2.00059
H	-4.05486	-2.33789	-0.98067
H	-4.21570	-0.81145	-0.07521
H	-3.25312	-2.15533	0.60074
H	-0.40016	-1.98648	-1.86292
H	-0.94718	-2.72524	-0.32860
H	-1.80046	-3.09283	-1.85289
H	1.74252	1.28060	-3.84369
H	3.34904	-2.04792	-2.26376
H	4.82675	-1.72216	-1.31025
H	3.23538	-1.74599	-0.50001
H	3.97404	-0.12408	-3.84556
H	4.29131	1.51116	-3.18146
H	5.43989	0.18100	-2.87626
H	5.27129	0.57849	-0.36771
H	4.12223	1.91965	-0.65247
H	3.67487	0.57058	0.43711
H	-1.83892	0.91754	-3.18401
H	-1.19957	2.57923	-2.96583
H	-0.60997	1.55469	-4.31518
H	-0.52629	0.33602	5.02977
H	-0.46836	-2.27475	4.33045
H	-2.50412	-2.74075	2.60339
H	-3.74907	-0.37360	2.15122
H	-2.56657	1.52486	3.67809
C	0.68126	1.33999	2.02745
C	1.31640	0.12635	2.41567
C	1.38638	-1.04714	1.58876
H	0.60222	2.11449	2.79528
H	0.78700	1.72589	1.01587
H	1.71697	0.03893	3.43335
H	1.52892	-0.42874	0.19794
H	0.42979	-1.27546	0.99001
C	2.00325	-2.29462	2.18778
H	1.64748	-3.20224	1.67472
H	1.78409	-2.40320	3.26666
H	3.10160	-2.26500	2.07731

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auf67b auf67b.fchk

Ru	-0.54619	-0.20503	-1.73540
P	-1.03195	0.02574	0.58057
C	0.39634	0.33621	1.69168
N	0.50812	0.99187	2.90038
C	1.80488	0.80078	3.33021
C	2.44160	0.03396	2.37849
N	1.55116	-0.24231	1.37245
C	3.86828	-0.45825	2.33258
C	-0.47536	1.74618	3.67068
C	-1.74440	-1.55368	1.30142
C	-0.78863	-2.72643	1.05260
C	-2.08264	-1.41136	2.78963
C	-2.28631	1.34035	1.02670
C	-1.81905	2.70542	0.51338
C	-3.71136	1.01426	0.56300
C	4.57313	0.15829	1.10802
C	3.86877	-1.99313	2.20074
C	4.60990	-0.04761	3.61222
H	-2.31022	1.35175	2.12257
H	-2.67234	-1.72013	0.72746
H	2.15272	1.23279	4.26316
H	-0.62803	-2.88764	-0.02521
H	-1.21342	-3.64821	1.48297
H	0.19052	-2.53906	1.52265
H	-2.50976	-2.35547	3.16612
H	-2.81766	-0.61220	2.97582
H	-1.17089	-1.19938	3.37312
H	-1.81119	2.71487	-0.58753
H	-0.79907	2.94669	0.85598
H	-2.50157	3.49662	0.86549
H	-3.81291	1.07241	-0.52842
H	-4.40289	1.75610	0.99549
H	-4.04078	0.01774	0.89669
H	4.59193	1.25864	1.17880
H	4.05445	-0.12124	0.17646
H	5.61218	-0.20588	1.04870
H	4.90466	-2.36505	2.13604
H	3.38332	-2.46172	3.07298
H	3.32701	-2.30454	1.29270
H	5.64895	-0.41132	3.57634
H	4.63600	1.04980	3.72059
H	4.12627	-0.47781	4.50517
H	-0.85200	2.60334	3.09491
H	0.01823	2.12077	4.57697
H	-1.31366	1.09980	3.96943
C	-2.68483	-0.72096	-2.14548
C	-1.87575	-1.66731	-2.82465
C	-1.05525	-0.95650	-3.76752
C	-1.37472	0.43263	-3.66688
C	-2.36798	0.59651	-2.64586
H	-3.41043	-0.94956	-1.37055
H	-1.86691	-2.74069	-2.64898
H	-0.32561	-1.39982	-4.44161
H	-0.92215	1.23528	-4.24385
H	-2.84532	1.53033	-2.36602
C	1.67159	-0.96125	-1.58549
C	1.44450	0.35382	-2.22176
C	0.99832	1.45748	-1.47486
H	0.63572	-1.46821	-1.19766
H	2.05925	-1.71939	-2.27612
H	1.60517	0.45113	-3.29908
H	1.23276	1.47663	-0.41095
H	2.16913	-0.92127	-0.60934
C	0.77925	2.79348	-2.13714
H	0.55785	2.68151	-3.21046
H	-0.04785	3.34738	-1.66783
H	1.68616	3.41813	-2.04132

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auf67a auf67a.fchk

Ru	-0.61545	-0.15522	-1.69622
P	-1.11528	-0.04206	0.54084
C	0.30398	0.26577	1.76511
N	0.44082	0.86001	2.97820
C	1.76959	0.79685	3.38088
C	2.47753	0.15032	2.40645
N	1.54289	-0.15874	1.44471
C	3.93272	-0.19289	2.23849
C	-0.58198	1.50727	3.80545
C	-1.82955	-1.60817	1.30753
C	-0.89190	-2.79429	1.05882
C	-2.21211	-1.49337	2.78551
C	-2.31368	1.29541	1.09604
C	-1.78013	2.66484	0.66417
C	-3.73759	1.04236	0.58343
C	4.46672	0.53967	0.98875
C	4.06933	-1.71654	2.04144
C	4.70829	0.25150	3.48543
H	-2.36784	1.24540	2.18905
H	-2.74238	-1.75620	0.70372
H	2.09308	1.22145	4.32448
H	-0.66162	-2.89398	-0.01198
H	-1.36378	-3.72431	1.41644
H	0.05571	-2.66897	1.61313
H	-2.67527	-2.43485	3.12473
H	-2.93193	-0.68111	2.97308
H	-1.31495	-1.32946	3.40793
H	-1.66980	2.70008	-0.43152
H	-0.78692	2.87446	1.09891
H	-2.47298	3.46192	0.98223
H	-3.80709	1.14978	-0.50549
H	-4.41398	1.78661	1.03567
H	-4.10566	0.04206	0.86220
H	4.38561	1.63223	1.10837
H	3.91262	0.24584	0.08060
H	5.52683	0.28084	0.83892
H	5.13187	-1.97409	1.90890
H	3.68128	-2.26616	2.91427
H	3.52797	-2.05505	1.14091
H	5.77394	0.00506	3.36215
H	4.62499	1.34046	3.63685
H	4.33881	-0.26382	4.38740
H	-0.96004	2.40756	3.30298
H	-0.11183	1.79025	4.75570
H	-1.40287	0.80768	4.00286
C	-2.74971	-0.53970	-2.25206
C	-1.93525	-1.44634	-2.98785
C	-1.06150	-0.66426	-3.81293
C	-1.36707	0.72190	-3.60497
C	-2.41398	0.81164	-2.64476
H	-3.52813	-0.82304	-1.54850
H	-1.96428	-2.53113	-2.92647
H	-0.30426	-1.05554	-4.48873
H	-0.87521	1.56149	-4.08953
H	-2.90097	1.72559	-2.31879
C	1.12410	-1.44840	-1.44495
C	1.48843	-0.18470	-2.02865
C	1.21153	1.09267	-1.45117
H	1.35186	-1.76894	-0.42519
H	1.18528	-2.30503	-2.12358
H	1.72409	-0.18970	-3.09827
H	1.39116	1.26945	-0.39170
H	1.75925	-0.60228	0.55565
C	1.41175	2.33527	-2.29086
H	1.26071	2.11950	-3.36082
H	0.70145	3.12707	-2.00023
H	2.43243	2.74460	-2.16939

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auf67 auf67.fchk

Ru	-0.80262	-0.32102	-2.16120
P	-1.35356	-0.11037	0.09675
C	0.11087	0.11589	1.23714
N	0.25562	0.67919	2.47135
C	1.58489	0.58088	2.84401
C	2.25824	-0.05022	1.82844
N	1.32477	-0.32605	0.85973
C	3.71071	-0.40652	1.65186
C	-0.74842	1.33671	3.30937
C	-2.16192	-1.64351	0.81755
C	-1.26104	-2.86246	0.58209
C	-2.56244	-1.52538	2.29057
C	-2.48064	1.30326	0.57748
C	-1.82678	2.63996	0.21417
C	-3.85061	1.15531	-0.09580
C	4.26487	0.38257	0.44675
C	3.82609	-1.91779	1.36900
C	4.48958	-0.04440	2.92317
H	-2.63534	1.24305	1.66248
H	-3.07004	-1.75017	0.19846
H	1.93196	0.96844	3.79559
H	-1.04189	-2.99656	-0.48805
H	-1.75877	-3.77133	0.95799
H	-0.30482	-2.75378	1.12298
H	-3.09120	-2.44013	2.60548
H	-3.23189	-0.67113	2.47879
H	-1.66641	-1.42865	2.92713
H	-1.67657	2.70023	-0.87434
H	-0.84163	2.76739	0.69342
H	-2.47682	3.47342	0.52800
H	-3.76487	1.26407	-1.18593
H	-4.51995	1.95014	0.27205
H	-4.32415	0.18580	0.12846
H	4.19532	1.46871	0.62264
H	3.70804	0.13593	-0.47222
H	5.32407	0.12076	0.29198
H	4.88563	-2.18532	1.22869
H	3.42459	-2.50923	2.20834
H	3.27923	-2.18678	0.44976
H	5.55167	-0.30240	2.79123
H	4.42541	1.03624	3.13416
H	4.10699	-0.60003	3.79555
H	-1.06811	2.28256	2.85028
H	-0.29002	1.54389	4.28476
H	-1.61266	0.67800	3.45290
C	-2.90117	-0.77023	-2.74262
C	-2.08473	-1.83635	-3.21970
C	-1.13812	-1.27112	-4.14045
C	-1.39421	0.13085	-4.24739
C	-2.47783	0.45730	-3.36697
H	-3.71740	-0.86745	-2.03207
H	-2.16471	-2.88360	-2.93985
H	-0.35606	-1.81678	-4.66403
H	-0.84668	0.83249	-4.87121
H	-2.93575	1.43530	-3.24766
C	1.38227	-1.09576	-1.70832
C	1.28680	0.17588	-2.38316
C	0.66688	1.33499	-1.84421
H	0.44097	-1.45182	-1.15487
H	1.75697	-1.90813	-2.33952
H	1.66627	0.23205	-3.41042
H	0.75924	1.52407	-0.77481
H	1.55472	-0.76997	-0.21234
C	0.58121	2.58567	-2.68946
H	0.55111	2.33751	-3.76235
H	-0.32012	3.17498	-2.45602
H	1.45494	3.24091	-2.51558

67			
auf65b auf65b.fchk			
Ru	0.06064	-0.19709	-1.07514
P	-1.38676	0.50455	0.68587
C	0.17114	0.67605	1.60832
N	0.64096	0.88556	2.86070
C	1.88224	0.29036	2.92347
C	2.13180	-0.30429	1.69646
N	1.06126	-0.01562	0.87898
C	3.21357	-1.31439	1.38021
C	-0.04060	1.59087	3.93853
C	-2.22493	-0.94643	1.56356
C	-1.17452	-1.98961	1.97315
C	-3.08291	-0.55737	2.77402
C	-2.53398	1.94564	0.99989
C	-1.92206	3.33478	0.78968
C	-3.81874	1.74868	0.18058
C	3.72643	-1.19719	-0.06210
C	2.57898	-2.70989	1.58721
C	4.38988	-1.15468	2.35596
H	-2.78566	1.84691	2.06842
H	-2.87779	-1.37917	0.78479
H	2.48703	0.33260	3.82339
H	-0.48129	-2.22666	1.15608
H	-1.68253	-2.91397	2.29257
H	-0.57607	-1.61893	2.82173
H	-3.48584	-1.47232	3.23907
H	-3.93453	0.08424	2.50454
H	-2.47807	-0.03754	3.53687
H	-1.78067	3.55891	-0.27581
H	-0.95149	3.44109	1.30163
H	-2.61191	4.08930	1.20291
H	-3.60902	1.80726	-0.89990
H	-4.54186	2.54245	0.42944
H	-4.29726	0.77742	0.38720
H	4.36849	-0.31137	-0.17325
H	2.89374	-1.12026	-0.77666
H	4.32952	-2.08632	-0.30683
H	3.31700	-3.49540	1.35525
H	2.24702	-2.83531	2.63079
H	1.70324	-2.84309	0.93401
H	5.16656	-1.89907	2.12018
H	4.83603	-0.14996	2.27582
H	4.07387	-1.32086	3.39918
H	0.57557	2.43317	4.28785
H	-0.23268	0.90514	4.77808
H	-0.99461	1.97660	3.55535
C	-0.90412	-2.17342	-1.44943
C	0.49380	-2.35511	-1.64216
C	0.92917	-1.48654	-2.68487
C	-0.22908	-0.77252	-3.16563
C	-1.35981	-1.18856	-2.40783
H	-1.52298	-2.70801	-0.73477
H	1.13660	-3.00955	-1.05961
H	1.94295	-1.40100	-3.06656
H	-0.23675	-0.04578	-3.97272
H	-2.38300	-0.85007	-2.55081
C	2.64386	1.82885	-1.10829
C	1.37331	1.47157	-1.83578
C	0.13140	2.00621	-1.46776
H	2.49317	1.90017	-0.02122
H	3.44625	1.10929	-1.30822
H	1.51291	1.23993	-2.89657
H	0.13881	2.55816	-0.52349
H	2.98796	2.81595	-1.46998
C	-0.90116	2.47181	-2.47094
H	-0.76732	1.97427	-3.44243
H	-1.93145	2.28373	-2.13255
H	-0.79788	3.56053	-2.63668

