Title

BIS (PENTAMETHYLCYCLOPENTADIENYL) YTTERBIUM (II) AS A LEWIS ACID AND AN ELECTRON-TRANSFER LIGAND; PREPARATION, CRYSTAL STRUCTURE, AND SOLUTION DYNAMICS OF [Yb(C5Me5)2(u-OC)2Mo-(CO) (C5H4)]2

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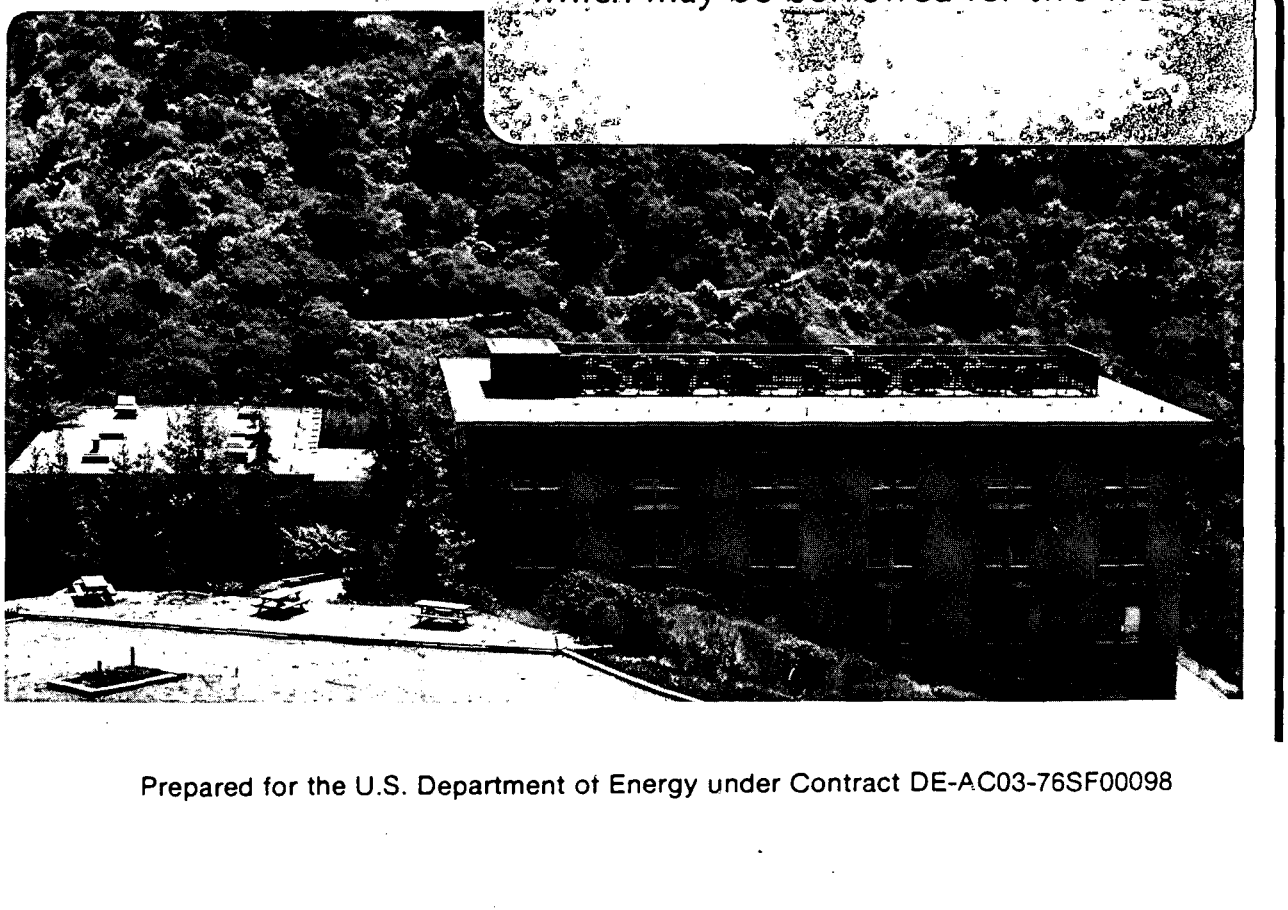

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Bis(Pentamethylcyclopentadienyl) Ytterbium(II) as a Lewis Acid and an Electron-Transfer Ligand; Preparation, Crystal Structure, and Solution Dynamics of $[Yb(C_5Me_5)_2(\mu\text{-}OC)_2Mo\text{-}(CO)(C_5H_4R)]_2$

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Abstract

The divalent ytterbium metallocene, $Yb(C_5Me_5)_2(OEt_2)$, reacts with the metal-metal bonded compound $(RC_5H_4)_2Mo_2(CO)_6$, to give dimers of composition $Mo_2(C_5H_4R)_2(CO)_6Yb_2(C_5Me_5)_4$, where R is H or Me_3Si. X-Ray crystallographic studies on the Me_3Si complex show that the molecule is a centrosymmetric dimer with the $C_5H_4SiMe_3$ groups on the molybdenum atoms trans-disposed. The space group is $P2_1/n$ with a = 13.771(1)Å, b = 15.294(2), c = 15.607(1), β = 93.434(8)°, V = 3294Å^3, and Z = 2. Variable temperature ^{1}HNMR spectroscopic studies show that in toluene solution the compound exists in an equilibrium between trans and cis isomers, and the activation energy for interconversion is ca. 20 kcal mol^{-1}. The mechanism for the interconversion is shown by cross-over studies to be intermolecular. Related intermolecular exchange processes have been discovered in the $M_2(C_5H_4R)_2(\mu\text{-}CO)_4Yb_2(C_5Me_5)_4$ dimers, where M is Fe or Ru and R is Me or $SiMe_3$.

In a previous paper, we described the synthesis and X-ray crystal structure of $Yb_2(C_5Me_5)_4(MeC_5H_4)_2Fe_2(\mu\text{-}CO)_4$[1a] which is structurally similar to the dimeric form of the electronically equivalent $Yb_2(C_5Me_5)_4(\mu\text{-}CO)_4Mn_2(CO)_6$.[1b] The motivation of these studies was crystallographic characterization of the tight ion-pair molecules, which were derived from electron-transfer to the neutral transition metal carbonyl dimers, so that the structural ramifications of coordination and electron transfer could be elucidated. In addition, we wanted to address the question of solution properties, i.e., what, if any, ion-pair equilibria are involved in hydrocarbon solution and how this compares with equilibria in ether solvents of the alkali-metal transition metal carbonyl anions.[2] The ytterbium-transition metal complexes are particularly convenient molecules for study since the complexes are tight ion-pairs of known composition in the solid state and they are soluble in aliphatic hydrocarbon and ether solvents. In a continuation of these studies we decided to make $Yb_2(C_5Me_5)_4(RC_5H_4)_2Mo_2(\mu\text{-}CO)_4(CO)_2$, which is electronically equivalent