67			
auf65a auf65a.fchk			
Ru	-0.49447	-0.14912	-1.75179
P	-0.98928	0.24161	0.53862
C	0.44260	0.34693	1.67468
N	0.55286	0.88261	2.94351
C	1.79823	0.51893	3.40963
C	2.40069	-0.23322	2.42319
N	1.54260	-0.32950	1.35706
C	3.75781	-0.89601	2.41640
C	-0.38380	1.68093	3.72975
C	-1.92376	-1.24558	1.22408
C	-0.99743	-2.47013	1.23834
C	-2.52758	-1.02886	2.61512
C	-2.06536	1.71245	0.96894
C	-1.34661	3.05778	0.79595
C	-3.37548	1.68468	0.17501
C	4.56943	-0.38356	1.21156
C	3.56613	-2.41969	2.28701
C	4.50845	-0.57649	3.71664
H	-2.30982	1.58149	2.03149
H	-2.73898	-1.41091	0.50026
H	2.14103	0.83398	4.39017
H	-0.49026	-2.61796	0.27360
H	-1.58556	-3.37208	1.47622
H	-0.21779	-2.35128	2.00697
H	-3.06162	-1.94266	2.92470
H	-3.24624	-0.19558	2.64715
H	-1.73037	-0.85025	3.35498
H	-1.30370	3.34756	-0.26131
H	-0.31630	3.04020	1.18533
H	-1.90582	3.84151	1.33345
H	-3.17621	1.78805	-0.90377
H	-4.01416	2.52719	0.48714
H	-3.94119	0.75367	0.34356
H	4.71058	0.70897	1.26694
H	4.05365	-0.62501	0.26821
H	5.56195	-0.86324	1.19497
H	4.54698	-2.92127	2.23803
H	3.01317	-2.81895	3.15370
H	3.00047	-2.65886	1.37184
H	5.49465	-1.06703	3.71020
H	4.66601	0.50959	3.82740
H	3.95135	-0.94228	4.59551
H	-0.58133	2.64887	3.25014
H	0.06900	1.86112	4.71354
H	-1.33074	1.14392	3.87532
C	-1.82501	-1.90539	-2.04891
C	-0.87681	-1.89129	-3.11931
C	-1.04667	-0.68704	-3.86395
C	-2.10065	0.06894	-3.24914
C	-2.58822	-0.68701	-2.13950
H	-1.97079	-2.70622	-1.33154
H	-0.13190	-2.65993	-3.31703
H	-0.46752	-0.38628	-4.73343
H	-2.46696	1.04064	-3.57051
H	-3.40844	-0.39485	-1.49254
C	1.84539	-0.03738	-1.66596
C	1.15180	0.98736	-2.47086
C	0.35391	1.96231	-1.84892
H	1.08207	-0.80053	-1.11261
H	2.47426	-0.71443	-2.25628
H	1.25187	0.96938	-3.55830
H	0.59845	2.23854	-0.82271
H	2.34027	0.32545	-0.75871
C	-0.35519	3.00152	-2.68367
H	-0.43289	2.67358	-3.73296
H	-1.37518	3.20265	-2.32020
H	0.19596	3.95872	-2.66336

67			
auf65 auf65.fchk			
Ru	-0.55861	-0.32285	-2.05953
P	-1.27829	0.18945	0.15228
C	0.19897	0.23987	1.21378
N	0.38744	0.68534	2.50027
C	1.65227	0.28169	2.86870
C	2.18743	-0.41269	1.80171
N	1.26726	-0.42613	0.78072
C	3.52511	-1.10754	1.69839
C	-0.48837	1.49347	3.34196
C	-2.27467	-1.25415	0.85439
C	-1.33969	-2.45369	1.07098
C	-3.05972	-0.96233	2.13742
C	-2.30353	1.69591	0.56146
C	-1.54024	3.02374	0.45466
C	-3.57814	1.68614	-0.29300
C	4.32228	-0.53275	0.51275
C	3.28524	-2.61198	1.46458
C	4.32193	-0.90687	2.99554
H	-2.59311	1.55566	1.61282
H	-2.99484	-1.48756	0.05256
H	2.05695	0.52755	3.84547
H	-0.67976	-2.63469	0.20957
H	-1.93926	-3.35920	1.26235
H	-0.69349	-2.27721	1.94586
H	-3.62560	-1.86487	2.42311
H	-3.78078	-0.13888	2.02370
H	-2.37690	-0.73370	2.97143
H	-1.44622	3.35393	-0.58621
H	-0.52757	2.95797	0.88270
H	-2.09546	3.80377	1.00149
H	-3.32993	1.74627	-1.36509
H	-4.20912	2.55312	-0.03741
H	-4.17408	0.77348	-0.12602
H	4.47635	0.55314	0.62899
H	3.79335	-0.71397	-0.43498
H	5.30905	-1.02111	0.45566
H	4.24987	-3.13431	1.35218
H	2.74334	-3.05873	2.31488
H	2.69012	-2.76823	0.55016
H	5.29124	-1.42460	2.92190
H	4.51795	0.16287	3.17955
H	3.77941	-1.31935	3.86267
H	-0.55049	2.52695	2.97045
H	-0.07409	1.50330	4.35881
H	-1.49639	1.06169	3.38015
C	-1.80423	-2.15751	-2.26617
C	-0.67338	-2.32498	-3.11602
C	-0.65711	-1.27976	-4.08441
C	-1.77888	-0.42175	-3.81949
C	-2.49499	-0.96582	-2.69592
H	-2.09520	-2.82112	-1.45973
H	0.08414	-3.10011	-3.01160
H	0.08750	-1.14410	-4.86412
H	-2.05373	0.47210	-4.37366
H	-3.41479	-0.56248	-2.27970
C	2.16388	0.36520	-2.33685
C	0.93641	1.00050	-2.94026
C	0.08565	1.85348	-2.23044
H	1.94353	-0.12176	-1.36305
H	2.60553	-0.37932	-3.01482
H	0.86276	1.00678	-4.03084
H	0.39911	2.17073	-1.23338
H	2.92563	1.13175	-2.10315
C	-0.86207	2.77130	-2.97192
H	-0.94616	2.46990	-4.02809
H	-1.87536	2.77930	-2.54320
H	-0.48550	3.80976	-2.94699

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73			
buf51b buf51b.fchk			
Ru	-0.32048	-0.59151	1.54198
P	-1.11002	-0.09001	-0.63769
C	-2.42369	1.25979	-0.67426
C	-3.74283	0.91658	0.02725
C	-1.85996	2.57150	-0.11184
C	-1.79450	-1.49890	-1.68160
C	-2.36057	-1.05598	-3.03446
C	-2.78741	-2.38862	-0.92286
C	0.19744	0.64335	-1.71228
N	1.46027	0.32486	-1.45580
C	2.24334	0.96018	-2.38441
C	1.43103	1.69440	-3.22080
N	0.13081	1.49398	-2.80262
C	3.74591	0.80805	-2.37908
C	4.30819	1.43934	-1.08950
C	4.10072	-0.69101	-2.40134
C	4.35703	1.50754	-3.60055
C	-0.99922	2.18551	-3.41611
C	-0.44876	-1.70770	3.47680
C	-1.43882	-2.23249	2.56608
C	-2.35906	-1.18230	2.28204
C	-1.92574	-0.00096	2.96076
C	-0.74668	-0.34547	3.72060
N	0.61997	1.20513	1.42116
C	1.20262	2.20065	1.32702
C	1.94464	3.44103	1.15373
H	-2.65342	1.39659	-1.73909
H	-4.45911	1.73639	-0.15019
H	-3.61044	0.82835	1.11376
H	-4.19824	-0.00832	-0.35154
H	-1.67676	2.47475	0.96944
H	-2.59069	3.38276	-0.26743
H	-0.91058	2.85718	-0.59194
H	-0.89197	-2.09651	-1.87228
H	-1.59159	-0.56415	-3.64871
H	-3.22184	-0.37713	-2.91693
H	-2.71261	-1.94222	-3.58851
H	-2.39956	-2.67765	0.06308
H	-3.76456	-1.90002	-0.79055
H	-2.95735	-3.30917	-1.50495
H	1.65125	2.33294	-4.07078
H	3.84028	0.98531	-0.20015
H	5.39778	1.28112	-1.03013
H	4.12030	2.52760	-1.07970
H	3.65676	-1.20586	-1.53468
H	3.71899	-1.16704	-3.31978
H	5.19528	-0.82000	-2.36941
H	5.45288	1.39539	-3.59025
H	3.97471	1.06931	-4.53728
H	4.12469	2.58623	-3.59829
H	-0.64697	2.65382	-4.34485
H	-1.80393	1.48362	-3.66549
H	-1.39079	2.96812	-2.74912
H	0.40105	-2.25599	3.87739
H	-1.49939	-3.25455	2.20298
H	-3.22773	-1.26444	1.63722
H	-2.42649	0.96337	2.95839
H	-0.16852	0.33119	4.34585
H	2.76728	3.26493	0.44161
H	1.27959	4.22598	0.75777
H	2.36318	3.77544	2.11667
C	1.83912	-1.19024	1.32749
C	1.14986	-2.31186	0.88151
C	1.23774	-2.85476	-0.52573
H	2.31509	-0.54733	0.58746
H	2.20260	-1.13414	2.35650
H	0.91294	-3.07873	1.62628
H	1.07420	-2.05697	-1.26122
H	2.28929	-3.16705	-0.67289
C	0.34092	-4.07369	-0.75192
H	0.63677	-4.89869	-0.08133
H	0.41957	-4.44080	-1.78815
H	-0.71534	-3.84573	-0.54732

73			
buf51a buf51a.fchk			
Ru	-0.46759	-0.13785	1.65860
P	-1.28558	-0.02619	-0.46506
C	-2.66078	1.21469	-0.77792
C	-3.97695	0.76496	-0.13070
C	-2.22442	2.58590	-0.24913
C	-1.79194	-1.59233	-1.38406
C	-2.49816	-1.34611	-2.72003
C	-2.59157	-2.52655	-0.46735
C	0.02336	0.60499	-1.66179
N	1.30351	0.29236	-1.39281
C	2.17718	0.85821	-2.29499
C	1.37982	1.55815	-3.16223
N	0.06094	1.38747	-2.76780
C	3.67108	0.64284	-2.28043
C	4.16193	0.39031	-0.84451
C	4.00463	-0.57953	-3.16376
C	4.36229	1.89092	-2.85479
C	-1.05791	2.01451	-3.47557
C	-0.42428	-0.74518	3.81148
C	-1.28059	-1.63556	3.07059
C	-2.37243	-0.86657	2.56873
C	-2.21961	0.49684	3.00845
C	-1.00837	0.55746	3.75352
N	0.82482	1.36204	1.35693
C	1.59697	2.22815	1.26553
C	2.55286	3.32616	1.16754
H	-2.82972	1.26186	-1.86212
H	-4.74566	1.53718	-0.30170
H	-3.86562	0.63476	0.95437
H	-4.34440	-0.17810	-0.56170
H	-2.06097	2.53098	0.83884
H	-3.00283	3.33885	-0.45854
H	-1.27700	2.92633	-0.70172
H	-0.81875	-2.07185	-1.57338
H	-1.85724	-0.78608	-3.42063
H	-3.44596	-0.79836	-2.58957
H	-2.73539	-2.31222	-3.19636
H	-2.06273	-2.69049	0.48229
H	-3.59376	-2.12679	-0.24427
H	-2.72274	-3.49963	-0.96935
H	1.63537	2.16057	-4.02681
H	3.73652	-0.53528	-0.42441
H	5.25694	0.27872	-0.85052
H	3.90118	1.22810	-0.17762
H	3.49877	-1.48656	-2.79749
H	3.69423	-0.40303	-4.20622
H	5.09213	-0.75811	-3.14770
H	5.45188	1.73249	-2.86942
H	4.03799	2.08738	-3.89005
H	4.14674	2.78327	-2.24372
H	-0.66205	2.47126	-4.39154
H	-1.80618	1.25913	-3.74378
H	-1.51877	2.78850	-2.84753
H	0.49500	-1.01398	4.32510
H	-1.13299	-2.70393	2.93286
H	-3.20129	-1.25990	1.98747
H	-2.90612	1.31908	2.82769
H	-0.57855	1.45848	4.18740
H	2.85862	3.46949	0.11775
H	2.10121	4.26235	1.53622
H	3.45062	3.10555	1.76866
C	1.19185	-1.50307	1.22032
C	0.92202	-2.61067	0.27099
C	1.57480	-2.87390	-0.87551
H	2.12650	-0.97022	0.94621
H	1.39190	-1.91623	2.22296
H	0.06904	-3.25469	0.52255
H	1.54372	-0.25943	-0.56609
H	2.44905	-2.26162	-1.13323
C	1.20186	-3.95474	-1.85035
H	2.03201	-4.66582	-2.01304
H	0.94705	-3.53861	-2.84527
H	0.33025	-4.52623	-1.48893

73			
an51 buf51.fchk			
Ru	-0.73813	-0.24123	2.35102
P	-1.44231	-0.07911	0.14264
C	-2.83044	1.15580	-0.14507
C	-4.18771	0.69448	0.40031
C	-2.42798	2.51476	0.44283
C	-1.94791	-1.62630	-0.80261
C	-2.62584	-1.33129	-2.14440
C	-2.76651	-2.58174	0.07380
C	-0.14406	0.57149	-1.04328
N	1.11104	0.12431	-0.89262
C	1.94595	0.77369	-1.77946
C	1.16261	1.64952	-2.48633
N	-0.13899	1.51246	-2.03709
C	3.43320	0.52550	-1.87611
C	4.05283	0.55100	-0.46591
C	3.70261	-0.84117	-2.53766
C	4.07571	1.62626	-2.73541
C	-1.24598	2.21884	-2.68607
C	-0.87773	-0.70712	4.52902
C	-1.72726	-1.60248	3.77880
C	-2.73158	-0.82239	3.14222
C	-2.52312	0.56162	3.49354
C	-1.37741	0.61323	4.34039
N	0.65402	1.17618	2.02399
C	1.45851	2.00336	1.89589
C	2.45087	3.05976	1.73637
H	-2.94583	1.23855	-1.23257
H	-4.94487	1.45976	0.15930
H	-4.17552	0.57382	1.49021
H	-4.51353	-0.25242	-0.05384
H	-2.35318	2.44685	1.53744
H	-3.18164	3.27752	0.18358
H	-1.44425	2.85376	0.07856
H	-0.97557	-2.10254	-1.00257
H	-1.99688	-0.68610	-2.78055
H	-3.60349	-0.84209	-2.00518
H	-2.79842	-2.27277	-2.69221
H	-2.26789	-2.75776	1.03938
H	-3.77501	-2.18775	0.27639
H	-2.88389	-3.54793	-0.44482
H	1.41139	2.35322	-3.27322
H	3.57073	-0.18430	0.19654
H	5.12705	0.31391	-0.52811
H	3.94590	1.54952	-0.01302
H	3.30946	-1.66786	-1.93216
H	3.24018	-0.88891	-3.53704
H	4.78970	-0.98477	-2.65034
H	5.16329	1.46337	-2.78983
H	3.67994	1.60934	-3.76438
H	3.89571	2.62558	-2.30506
H	-0.82834	2.79286	-3.52322
H	-1.97464	1.49810	-3.08169
H	-1.74243	2.90782	-1.99248
H	-0.01559	-0.98755	5.12826
H	-1.62728	-2.68377	3.71928
H	-3.53481	-1.21609	2.52687
H	-3.15155	1.40206	3.21631
H	-0.93314	1.51970	4.74698
H	2.54984	3.32161	0.67049
H	2.14515	3.95608	2.30082
H	3.43077	2.71993	2.10864
C	0.96658	-1.72096	2.27307
C	0.80232	-2.46444	1.07266
C	1.60720	-2.38349	-0.06693
H	1.92520	-1.19146	2.35884
H	0.72009	-2.29056	3.17595
H	-0.09224	-3.09884	1.01749
H	1.32700	-1.03675	-0.40554
H	2.65715	-2.12547	0.13287
C	1.34923	-3.27205	-1.27314
H	2.12879	-4.04434	-1.38936
H	1.32100	-2.69749	-2.21706
H	0.38193	-3.79427	-1.17440

73			
buf53b buf53b.fchk			
Ru	-0.72304	-0.14020	1.57700
P	-1.23524	0.07592	-0.63839
C	-2.38403	1.48424	-1.11108
C	-3.81268	1.21784	-0.62084
C	-1.83501	2.79364	-0.53388
C	-1.81850	-1.41595	-1.63228
C	-2.33820	-1.09670	-3.03652
C	-2.81651	-2.25167	-0.82138
C	0.29356	0.54473	-1.63066
N	1.48082	0.14913	-1.14198
C	2.53253	0.59620	-1.91185
C	1.94788	1.30180	-2.92985
N	0.57219	1.26099	-2.74656
C	3.97878	0.35268	-1.56510
C	4.30157	1.10173	-0.25526
C	4.23007	-1.15292	-1.35984
C	4.86592	0.88364	-2.70019
C	-0.36134	1.97363	-3.62141
C	-1.44890	0.53553	3.62265
C	-1.04034	-0.82977	3.68543
C	-1.88770	-1.57739	2.79157
C	-2.80317	-0.65686	2.19716
C	-2.54787	0.65803	2.72349
N	0.69665	1.27437	1.52411
C	1.49013	2.11941	1.63221
C	2.44987	3.20376	1.81049
H	-2.41565	1.53826	-2.20795
H	-4.45594	2.06995	-0.89737
H	-3.84343	1.11173	0.47229
H	-4.23952	0.31060	-1.07401
H	-1.79310	2.72765	0.56530
H	-2.48668	3.63687	-0.81832
H	-0.81177	3.00823	-0.88853
H	-0.89572	-2.00901	-1.71573
H	-1.55098	-0.65798	-3.67039
H	-3.20286	-0.41317	-3.01486
H	-2.66486	-2.02935	-3.52647
H	-2.40914	-2.49023	0.17071
H	-3.78070	-1.73409	-0.69120
H	-3.01150	-3.19544	-1.35725
H	2.39055	1.83048	-3.76651
H	3.66374	0.74434	0.57025
H	5.35332	0.92343	0.02067
H	4.15045	2.18653	-0.37719
H	3.65631	-1.54199	-0.50355
H	3.95584	-1.72976	-2.25747
H	5.29897	-1.31662	-1.15081
H	5.92430	0.72059	-2.44547
H	4.65432	0.35903	-3.64617
H	4.71485	1.96548	-2.85196
H	0.19575	2.31299	-4.50402
H	-1.16990	1.30632	-3.93991
H	-0.78256	2.84115	-3.09438
H	-0.97441	1.35778	4.15520
H	-0.23578	-1.23054	4.29636
H	-1.85677	-2.65068	2.62224
H	-3.58711	-0.91890	1.49312
H	-3.09969	1.56697	2.50100
H	3.43019	2.80285	2.11462
H	2.57552	3.76355	0.86933
H	2.09069	3.89720	2.58915
C	0.85094	-1.65172	1.31060
C	0.48418	-2.78654	0.42800
C	1.05783	-3.16224	-0.72918
H	1.85906	-1.25605	1.05473
H	0.97140	-2.01112	2.34571
H	-0.39687	-3.35636	0.75289
H	1.52801	-0.38857	-0.26854
H	1.94283	-2.62532	-1.08850
C	0.55642	-4.28142	-1.59892
H	1.33251	-5.04978	-1.76756
H	0.25602	-3.91718	-2.60183
H	-0.31870	-4.77414	-1.14248

73			
buf53a buf53a.fchk			
Ru	-0.77270	-0.07963	1.67731
P	-1.16616	0.21056	-0.63684
C	-2.41370	1.53753	-1.05567
C	-3.84367	1.17151	-0.64136
C	-1.97011	2.85831	-0.41356
C	-1.62328	-1.33081	-1.60649
C	-2.03858	-1.02153	-3.04835
C	-2.63871	-2.22474	-0.88778
C	0.36931	0.73257	-1.50627
N	1.51724	0.24621	-1.04794
C	2.51256	0.71481	-1.86937
C	1.94799	1.50946	-2.84451
N	0.58575	1.51809	-2.61940
C	3.96338	0.36303	-1.63640
C	4.41138	0.95203	-0.28408
C	4.11285	-1.16889	-1.58793
C	4.83765	0.93435	-2.76084
C	-0.35454	2.26006	-3.45251
C	-1.52491	0.47022	3.68649
C	-1.14032	-0.89155	3.72343
C	-1.94046	-1.60404	2.74676
C	-2.82560	-0.67393	2.13919
C	-2.54750	0.63647	2.68277
N	0.57043	1.44489	1.59777
C	1.36581	2.28402	1.52765
C	2.37343	3.32713	1.39942
H	-2.40476	1.63694	-2.14942
H	-4.52539	1.98255	-0.94767
H	-3.93211	1.05814	0.44806
H	-4.18851	0.24407	-1.12203
H	-1.99089	2.77071	0.68453
H	-2.65036	3.67190	-0.71603
H	-0.94301	3.13324	-0.70468
H	-0.66090	-1.86817	-1.61677
H	-1.24319	-0.48373	-3.58767
H	-2.96417	-0.42288	-3.08656
H	-2.22937	-1.96404	-3.58844
H	-2.29950	-2.46758	0.12849
H	-3.63496	-1.75838	-0.82549
H	-2.74713	-3.16756	-1.44938
H	2.38109	2.06155	-3.67288
H	3.75032	0.60027	0.52552
H	5.44476	0.64165	-0.05628
H	4.38239	2.05428	-0.31330
H	3.49751	-1.58560	-0.77565
H	3.78870	-1.62478	-2.53817
H	5.16617	-1.44081	-1.40881
H	5.89457	0.67967	-2.58289
H	4.54330	0.51886	-3.73883
H	4.75491	2.03352	-2.80855
H	0.20606	2.70677	-4.28431
H	-1.12233	1.59238	-3.86767
H	-0.84121	3.06288	-2.87999
H	-1.07503	1.27256	4.26785
H	-0.36694	-1.32172	4.35565
H	-1.88824	-2.66903	2.53338
H	-3.56415	-0.90772	1.37942
H	-3.07708	1.55725	2.45497
H	3.27682	3.04710	1.96436
H	2.64339	3.43966	0.33736
H	1.98389	4.28237	1.78694
C	1.15668	-1.96371	1.30657
C	0.53737	-3.06850	0.51080
C	1.05874	-3.57296	-0.61396
H	2.22517	-1.83156	1.07672
H	1.03493	-2.08683	2.38929
H	-0.42788	-3.44861	0.86261
H	0.78089	-0.95392	0.93075
H	2.01696	-3.17771	-0.97229
C	0.40488	-4.63273	-1.44939
H	1.06095	-5.51362	-1.56595
H	0.20338	-4.25667	-2.47035
H	-0.54852	-4.96422	-1.00576

73			
an53 buf53.fchk			
Ru	-0.81460	-0.06984	2.01639
P	-1.45913	0.13693	-0.20206
C	-2.59995	1.55380	-0.62785
C	-4.00575	1.30600	-0.06606
C	-2.01330	2.86342	-0.08835
C	-2.08655	-1.37240	-1.12890
C	-2.64759	-1.05914	-2.51924
C	-3.06042	-2.20546	-0.28785
C	0.09112	0.54163	-1.12181
N	1.21370	0.12120	-0.53865
C	2.29399	0.56617	-1.26768
C	1.79056	1.27991	-2.33216
N	0.41030	1.25352	-2.23618
C	3.72822	0.30836	-0.87309
C	3.95459	0.82673	0.56111
C	4.03308	-1.20123	-0.92458
C	4.66649	1.04689	-1.83943
C	-0.48346	1.96654	-3.14493
C	-1.37217	0.43221	4.13650
C	-1.00394	-0.93508	4.08961
C	-1.90103	-1.60677	3.17659
C	-2.82955	-0.63570	2.69648
C	-2.49785	0.64168	3.26749
N	0.41189	1.53169	1.88124
C	1.10933	2.45937	1.88868
C	1.98513	3.62455	1.90569
H	-2.67032	1.59930	-1.72495
H	-4.66013	2.15420	-0.32719
H	-3.98027	1.22384	1.03118
H	-4.45777	0.39030	-0.47639
H	-1.94824	2.82169	1.01057
H	-2.65953	3.71001	-0.37444
H	-0.99742	3.05205	-0.47364
H	-1.16349	-1.96296	-1.23583
H	-1.88614	-0.60171	-3.17036
H	-3.52343	-0.39123	-2.47073
H	-2.97006	-1.99645	-3.00273
H	-2.61009	-2.47796	0.67639
H	-4.00826	-1.67509	-0.09988
H	-3.29977	-3.13345	-0.83308
H	2.28852	1.80067	-3.14346
H	3.26406	0.34516	1.27178
H	4.98787	0.60968	0.87711
H	3.80080	1.91748	0.60670
H	3.42604	-1.75774	-0.19551
H	3.83257	-1.60921	-1.92862
H	5.09536	-1.37043	-0.68439
H	5.71293	0.87645	-1.54247
H	4.54089	0.67959	-2.87139
H	4.47739	2.13343	-1.82679
H	0.08365	2.23349	-4.04636
H	-1.32606	1.32623	-3.43154
H	-0.86648	2.88190	-2.66918
H	-0.85487	1.20667	4.69938
H	-0.17790	-1.39205	4.62948
H	-1.90115	-2.66762	2.94096
H	-3.65003	-0.83072	2.01314
H	-3.03715	1.57410	3.12466
H	2.90423	3.39724	2.46983
H	2.26173	3.90148	0.87556
H	1.47322	4.47698	2.38174
C	0.95051	-1.61637	1.52994
C	0.40808	-2.78137	0.77444
C	0.84120	-3.24552	-0.40869
H	2.03220	-1.48634	1.33866
H	0.91527	-1.78059	2.61268
H	-0.48092	-3.25498	1.20876
H	0.98849	-0.52289	0.61282
H	1.71692	-2.78283	-0.87685
C	0.18343	-4.36417	-1.16598
H	0.88564	-5.19548	-1.35743
H	-0.17328	-4.02409	-2.15792
H	-0.68134	-4.76568	-0.61095

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73			
duf73b duf73b.fchk			
Ru	-0.60755	-0.33944	1.63671
P	-1.44842	0.17842	-0.40868
C	-2.73975	1.53722	-0.54422
C	-4.06007	1.17489	0.14770
C	-2.15759	2.83359	0.03392
C	-2.08923	-1.26880	-1.43826
C	-2.70104	-0.88576	-2.78819
C	-3.03521	-2.15094	-0.61146
C	-0.17304	0.82057	-1.65251
N	1.09479	0.37104	-1.57397
C	1.88958	0.89338	-2.57467
C	1.06715	1.72181	-3.28542
N	-0.19659	1.66588	-2.71584
C	3.33347	0.51527	-2.77245
C	4.11097	0.76233	-1.46615
C	3.40254	-0.97819	-3.15637
C	3.93166	1.36580	-3.90213
C	-1.32044	2.42728	-3.26859
C	-0.86831	0.45301	3.74011
C	-0.53660	-0.94677	3.78156
C	-1.60257	-1.65044	3.12917
C	-2.55757	-0.69934	2.67261
C	-2.11101	0.61592	3.07826
N	1.12686	0.63745	1.42537
C	2.13900	1.20794	1.49085
C	3.40546	1.91083	1.65565
H	-2.96637	1.66743	-1.60978
H	-4.75861	2.02205	0.04195
H	-3.91964	0.98943	1.22005
H	-4.53435	0.29149	-0.30294
H	-1.94361	2.70364	1.10620
H	-2.87907	3.65920	-0.08708
H	-1.20993	3.12370	-0.45146
H	-1.16327	-1.84570	-1.61050
H	-1.97538	-0.36531	-3.43427
H	-3.58830	-0.24326	-2.65811
H	-3.02710	-1.79350	-3.32320
H	-2.62113	-2.35099	0.38711
H	-4.02431	-1.68234	-0.49183
H	-3.18312	-3.11139	-1.13244
H	1.26919	2.34334	-4.15025
H	3.68701	0.17430	-0.63738
H	5.16117	0.45779	-1.60087
H	4.08983	1.83115	-1.19878
H	2.94082	-1.61205	-2.38411
H	2.88492	-1.15714	-4.11266
H	4.45594	-1.28169	-3.26723
H	4.98617	1.08693	-4.05055
H	3.39875	1.19611	-4.85220
H	3.89013	2.43999	-3.65707
H	-0.96235	2.94030	-4.17016
H	-2.13824	1.74946	-3.54220
H	-1.67373	3.17059	-2.54311
H	-0.25254	1.25967	4.13330
H	0.33764	-1.39096	4.25004
H	-1.65524	-2.72559	2.97491
H	-3.48876	-0.93601	2.16628
H	-2.63662	1.55399	2.92546
H	3.45624	2.35243	2.66484
H	4.24581	1.20892	1.53051
H	3.50315	2.71637	0.91079
C	0.26228	-2.21979	0.88700
C	1.44344	-2.20190	-0.00624
C	2.73296	-2.03478	0.36570
H	0.52627	-2.72850	1.82687
H	-0.54718	-2.79071	0.40951
H	1.25656	-2.36974	-1.07766
H	1.40797	-0.30288	-0.85663
H	3.51518	-2.09955	-0.39710
C	3.18811	-1.85736	1.78726
H	3.99323	-1.10414	1.86350
H	3.60663	-2.80027	2.18690
H	2.35496	-1.54984	2.43701

73			
duf73a duf73a.fchk			
Ru	-0.64042	-0.49685	1.56993
P	-1.45023	0.25026	-0.51686
C	-2.67369	1.65935	-0.41204
C	-4.01753	1.27218	0.21698
C	-2.02439	2.82754	0.34186
C	-2.20767	-1.07887	-1.61146
C	-2.93180	-0.49125	-2.82765
C	-3.07577	-2.08336	-0.84684
C	-0.13694	0.86724	-1.65117
N	1.00790	0.19023	-1.67991
C	1.75915	0.71686	-2.70581
C	1.05165	1.74051	-3.29610
N	-0.15407	1.83698	-2.63436
C	3.12621	0.18707	-3.07430
C	4.11670	0.47737	-1.92960
C	3.02921	-1.33218	-3.31078
C	3.63099	0.86761	-4.35537
C	-1.17990	2.80266	-3.01616
C	-0.94745	-0.26751	3.75078
C	-0.71256	-1.63874	3.49162
C	-1.74481	-2.10545	2.58842
C	-2.62439	-1.02209	2.32965
C	-2.11293	0.14746	3.00918
N	0.87881	0.83735	1.43827
C	1.85225	1.45393	1.32494
C	3.08747	2.20469	1.16727
H	-2.87979	1.95539	-1.44835
H	-4.70374	2.13269	0.14659
H	-3.91270	1.02306	1.28126
H	-4.49010	0.42434	-0.30066
H	-1.84013	2.54600	1.39059
H	-2.69140	3.70566	0.32443
H	-1.05421	3.11488	-0.09542
H	-1.30275	-1.60609	-1.96121
H	-2.26603	0.15948	-3.41595
H	-3.82014	0.08788	-2.52525
H	-3.27306	-1.30651	-3.48707
H	-2.52126	-2.52524	-0.00625
H	-3.99536	-1.62002	-0.45489
H	-3.37947	-2.89382	-1.53005
H	1.29087	2.40508	-4.12015
H	3.74527	0.06956	-0.97801
H	5.09781	0.02430	-2.15020
H	4.26277	1.56684	-1.82132
H	2.59318	-1.83666	-2.43562
H	2.38661	-1.54548	-4.18110
H	4.03023	-1.75163	-3.50522
H	4.62388	0.47204	-4.62255
H	2.94681	0.67941	-5.19913
H	3.72553	1.95786	-4.21591
H	-0.77576	3.42161	-3.82807
H	-2.08394	2.29436	-3.38289
H	-1.44279	3.45565	-2.17337
H	-0.31723	0.38285	4.35391
H	0.10968	-2.23250	3.88355
H	-1.84494	-3.11647	2.20033
H	-3.51113	-1.06429	1.70687
H	-2.57582	1.12940	3.04423
H	3.82179	1.87160	1.91852
H	3.49115	2.01509	0.16050
H	2.89965	3.28285	1.29630
C	1.25068	-2.27671	0.65954
C	2.67891	-1.83860	0.55590
C	3.43784	-1.37620	1.56075
H	0.99181	-2.64980	1.65573
H	1.00916	-3.05609	-0.07919
H	3.12463	-1.90611	-0.43737
H	0.57814	-1.42506	0.30043
H	4.47797	-1.11854	1.32901
C	3.00764	-1.19237	2.98821
H	3.36493	-0.22551	3.38619
H	3.44340	-1.97440	3.63709
H	1.91337	-1.21911	3.09106

73			
duf73 duf73.fchk			
Ru	-0.73588	-0.62814	1.82808
P	-1.75051	0.07894	-0.10719
C	-2.88351	1.56173	0.01113
C	-4.16511	1.25040	0.79390
C	-2.11507	2.71887	0.66282
C	-2.60391	-1.21351	-1.17882
C	-3.32670	-0.62477	-2.39469
C	-3.51120	-2.14980	-0.37177
C	-0.44471	0.64754	-1.28269
N	0.73630	0.02456	-1.19779
C	1.56377	0.50335	-2.19950
C	0.84950	1.45719	-2.88293
N	-0.40424	1.53943	-2.30873
C	2.96436	0.01288	-2.47242
C	3.88737	0.39796	-1.29844
C	2.92458	-1.51414	-2.68725
C	3.50194	0.67518	-3.75196
C	-1.42798	2.48427	-2.75301
C	-0.86065	-0.60378	4.07207
C	-0.67457	-1.94728	3.66392
C	-1.78266	-2.31599	2.81499
C	-2.65660	-1.19074	2.74220
C	-2.08312	-0.10991	3.49724
N	0.66418	0.82853	1.72738
C	1.60617	1.50464	1.72656
C	2.82307	2.30419	1.74203
H	-3.17331	1.83214	-1.01404
H	-4.80543	2.14794	0.80866
H	-3.93637	0.98568	1.83617
H	-4.74302	0.43207	0.33878
H	-1.83867	2.45125	1.69511
H	-2.74679	3.62243	0.68667
H	-1.18209	2.95694	0.12549
H	-1.74201	-1.80788	-1.53096
H	-2.63277	-0.08082	-3.05404
H	-4.14112	0.05430	-2.09176
H	-3.77591	-1.43872	-2.98770
H	-2.95913	-2.62217	0.45172
H	-4.38484	-1.62232	0.04334
H	-3.88923	-2.94355	-1.03712
H	1.12314	2.07844	-3.72883
H	3.50667	0.02545	-0.33757
H	4.89239	-0.02485	-1.46136
H	3.98454	1.49668	-1.24748
H	2.41140	-2.03093	-1.86439
H	2.38818	-1.75025	-3.62115
H	3.94985	-1.91015	-2.76581
H	4.51851	0.30412	-3.95515
H	2.86863	0.43561	-4.62176
H	3.55657	1.77115	-3.64200
H	-1.05149	2.99252	-3.65012
H	-2.35696	1.95810	-3.00586
H	-1.62818	3.22962	-1.97098
H	-0.16798	-0.02548	4.67978
H	0.17649	-2.57532	3.91393
H	-1.95013	-3.29183	2.36639
H	-3.59836	-1.15979	2.20391
H	-2.52557	0.86766	3.66803
H	3.47131	1.96515	2.56688
H	3.35993	2.16484	0.79039
H	2.58773	3.37173	1.88109
C	0.97080	-1.96763	0.68859
C	2.44735	-1.85599	0.89728
C	3.17192	-1.53289	1.98626
H	0.51514	-2.54023	1.50808
H	0.76122	-2.58110	-0.20511
H	3.04548	-2.06027	0.00537
H	0.79197	-0.81984	-0.21471
H	4.26083	-1.53906	1.86043
C	2.68163	-1.22060	3.37119
H	3.30814	-0.44504	3.84740
H	2.74365	-2.11058	4.02728
H	1.64111	-0.87810	3.36454

73			
duf71b duf71b.fchk			
Ru	-0.46389	-0.55517	1.76544
P	-1.16825	-0.02350	-0.47450
C	-2.55714	1.24496	-0.64140
C	-3.92633	0.92776	-0.02330
C	-2.06042	2.63470	-0.21731
C	-1.75149	-1.55080	-1.41654
C	-2.30625	-1.26236	-2.81433
C	-2.71606	-2.42571	-0.60351
C	0.05571	0.72528	-1.65743
N	1.35627	0.49000	-1.50808
C	2.00742	1.07846	-2.56518
C	1.07854	1.70284	-3.36349
N	-0.16169	1.48044	-2.80872
C	3.49062	0.92632	-2.81773
C	4.27856	1.13637	-1.51614
C	3.74365	-0.49718	-3.35651
C	3.95888	1.94771	-3.86563
C	-1.35832	2.03998	-3.43826
C	-0.85916	-0.93208	3.95160
C	-1.82174	-1.64164	3.13674
C	-2.57927	-0.68437	2.41948
C	-2.07687	0.62987	2.76334
C	-1.03558	0.45583	3.71786
N	1.19099	0.59093	1.56398
C	2.10762	1.29763	1.55387
C	3.25480	2.19380	1.54076
H	-2.73257	1.25620	-1.72145
H	-4.66535	1.61791	-0.46400
H	-3.95541	1.08397	1.06140
H	-4.26224	-0.09514	-0.24079
H	-1.82321	2.66678	0.85640
H	-2.84398	3.38522	-0.41640
H	-1.14890	2.93047	-0.75912
H	-0.80856	-2.10681	-1.53267
H	-1.55854	-0.76316	-3.44846
H	-3.21717	-0.64169	-2.76947
H	-2.57997	-2.21255	-3.30272
H	-2.37510	-2.55564	0.43336
H	-3.73320	-2.00403	-0.58680
H	-2.78514	-3.41996	-1.07522
H	1.18338	2.28099	-4.27587
H	3.91886	0.45261	-0.73428
H	5.35031	0.94543	-1.68981
H	4.16680	2.17512	-1.16414
H	3.35478	-1.25279	-2.65809
H	3.24000	-0.63480	-4.32767
H	4.82473	-0.66651	-3.49660
H	5.03983	1.83051	-4.04383
H	3.44227	1.79618	-4.82801
H	3.77205	2.98016	-3.52577
H	-1.05289	2.48126	-4.39615
H	-2.10210	1.26063	-3.64495
H	-1.80580	2.82919	-2.81834
H	-0.13451	-1.37821	4.62669
H	-1.95071	-2.72080	3.09169
H	-3.40538	-0.90736	1.75486
H	-2.46948	1.58220	2.42907
H	-0.43340	1.25229	4.14991
H	3.15025	2.91296	0.71386
H	3.31999	2.73731	2.49718
H	4.17769	1.61478	1.38286
C	0.92208	-2.28576	2.12680
C	0.53267	-2.46023	0.80125
C	1.53129	-2.42697	-0.34339
H	1.92629	-1.92688	2.35588
H	0.44283	-2.86058	2.91804
H	-0.34202	-3.08882	0.62061
H	1.21045	-1.76118	-1.15313
H	1.53399	-3.45263	-0.75921
C	2.95612	-2.05258	0.06271
H	3.62656	-2.08469	-0.80781
H	3.35202	-2.74797	0.82118
H	2.98458	-1.03335	0.47340

73			
duf71a duf71a.fchk			
Ru	-0.52163	-0.38552	1.53811
P	-1.41269	0.05860	-0.50386
C	-2.76791	1.35287	-0.64321
C	-4.05862	0.94073	0.07579
C	-2.23896	2.68468	-0.09533
C	-1.99813	-1.43518	-1.49939
C	-2.64973	-1.10577	-2.84479
C	-2.88587	-2.34794	-0.64181
C	-0.18595	0.73905	-1.77555
N	1.10388	0.35579	-1.70474
C	1.85931	0.89823	-2.72504
C	0.98738	1.66975	-3.44090
N	-0.26502	1.56113	-2.85427
C	3.31874	0.59194	-2.93316
C	4.09692	0.90782	-1.64217
C	3.46302	-0.90380	-3.28592
C	3.85800	1.44802	-4.08803
C	-1.43202	2.25617	-3.40506
C	-0.39286	-0.96184	3.68867
C	-1.43349	-1.72304	3.05990
C	-2.43873	-0.82355	2.60671
C	-2.04906	0.51615	2.98984
C	-0.79080	0.41994	3.63537
N	1.15499	0.67904	1.28801
C	2.13526	1.30472	1.33016
C	3.36307	2.07890	1.46531
H	-3.01604	1.45394	-1.70708
H	-4.79889	1.75117	-0.03362
H	-3.89200	0.78247	1.14865
H	-4.49643	0.02711	-0.35086
H	-2.00029	2.58188	0.97478
H	-3.00145	3.47268	-0.21552
H	-1.31516	3.01217	-0.60244
H	-1.04804	-1.96930	-1.67796
H	-1.95958	-0.56524	-3.51294
H	-3.56317	-0.50198	-2.71051
H	-2.94272	-2.03734	-3.35750
H	-2.44327	-2.51375	0.35078
H	-3.89320	-1.92392	-0.50848
H	-2.99896	-3.32171	-1.14655
H	1.14734	2.28371	-4.31983
H	3.71448	0.31557	-0.79633
H	5.16027	0.65675	-1.78387
H	4.02182	1.97944	-1.39660
H	3.04748	-1.54416	-2.49310
H	2.94263	-1.13185	-4.23018
H	4.52971	-1.15235	-3.40613
H	4.92408	1.22216	-4.24366
H	3.32405	1.22966	-5.02753
H	3.76219	2.52362	-3.86537
H	-1.11191	2.76716	-4.32195
H	-2.22009	1.53466	-3.65271
H	-1.81028	2.99639	-2.68899
H	0.50778	-1.35845	4.14978
H	-1.43780	-2.80138	2.91959
H	-3.36499	-1.10991	2.11721
H	-2.62027	1.42657	2.83337
H	-0.20808	1.25958	4.00945
H	3.40926	2.87125	0.70156
H	3.39973	2.54566	2.46372
H	4.23922	1.42106	1.34639
C	0.43492	-2.22916	0.80235
C	1.61013	-2.16346	-0.09683
C	2.89030	-1.92103	0.26570
H	0.72800	-2.71408	1.74621
H	-0.34740	-2.84492	0.33545
H	1.42841	-2.35985	-1.16423
H	1.45920	-0.28705	-0.97857
H	3.67161	-1.95667	-0.50002
C	3.34120	-1.69515	1.68170
H	4.10344	-0.89716	1.74150
H	3.81331	-2.60668	2.09422
H	2.49508	-1.42372	2.33076

73			
an71 duf71.fchk			
Ru	-0.85181	-0.47718	2.23605
P	-1.54764	-0.12352	0.04034
C	-2.87160	1.19933	-0.16822
C	-4.22006	0.86016	0.48235
C	-2.34191	2.55077	0.32585
C	-2.21346	-1.61802	-0.91298
C	-3.06829	-1.28543	-2.13971
C	-2.92385	-2.58491	0.04290
C	-0.27494	0.50792	-1.20140
N	1.02114	0.15800	-1.08929
C	1.75854	0.78389	-2.07890
C	0.87846	1.53978	-2.80438
N	-0.38154	1.36210	-2.27094
C	3.25547	0.67345	-2.25952
C	3.94891	1.06447	-0.94221
C	3.65425	-0.75704	-2.66987
C	3.70329	1.64146	-3.36748
C	-1.53554	2.02781	-2.88400
C	-1.01712	-0.92711	4.40667
C	-2.05647	-1.63096	3.69716
C	-2.90799	-0.67531	3.08659
C	-2.41955	0.64230	3.42081
C	-1.25874	0.46877	4.22872
N	0.84898	0.58018	2.01133
C	1.81358	1.22523	2.05909
C	3.02839	2.02301	2.17117
H	-3.06592	1.24977	-1.24383
H	-4.97931	1.56163	0.09743
H	-4.19299	0.97597	1.57171
H	-4.55678	-0.15944	0.24423
H	-2.13521	2.50744	1.40518
H	-3.09008	3.34046	0.14164
H	-1.40086	2.83833	-0.17092
H	-1.29026	-2.10341	-1.26968
H	-2.49870	-0.70631	-2.88336
H	-3.97659	-0.72396	-1.86897
H	-3.38866	-2.22049	-2.62908
H	-2.29656	-2.80615	0.92010
H	-3.87594	-2.16498	0.40568
H	-3.15245	-3.52568	-0.48489
H	1.03846	2.19149	-3.65577
H	3.59774	0.43789	-0.11182
H	5.03926	0.93528	-1.03974
H	3.74436	2.12068	-0.70154
H	3.41014	-1.48566	-1.88758
H	3.14092	-1.05187	-3.59965
H	4.74144	-0.79577	-2.84744
H	4.79644	1.58159	-3.48377
H	3.24440	1.37899	-4.33486
H	3.43954	2.68305	-3.12034
H	-1.18524	2.50513	-3.80815
H	-2.31379	1.30031	-3.14287
H	-1.94730	2.79791	-2.21998
H	-0.21079	-1.37630	4.98027
H	-2.16912	-2.71021	3.63346
H	-3.79247	-0.90935	2.50405
H	-2.87861	1.59088	3.16228
H	-0.63431	1.27255	4.61393
H	3.03688	2.81712	1.40845
H	3.08133	2.48268	3.17180
H	3.91265	1.38331	2.02039
C	0.37801	-2.36734	2.06779
C	0.70489	-2.55070	0.70124
C	1.88332	-2.17436	0.05246
H	1.23059	-2.20905	2.73802
H	-0.33651	-3.10552	2.44487
H	-0.07965	-2.99484	0.08033
H	1.40228	-0.87462	-0.47279
H	2.02666	-2.65838	-0.92244
C	3.14539	-1.92353	0.86531
H	3.99463	-1.66642	0.21482
H	3.43111	-2.81738	1.44998
H	3.00717	-1.09988	1.58393

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73			
cuf63b cuf63b.fchk			
Ru	-0.81227	-0.24132	1.37563
P	-1.16045	0.06385	-0.84634
C	-2.32527	1.42507	-1.41304
C	-3.76391	1.19389	-0.93500
C	-1.80219	2.76727	-0.88325
C	-1.55224	-1.48283	-1.84593
C	-1.82383	-1.26166	-3.33587
C	-2.66666	-2.28866	-1.16586
C	0.40937	0.61891	-1.74267
N	1.59445	0.33699	-1.17372
C	2.65721	0.78314	-1.92707
C	2.08570	1.38557	-3.01521
N	0.70624	1.27553	-2.89104
C	4.08815	0.56837	-1.51218
C	4.34376	1.32001	-0.18974
C	4.32630	-0.94127	-1.29999
C	5.02114	1.10345	-2.60671
C	-0.21915	1.87979	-3.85251
C	-1.55374	0.30715	3.44049
C	-1.29848	-1.09534	3.39413
C	-2.18637	-1.65893	2.41122
C	-2.97122	-0.59712	1.87478
C	-2.59799	0.63065	2.51879
N	0.61624	1.15964	1.50215
C	1.37377	2.01595	1.72609
C	2.29278	3.10389	2.04245
H	-2.33231	1.42576	-2.51210
H	-4.40651	1.99654	-1.33365
H	-3.81940	1.23101	0.16179
H	-4.17178	0.23206	-1.27894
H	-1.78024	2.74627	0.21886
H	-2.46600	3.58560	-1.20880
H	-0.77906	2.99110	-1.23069
H	-0.62014	-2.06298	-1.73043
H	-0.93806	-0.86531	-3.85749
H	-2.67481	-0.57855	-3.49883
H	-2.07816	-2.22354	-3.81164
H	-2.41720	-2.48201	-0.11478
H	-3.63978	-1.77532	-1.22470
H	-2.76756	-3.25884	-1.67960
H	2.53867	1.87818	-3.86832
H	3.68110	0.95005	0.60966
H	5.38543	1.15753	0.12968
H	4.17998	2.40286	-0.31492
H	3.67398	-1.34459	-0.50815
H	4.14212	-1.50290	-2.22999
H	5.37141	-1.10613	-0.99343
H	6.06830	0.94803	-2.30514
H	4.85640	0.57503	-3.55993
H	4.86820	2.18376	-2.76729
H	0.35763	2.16616	-4.74127
H	-0.99111	1.15863	-4.14024
H	-0.68732	2.77148	-3.41246
H	-1.01494	1.02296	4.05869
H	-0.57683	-1.63725	3.99896
H	-2.26051	-2.70620	2.13735
H	-3.74467	-0.71587	1.12220
H	-3.03341	1.61267	2.35518
H	3.24105	2.70376	2.43741
H	2.51067	3.69604	1.13875
H	1.84381	3.76758	2.80026
C	1.99766	-1.58767	1.73109
C	0.70013	-1.81868	0.93152
C	0.15534	-3.16362	1.26609
H	1.78101	-1.57855	2.81277
H	2.74578	-2.38122	1.54132
H	0.94924	-1.87227	-0.14522
H	2.47856	-0.61720	1.51218
H	0.04722	-3.37474	2.33795
C	-0.19085	-4.12410	0.39509
H	1.64507	-0.13860	-0.27478
H	-0.58599	-5.08698	0.72915
H	-0.08673	-3.97090	-0.68504

73			
cuf63a cuf63a.fchk			
Ru	-1.00031	-0.10834	1.44933
P	-1.14709	0.27284	-0.87239
C	-2.41604	1.53343	-1.40537
C	-3.85603	1.08487	-1.12945
C	-2.10921	2.86561	-0.70833
C	-1.41794	-1.28954	-1.88477
C	-1.76074	-0.98943	-3.34760
C	-2.40639	-2.26632	-1.23905
C	0.44159	0.84962	-1.59907
N	1.55996	0.33030	-1.10010
C	2.59436	0.76902	-1.89201
C	2.08421	1.57978	-2.88361
N	0.71772	1.62885	-2.70337
C	4.03198	0.37312	-1.64053
C	4.54170	1.06652	-0.36183
C	4.11800	-1.15319	-1.45518
C	4.91099	0.79930	-2.82558
C	-0.17152	2.38799	-3.57645
C	-1.91701	0.36982	3.39510
C	-1.52233	-0.99124	3.42113
C	-2.23374	-1.67348	2.35865
C	-3.07917	-0.73596	1.71123
C	-2.85650	0.55972	2.31601
N	0.43607	1.31381	1.59697
C	1.27577	2.10579	1.69844
C	2.34696	3.08647	1.79816
H	-2.30767	1.64690	-2.49230
H	-4.55107	1.84234	-1.52856
H	-4.04743	0.99514	-0.05106
H	-4.09167	0.12441	-1.61188
H	-2.23773	2.75881	0.38097
H	-2.79671	3.64867	-1.06930
H	-1.07349	3.19812	-0.88752
H	-0.41413	-1.74731	-1.84358
H	-0.98472	-0.36917	-3.82281
H	-2.73173	-0.47421	-3.43563
H	-1.83015	-1.93249	-3.91493
H	-2.09041	-2.52960	-0.21951
H	-3.42731	-1.85392	-1.19823
H	-2.44563	-3.19019	-1.83998
H	2.56038	2.12169	-3.69466
H	3.91726	0.79437	0.50372
H	5.57908	0.75902	-0.14883
H	4.52789	2.16374	-0.48527
H	3.49815	-1.47456	-0.60515
H	3.76817	-1.67525	-2.36118
H	5.16223	-1.45008	-1.26263
H	5.95658	0.50480	-2.64228
H	4.57433	0.31852	-3.75872
H	4.88638	1.89325	-2.96644
H	0.44438	2.89677	-4.32973
H	-0.87861	1.72353	-4.09410
H	-0.73107	3.14366	-3.00811
H	-1.52548	1.15824	4.03489
H	-0.80018	-1.43887	4.09959
H	-2.12445	-2.72316	2.09646
H	-3.75023	-0.95362	0.88736
H	-3.37019	1.48559	2.07183
H	2.83846	3.01200	2.78193
H	3.08840	2.88891	1.00798
H	1.94005	4.10357	1.67669
C	2.22555	-1.47022	1.82011
C	1.13161	-2.11636	0.98035
C	0.55455	-3.37113	1.55512
H	1.87882	-1.29314	2.85129
H	3.10963	-2.12774	1.85682
H	1.46846	-2.26619	-0.05650
H	2.51394	-0.51104	1.37053
H	0.32518	-3.34947	2.62745
C	0.32482	-4.48305	0.84915
H	0.27855	-1.37519	0.81537
H	-0.08607	-5.38281	1.31491
H	0.55652	-4.52811	-0.22061

73			
an63 cuf63.fchk			
Ru	-0.99065	-0.27454	1.75324
P	-1.54611	-0.00076	-0.47649
C	-2.63982	1.44625	-0.96153
C	-4.01736	1.41319	-0.28618
C	-1.93226	2.75921	-0.59072
C	-2.12408	-1.53907	-1.38713
C	-2.09084	-1.42753	-2.91450
C	-3.49512	-2.04215	-0.91643
C	0.01914	0.41059	-1.35903
N	1.12718	0.09233	-0.69615
C	2.22142	0.48676	-1.43721
C	1.73617	1.07762	-2.58236
N	0.35537	1.01720	-2.52977
C	3.64973	0.25665	-1.00661
C	3.82963	0.71991	0.45081
C	3.98843	-1.24439	-1.12378
C	4.59594	1.05362	-1.91792
C	-0.52759	1.60663	-3.53190
C	-1.53244	-0.19855	3.94719
C	-1.46185	-1.56122	3.57296
C	-2.41012	-1.81271	2.52796
C	-3.10935	-0.58052	2.29553
C	-2.55705	0.42739	3.14185
N	0.16721	1.37946	1.78849
C	0.86156	2.30489	1.88000
C	1.74150	3.46155	1.99394
H	-2.77866	1.38722	-2.05342
H	-4.63285	2.23682	-0.68419
H	-3.91196	1.56804	0.79861
H	-4.55877	0.47225	-0.45713
H	-1.80266	2.81314	0.50229
H	-2.54977	3.61515	-0.91014
H	-0.93663	2.85636	-1.05089
H	-1.35999	-2.26691	-1.05831
H	-1.08602	-1.17967	-3.28952
H	-2.80965	-0.67149	-3.27606
H	-2.38518	-2.39387	-3.35719
H	-3.57131	-2.09255	0.17727
H	-4.30930	-1.40797	-1.30254
H	-3.65594	-3.05806	-1.31389
H	2.24828	1.53148	-3.42470
H	3.16092	0.17278	1.13084
H	4.86891	0.54210	0.77105
H	3.61866	1.79865	0.54291
H	3.33661	-1.86172	-0.48526
H	3.87556	-1.58743	-2.16513
H	5.03185	-1.41468	-0.81150
H	5.63794	0.89311	-1.60020
H	4.50817	0.72470	-2.96664
H	4.38029	2.13392	-1.86815
H	0.03409	1.71059	-4.46987
H	-1.38755	0.95076	-3.70302
H	-0.87772	2.59702	-3.20333
H	-0.91561	0.29146	4.69674
H	-0.77529	-2.29510	3.98285
H	-2.61137	-2.77259	2.06221
H	-3.92378	-0.43940	1.59356
H	-2.87890	1.46429	3.19964
H	2.67539	3.17493	2.50440
H	1.98884	3.84557	0.99090
H	1.24759	4.25986	2.57175
C	1.74006	-1.34029	2.84355
C	1.01625	-1.58516	1.50667
C	0.42755	-2.94757	1.31874
H	1.13011	-1.60289	3.71730
H	2.66957	-1.93627	2.89660
H	1.84443	-1.56975	0.77632
H	2.01255	-0.27803	2.94984
H	-0.12221	-3.36993	2.16520
C	0.52691	-3.67820	0.19626
H	0.85520	-0.55099	0.47966
H	0.06260	-4.66400	0.11345
H	1.08415	-3.30753	-0.67182

73			
cuf61b cuf61b.fchk			
Ru	-0.54911	-0.58282	1.49628
P	-1.15008	-0.23074	-0.77380
C	-2.47156	1.08947	-0.99361
C	-3.86178	0.71279	-0.46760
C	-2.00668	2.42141	-0.39331
C	-1.74970	-1.69954	-1.78740
C	-2.43298	-1.30917	-3.10211
C	-2.60521	-2.66676	-0.95988
C	0.23116	0.44898	-1.79520
N	1.46510	0.08491	-1.46870
C	2.32632	0.70533	-2.33580
C	1.59135	1.47570	-3.21054
N	0.26088	1.31364	-2.87561
C	3.81913	0.49730	-2.23856
C	4.31451	1.03057	-0.87927
C	4.12126	-1.01115	-2.32486
C	4.53542	1.23916	-3.37471
C	-0.80875	2.00238	-3.59270
C	-0.89542	-1.46021	3.53889
C	-1.77780	-2.09877	2.59210
C	-2.65252	-1.10347	2.07583
C	-2.29505	0.15913	2.65005
C	-1.21126	-0.08119	3.57244
N	0.48541	1.14872	1.28281
C	1.11286	2.10009	1.07977
C	1.89939	3.27741	0.74079
H	-2.56896	1.20056	-2.08073
H	-4.58482	1.47408	-0.80553
H	-3.89372	0.69866	0.62949
H	-4.20398	-0.26132	-0.84559
H	-1.91630	2.33873	0.70060
H	-2.74228	3.21015	-0.62408
H	-1.02586	2.73131	-0.78784
H	-0.80740	-2.20883	-2.03394
H	-1.75711	-0.72734	-3.74729
H	-3.35514	-0.73029	-2.93274
H	-2.71001	-2.22315	-3.65354
H	-2.10834	-2.93026	-0.01532
H	-3.59477	-2.24321	-0.72593
H	-2.77042	-3.59060	-1.53864
H	1.88363	2.11048	-4.04144
H	3.77450	0.54232	-0.05116
H	5.39185	0.82737	-0.76197
H	4.16223	2.12103	-0.80820
H	3.60562	-1.55440	-1.51675
H	3.78365	-1.42176	-3.29082
H	5.20623	-1.18391	-2.23136
H	5.62366	1.08690	-3.29720
H	4.20545	0.86624	-4.35851
H	4.33826	2.32386	-3.32758
H	-0.36685	2.49276	-4.47016
H	-1.57201	1.29411	-3.94048
H	-1.28237	2.76687	-2.95976
H	-0.11515	-1.95063	4.11245
H	-1.80248	-3.15747	2.34977
H	-3.43980	-1.27807	1.35077
H	-2.79113	1.11000	2.47854
H	-0.70174	0.67293	4.16820
H	2.79898	3.33224	1.37440
H	2.21244	3.19619	-0.31326
H	1.30076	4.19193	0.88139
C	2.32708	-1.06206	2.72422
C	1.63302	-1.27852	1.40232
C	0.85750	-2.39189	1.09191
H	1.91190	-1.69611	3.52141
H	3.39700	-1.32021	2.61579
H	2.05336	-0.74703	0.54619
H	2.27582	-0.00935	3.04795
H	0.61828	-3.07020	1.91816
C	0.87276	-3.04592	-0.26449
H	1.11786	-2.31759	-1.04923
H	-0.07523	-3.55214	-0.49726
H	1.66035	-3.82284	-0.26338

73			
cuf61a cuf61a.fchk			
Ru	-0.53576	-0.23662	1.48598
P	-1.25608	-0.14769	-0.68675
C	-2.64312	1.06001	-1.07493
C	-3.99663	0.56557	-0.54717
C	-2.28213	2.44058	-0.51634
C	-1.70088	-1.71705	-1.62822
C	-2.34167	-1.48457	-2.99912
C	-2.52041	-2.66549	-0.74559
C	0.08236	0.50349	-1.84226
N	1.35090	0.19975	-1.52113
C	2.25663	0.73750	-2.40919
C	1.49251	1.40921	-3.32493
N	0.15842	1.25657	-2.96671
C	3.74678	0.58162	-2.25485
C	4.18715	1.30900	-0.96725
C	4.10421	-0.91278	-2.13872
C	4.44972	1.20005	-3.47120
C	-0.93349	1.87817	-3.72016
C	-0.67899	-0.67591	3.68149
C	-1.41564	-1.66353	2.93901
C	-2.48497	-0.99770	2.27200
C	-2.43794	0.40358	2.61603
C	-1.31467	0.58580	3.46355
N	0.78335	1.25506	1.27666
C	1.54572	2.13468	1.29082
C	2.46934	3.26238	1.35603
H	-2.72857	1.11114	-2.16839
H	-4.76214	1.33527	-0.74281
H	-3.97416	0.38122	0.53445
H	-4.31380	-0.36016	-1.04907
H	-2.17952	2.39022	0.57897
H	-3.06834	3.17128	-0.77086
H	-1.32066	2.80918	-0.91511
H	-0.71527	-2.18858	-1.76803
H	-1.67270	-0.91866	-3.66799
H	-3.30354	-0.95162	-2.92529
H	-2.53734	-2.45685	-3.48199
H	-1.99912	-2.85510	0.20356
H	-3.52292	-2.26622	-0.52391
H	-2.64897	-3.62560	-1.27261
H	1.77989	1.98314	-4.19872
H	3.67713	0.89010	-0.08340
H	5.27306	1.18522	-0.82781
H	3.96261	2.38607	-1.02969
H	3.66162	-1.36085	-1.23432
H	3.75382	-1.47637	-3.01826
H	5.19782	-1.02094	-2.06575
H	5.53979	1.09900	-3.35632
H	4.15265	0.68930	-4.40167
H	4.21460	2.27353	-3.56414
H	-0.50055	2.34872	-4.61206
H	-1.66232	1.11944	-4.03031
H	-1.42887	2.64184	-3.10567
H	0.18633	-0.85568	4.30982
H	-1.20539	-2.72916	2.90254
H	-3.23571	-1.47768	1.65172
H	-3.13531	1.17531	2.30547
H	-0.97330	1.53926	3.86252
H	3.49531	2.90742	1.54452
H	2.45960	3.82227	0.40666
H	2.17172	3.94271	2.17132
C	1.88023	-1.92470	2.49058
C	1.19399	-1.57500	1.15521
C	0.82672	-2.82068	0.43549
H	1.22582	-2.54324	3.12610
H	2.80585	-2.50481	2.31459
H	2.00129	-1.06234	0.58354
H	2.14059	-1.01620	3.05734
H	0.12857	-3.47126	0.97878
C	1.25935	-3.22985	-0.76939
H	1.56541	-0.34374	-0.67844
H	0.91471	-4.16892	-1.21041
H	1.97400	-2.64033	-1.35216

73			
cuf61 cuf61.fchk			
Ru	-0.82757	-0.19805	2.12264
P	-1.42714	-0.15905	-0.12689
C	-2.85935	0.98673	-0.54124
C	-4.23060	0.43898	-0.12274
C	-2.59517	2.37573	0.05662
C	-1.78379	-1.74972	-1.06842
C	-2.36076	-1.50961	-2.46775
C	-2.62669	-2.72468	-0.23822
C	-0.10283	0.52531	-1.26356
N	1.13767	0.05352	-1.08345
C	2.01617	0.69593	-1.93081
C	1.27311	1.59777	-2.64710
N	-0.04674	1.48021	-2.23932
C	3.49123	0.38661	-1.98266
C	4.07070	0.42359	-0.55477
C	3.69876	-1.01156	-2.60160
C	4.20416	1.43284	-2.85261
C	-1.12375	2.18890	-2.93588
C	-1.14919	-0.53881	4.31945
C	-1.80397	-1.57081	3.55305
C	-2.81735	-0.95371	2.76856
C	-2.80240	0.46230	3.04380
C	-1.76787	0.69944	3.99073
N	0.44457	1.32309	1.77980
C	1.21054	2.17054	1.57215
C	2.17221	3.22830	1.28482
H	-2.87728	1.05576	-1.63641
H	-5.00286	1.18658	-0.37165
H	-4.29510	0.24182	0.95412
H	-4.47941	-0.48838	-0.65828
H	-2.65259	2.34366	1.15247
H	-3.34330	3.09536	-0.31691
H	-1.58914	2.75227	-0.19077
H	-0.77716	-2.18330	-1.17559
H	-1.72173	-0.83071	-3.05789
H	-3.37531	-1.08260	-2.42209
H	-2.42566	-2.46554	-3.01387
H	-2.17924	-2.88424	0.75447
H	-3.65689	-2.36081	-0.09852
H	-2.68245	-3.69554	-0.75807
H	1.55960	2.30323	-3.41946
H	3.55225	-0.28649	0.10792
H	5.14003	0.15962	-0.58060
H	3.97427	1.43314	-0.12193
H	3.18675	-1.79052	-2.01824
H	3.31278	-1.03821	-3.63369
H	4.77512	-1.24772	-2.62632
H	5.28245	1.21265	-2.88508
H	3.82366	1.41528	-3.88730
H	4.07134	2.44902	-2.44480
H	-0.66279	2.81336	-3.71192
H	-1.79861	1.46702	-3.41734
H	-1.69094	2.82976	-2.25207
H	-0.35013	-0.67970	5.03732
H	-1.58448	-2.63440	3.58554
H	-3.50537	-1.47159	2.10752
H	-3.48766	1.20472	2.65038
H	-1.47467	1.67408	4.37615
H	3.10821	3.05087	1.83917
H	2.39675	3.23850	0.20543
H	1.76434	4.20929	1.57910
C	1.38107	-2.03345	3.56755
C	1.09426	-1.42240	2.19545
C	0.80799	-2.36024	1.15320
H	0.57842	-2.70432	3.91239
H	2.30717	-2.63551	3.51377
H	1.92004	-0.75327	1.90707
H	1.53877	-1.25735	4.33099
H	-0.01545	-3.06183	1.33648
C	1.51361	-2.41220	-0.05289
H	1.30842	-1.04921	-0.57598
H	1.25243	-3.17556	-0.79351
H	2.58457	-2.18465	0.02007

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73			
eug81b eug81b.fchk			
Ru	-0.77246	-0.09839	1.63008
P	-1.22245	-0.27349	-0.60266
C	-2.60685	0.84243	-1.22015
C	-3.99673	0.38966	-0.75476
C	-2.32762	2.28315	-0.77280
C	-1.53297	-1.94470	-1.41863
C	-2.09453	-1.85588	-2.84071
C	-2.37993	-2.83772	-0.50300
C	0.17929	0.31247	-1.73842
N	1.44799	-0.01229	-1.41669
C	2.35979	0.55192	-2.28819
C	1.60526	1.26590	-3.17642
N	0.26949	1.10355	-2.84038
C	3.85121	0.34172	-2.22202
C	4.35039	0.58804	-0.78664
C	4.17584	-1.10404	-2.65280
C	4.53919	1.32504	-3.18173
C	-0.79234	1.65697	-3.68775
C	-1.12139	-0.35637	3.81932
C	-1.87905	-1.34613	3.09552
C	-2.83890	-0.66167	2.29871
C	-2.71027	0.75290	2.53408
C	-1.63776	0.92411	3.45685
N	0.56637	1.35019	1.27751
C	1.33946	2.20957	1.15219
C	2.32838	3.27330	1.02149
H	-2.60710	0.77445	-2.31453
H	-4.75404	1.05021	-1.20966
H	-4.10313	0.46463	0.33410
H	-4.22321	-0.64159	-1.06225
H	-2.37345	2.34672	0.32410
H	-3.07827	2.96684	-1.20434
H	-1.32322	2.63107	-1.06668
H	-0.51880	-2.37571	-1.46460
H	-1.44008	-1.25956	-3.49899
H	-3.10243	-1.41064	-2.85125
H	-2.17122	-2.86596	-3.27683
H	-1.96730	-2.85746	0.51766
H	-3.42249	-2.48681	-0.44416
H	-2.39393	-3.86587	-0.90105
H	1.90216	1.86745	-4.02772
H	3.88405	-0.10713	-0.07272
H	5.44020	0.43452	-0.74689
H	4.13277	1.61994	-0.46636
H	3.67652	-1.83574	-2.00143
H	3.85502	-1.27999	-3.69239
H	5.26377	-1.26829	-2.59062
H	5.62878	1.17554	-3.13632
H	4.21876	1.15615	-4.22300
H	4.32138	2.37071	-2.90781
H	-0.30975	2.14196	-4.54569
H	-1.43940	0.84897	-4.05322
H	-1.38737	2.39733	-3.14128
H	-0.30930	-0.54900	4.51530
H	-1.75037	-2.42389	3.15317
H	-3.57018	-1.14292	1.65605
H	-3.33120	1.54035	2.11749
H	-1.25525	1.87971	3.81058
H	1.96732	4.19426	1.50851
H	3.27529	2.96775	1.49710
H	2.52045	3.48680	-0.04283
C	2.20523	-0.88993	2.35465
C	0.91854	-1.53994	1.85212
C	1.10985	-2.45398	0.71565
H	2.65219	-0.22017	1.60116
H	2.00922	-0.27812	3.24936
H	0.48897	-2.14616	2.66531
H	2.97000	-1.64799	2.61140
H	0.23331	-3.05647	0.45310
C	2.23144	-2.62587	-0.02234
H	1.66737	-0.72175	-0.69348
H	2.26179	-3.33382	-0.85497
H	3.16602	-2.12237	0.23825

73			
eug81a eug81a.fchk			
Ru	-0.83339	-0.03110	1.63064
P	-1.29263	-0.08337	-0.68253
C	-2.71633	1.00081	-1.22018
C	-4.08265	0.51473	-0.72216
C	-2.44433	2.44084	-0.76380
C	-1.56007	-1.79075	-1.41643
C	-2.09878	-1.73277	-2.84982
C	-2.38800	-2.71151	-0.51381
C	0.12999	0.48917	-1.70127
N	1.34277	0.11866	-1.30189
C	2.23792	0.60994	-2.22312
C	1.54245	1.30309	-3.19160
N	0.20342	1.22060	-2.86898
C	3.71904	0.31016	-2.16663
C	4.23080	0.43065	-0.72264
C	3.93612	-1.13866	-2.65160
C	4.49144	1.27524	-3.07764
C	-0.84683	1.76365	-3.72520
C	-1.10084	-0.54852	3.78240
C	-1.86607	-1.45728	2.95243
C	-2.82893	-0.70078	2.23596
C	-2.64005	0.69487	2.56411
C	-1.58809	0.76063	3.54969
N	0.43378	1.51766	1.26801
C	1.19877	2.32770	0.95235
C	2.16439	3.30561	0.47376
H	-2.73502	0.95462	-2.31697
H	-4.86967	1.15001	-1.16172
H	-4.16633	0.59638	0.37002
H	-4.28753	-0.52519	-1.01692
H	-2.45900	2.49768	0.33566
H	-3.21977	3.11616	-1.16230
H	-1.45836	2.80327	-1.09687
H	-0.52516	-2.17491	-1.44241
H	-1.45043	-1.12157	-3.49813
H	-3.12034	-1.31871	-2.87829
H	-2.13762	-2.74905	-3.27591
H	-1.95641	-2.76516	0.49692
H	-3.43309	-2.37292	-0.42774
H	-2.40298	-3.72700	-0.94330
H	1.87025	1.83309	-4.08042
H	3.67081	-0.25363	-0.07059
H	5.29995	0.16575	-0.68110
H	4.11766	1.46024	-0.34399
H	3.37517	-1.84025	-2.01518
H	3.59634	-1.25360	-3.69433
H	5.00779	-1.39667	-2.60267
H	5.56884	1.04939	-3.03401
H	4.16990	1.17595	-4.12793
H	4.34463	2.32368	-2.76592
H	-0.36720	2.22512	-4.59846
H	-1.51455	0.96355	-4.07704
H	-1.43663	2.52765	-3.20114
H	-0.28307	-0.82104	4.44529
H	-1.73751	-2.53615	2.89933
H	-3.56101	-1.10570	1.54531
H	-3.24390	1.52855	2.21746
H	-1.19065	1.67405	3.98771
H	1.73433	4.31942	0.51286
H	3.07474	3.27520	1.09343
H	2.42845	3.04994	-0.56626
C	2.37853	-1.05105	2.48846
C	1.31633	-1.72549	1.62652
C	1.80787	-2.69606	0.58566
H	3.05261	-0.43346	1.87706
H	1.90525	-0.40189	3.23975
H	0.58636	-2.24992	2.25971
H	2.98665	-1.80889	3.00855
H	1.02385	-3.15445	-0.02763
C	3.08396	-3.03332	0.38477
H	0.79450	-0.93302	0.98986
H	3.35731	-3.76958	-0.37476
H	3.89548	-2.59237	0.96909

73			
eug81 eug81.fchk			
Ru	-1.01725	-0.05972	1.96510
P	-1.64894	-0.21737	-0.23931
C	-2.95238	0.99238	-0.82079
C	-4.32004	0.69331	-0.19421
C	-2.50058	2.41784	-0.47828
C	-2.10035	-1.90750	-0.92887
C	-2.68880	-1.86653	-2.34266
C	-2.98373	-2.70166	0.04121
C	-0.17734	0.23099	-1.26630
N	1.03563	0.00839	-0.73834
C	1.99648	0.48219	-1.61357
C	1.32310	1.00966	-2.69097
N	-0.02709	0.83924	-2.47380
C	3.49808	0.36516	-1.46599
C	3.91500	0.38486	0.00713
C	3.94858	-0.96510	-2.10755
C	4.17271	1.53590	-2.20306
C	-1.04634	1.30810	-3.41118
C	-1.14806	-0.65132	4.14105
C	-2.03602	-1.47019	3.34822
C	-3.00121	-0.60552	2.75190
C	-2.70474	0.74854	3.13211
C	-1.55857	0.69698	4.00342
N	0.14474	1.54484	1.56629
C	0.86383	2.43571	1.37955
C	1.79484	3.52641	1.11906
H	-3.04954	0.87697	-1.90906
H	-5.06325	1.40239	-0.59497
H	-4.28786	0.82222	0.89707
H	-4.66903	-0.32529	-0.42126
H	-2.41966	2.53078	0.61447
H	-3.23676	3.14585	-0.85783
H	-1.51449	2.65952	-0.90769
H	-1.11589	-2.40413	-0.97046
H	-1.97956	-1.43163	-3.06418
H	-3.63020	-1.29358	-2.37505
H	-2.91133	-2.89274	-2.67918
H	-2.51986	-2.76381	1.03559
H	-3.98391	-2.25179	0.14802
H	-3.11889	-3.72436	-0.34764
H	1.69108	1.47990	-3.59649
H	3.52035	-0.49182	0.53002
H	5.01404	0.36258	0.07636
H	3.55436	1.29332	0.51811
H	3.44866	-1.81662	-1.62141
H	3.70975	-0.97606	-3.18382
H	5.03887	-1.08252	-1.99026
H	5.26582	1.44807	-2.10188
H	3.93697	1.52958	-3.27985
H	3.86165	2.50750	-1.78212
H	-0.54690	1.55653	-4.35662
H	-1.78629	0.52121	-3.59789
H	-1.55098	2.20272	-3.01970
H	-0.29649	-1.00517	4.71670
H	-2.00812	-2.55408	3.26735
H	-3.82235	-0.92474	2.11780
H	-3.27997	1.63460	2.87719
H	-1.06063	1.55798	4.44470
H	1.26437	4.49255	1.10844
H	2.57283	3.55373	1.89952
H	2.27846	3.36709	0.14098
C	2.07526	-0.84863	2.59913
C	0.98799	-1.40400	1.66813
C	1.35779	-2.53189	0.75862
H	2.48002	0.11464	2.25581
H	1.65056	-0.66676	3.59864
H	0.20554	-1.87725	2.28375
H	2.92475	-1.54436	2.71552
H	0.49582	-3.01260	0.27783
C	2.57835	-3.01176	0.47504
H	0.97191	-0.53525	0.42487
H	2.69996	-3.86507	-0.19652
H	3.48525	-2.59941	0.92405

73			
euf81b euf81b.fchk			
Ru	-0.65374	-0.42719	1.63372
P	-1.07939	-0.25382	-0.70433
C	-2.44675	0.96487	-1.12718
C	-3.86144	0.56479	-0.68802
C	-2.07718	2.36683	-0.62784
C	-1.52120	-1.83652	-1.62075
C	-2.18290	-1.61026	-2.98426
C	-2.32340	-2.80147	-0.74020
C	0.31526	0.41788	-1.72260
N	1.55677	0.13445	-1.34730
C	2.40934	0.66004	-2.28497
C	1.65998	1.29289	-3.25143
N	0.33240	1.14139	-2.90571
C	3.90941	0.50235	-2.18339
C	4.43723	1.33452	-0.99761
C	4.24758	-0.98250	-1.95003
C	4.57807	0.98750	-3.47760
C	-0.73517	1.72300	-3.71708
C	-1.22583	-0.97746	3.75145
C	-2.00561	-1.76226	2.83042
C	-2.80278	-0.87197	2.06435
C	-2.50165	0.47354	2.47399
C	-1.53181	0.38892	3.53196
N	0.49981	1.20294	1.34282
C	1.16394	2.11969	1.10212
C	2.01036	3.24316	0.72943
H	-2.46301	0.96997	-2.22281
H	-4.58750	1.20424	-1.21740
H	-4.02238	0.71562	0.38628
H	-4.09628	-0.48060	-0.93673
H	-2.02482	2.38625	0.47104
H	-2.83855	3.09500	-0.95437
H	-1.09638	2.69199	-1.01069
H	-0.53019	-2.27743	-1.79828
H	-1.52796	-1.03502	-3.65597
H	-3.15098	-1.09187	-2.89556
H	-2.36997	-2.58593	-3.46302
H	-1.83832	-2.94171	0.23689
H	-3.35066	-2.43983	-0.57060
H	-2.39672	-3.77977	-1.24342
H	1.94248	1.82643	-4.15357
H	3.94086	1.03927	-0.06009
H	5.52247	1.17787	-0.88059
H	4.26467	2.41065	-1.17037
H	3.78188	-1.34806	-1.02217
H	3.88530	-1.60074	-2.78795
H	5.33981	-1.10902	-1.86922
H	5.67080	0.87080	-3.40186
H	4.22758	0.40480	-4.34541
H	4.36273	2.05399	-3.66120
H	-0.27474	2.16349	-4.61121
H	-1.45318	0.95837	-4.04161
H	-1.26491	2.51393	-3.16771
H	-0.51596	-1.36448	4.47760
H	-2.00716	-2.84590	2.75215
H	-3.51374	-1.17057	1.30257
H	-2.97813	1.38161	2.11934
H	-1.08137	1.23142	4.05241
H	2.92311	3.25131	1.34638
H	2.30214	3.12689	-0.32672
H	1.47085	4.19407	0.86687
C	2.64377	-0.75741	1.66152
C	1.37383	-1.40559	2.14247
C	0.66475	-2.33144	1.37282
H	2.56927	-0.48286	0.60280
H	2.88872	0.13908	2.25234
H	1.28421	-1.48061	3.22795
H	3.47723	-1.47431	1.78654
H	0.06141	-3.05571	1.92518
C	1.17880	-2.84834	0.05212
H	1.51039	-2.04203	-0.61393
H	0.42673	-3.46980	-0.45424
H	2.04968	-3.50112	0.25370

73			
euf81a euf81a.fchk			
Ru	-0.74821	-0.11114	1.58895
P	-1.22252	-0.25718	-0.64097
C	-2.60730	0.87375	-1.22998
C	-3.99451	0.42334	-0.75453
C	-2.31459	2.30726	-0.76842
C	-1.55086	-1.91693	-1.47314
C	-2.12784	-1.80826	-2.88761
C	-2.39210	-2.81647	-0.55863
C	0.16999	0.33525	-1.78471
N	1.44047	0.00119	-1.48004
C	2.34574	0.57165	-2.35425
C	1.58527	1.29927	-3.22621
N	0.25234	1.13878	-2.87827
C	3.83680	0.35415	-2.30604
C	4.35188	0.58079	-0.87306
C	4.15044	-1.08770	-2.75765
C	4.51928	1.34604	-3.26085
C	-0.81568	1.70697	-3.70792
C	-1.07566	-0.39492	3.77827
C	-1.84656	-1.37109	3.04999
C	-2.81069	-0.67101	2.27207
C	-2.67130	0.73969	2.52384
C	-1.58822	0.89296	3.43745
N	0.59407	1.33528	1.24007
C	1.37006	2.19246	1.11760
C	2.36277	3.25307	0.99044
H	-2.62006	0.81879	-2.32502
H	-4.75314	1.09243	-1.19452
H	-4.08884	0.48772	0.33610
H	-4.22963	-0.60352	-1.07008
H	-2.34560	2.35686	0.32971
H	-3.06712	3.00028	-1.18138
H	-1.31225	2.65364	-1.07100
H	-0.53950	-2.35245	-1.53563
H	-1.47759	-1.20751	-3.54601
H	-3.13338	-1.35763	-2.88143
H	-2.21483	-2.81263	-3.33485
H	-1.96805	-2.85041	0.45697
H	-3.43208	-2.46097	-0.48384
H	-2.41595	-3.83971	-0.96866
H	1.87606	1.90950	-4.07344
H	3.88951	-0.12065	-0.16270
H	5.44128	0.42160	-0.84644
H	4.14259	1.60981	-0.53830
H	3.65459	-1.82507	-2.11001
H	3.81809	-1.24962	-3.79590
H	5.23820	-1.25746	-2.70880
H	5.60859	1.19121	-3.22858
H	4.18734	1.19128	-4.30070
H	4.30904	2.38924	-2.97199
H	-0.33983	2.19904	-4.56560
H	-1.47082	0.90641	-4.07531
H	-1.40094	2.44420	-3.14685
H	-0.25742	-0.60100	4.46309
H	-1.72367	-2.45021	3.09280
H	-3.55145	-1.13985	1.63112
H	-3.29205	1.53592	2.12399
H	-1.19633	1.84176	3.79918
H	3.31400	2.93556	1.44929
H	2.54246	3.48192	-0.07285
H	2.01266	4.16826	1.49599
C	2.23263	-0.92516	2.27337
C	0.93799	-1.56315	1.77588
C	1.11379	-2.46431	0.62662
H	2.67525	-0.24838	1.52360
H	2.04819	-0.32331	3.17724
H	0.51380	-2.17740	2.58589
H	2.99632	-1.68976	2.51340
H	0.23202	-3.05992	0.36583
C	2.22711	-2.63212	-0.12473
H	1.66411	-0.71790	-0.76772
H	2.24595	-3.33021	-0.96598
H	3.16647	-2.13577	0.13235

73			
euf81 euf81.fchk			
Ru	-1.01559	-0.15725	2.12509
P	-1.46919	-0.25964	-0.15245
C	-2.86806	0.86374	-0.71733
C	-4.26079	0.41332	-0.25971
C	-2.57509	2.29964	-0.26210
C	-1.79805	-1.92450	-0.96959
C	-2.33896	-1.81358	-2.39837
C	-2.67171	-2.81796	-0.07983
C	-0.08981	0.34639	-1.27787
N	1.17075	-0.00007	-0.97401
C	2.04952	0.57738	-1.86728
C	1.28939	1.31284	-2.73791
N	-0.03884	1.15689	-2.38010
C	3.54316	0.36437	-1.82976
C	4.06387	0.59470	-0.39880
C	3.86664	-1.07595	-2.27887
C	4.22341	1.35411	-2.78818
C	-1.11088	1.71571	-3.20863
C	-1.39200	-0.40582	4.30945
C	-2.15137	-1.38784	3.57021
C	-3.08322	-0.69468	2.75166
C	-2.92137	0.72103	2.97499
C	-1.87488	0.87900	3.93252
N	0.34729	1.27932	1.77531
C	1.12604	2.12760	1.62914
C	2.11407	3.18353	1.44727
H	-2.87378	0.81168	-1.81230
H	-5.01216	1.08697	-0.70537
H	-4.37518	0.46869	0.82930
H	-4.49409	-0.60981	-0.58794
H	-2.60076	2.36093	0.83502
H	-3.33025	2.98942	-0.67551
H	-1.57565	2.64365	-0.57488
H	-0.78787	-2.36596	-1.00818
H	-1.67025	-1.21410	-3.03845
H	-3.34305	-1.35927	-2.41463
H	-2.41942	-2.81727	-2.84818
H	-2.29018	-2.84494	0.95262
H	-3.71468	-2.46524	-0.04887
H	-2.67867	-3.84463	-0.48181
H	1.57202	1.92454	-3.58762
H	3.56846	-0.07682	0.31827
H	5.14790	0.40138	-0.36337
H	3.88827	1.63598	-0.08347
H	3.39942	-1.81688	-1.61499
H	3.51009	-1.25026	-3.30720
H	4.95781	-1.23079	-2.25812
H	5.31417	1.20782	-2.75481
H	3.89273	1.19265	-3.82754
H	4.00517	2.39775	-2.50620
H	-0.64067	2.21094	-4.06783
H	-1.76149	0.91173	-3.57860
H	-1.70421	2.45133	-2.65325
H	-0.59685	-0.60983	5.02151
H	-2.04076	-2.46755	3.63519
H	-3.81025	-1.16503	2.09682
H	-3.52181	1.51740	2.54678
H	-1.48255	1.82974	4.28812
H	3.06705	2.89126	1.91793
H	2.28847	3.35221	0.37224
H	1.76082	4.12134	1.90654
C	2.01050	-0.96182	2.92361
C	0.72096	-1.62343	2.47178
C	0.74424	-2.36854	1.26035
H	2.42169	-0.30105	2.14495
H	1.84603	-0.35015	3.82471
H	0.22806	-2.18310	3.27425
H	2.78440	-1.71806	3.15654
H	-0.13542	-2.99294	1.07633
C	1.73920	-2.32306	0.28203
H	1.42188	-1.00749	-0.32964
H	1.68481	-3.04194	-0.54266
H	2.75154	-2.04973	0.60163

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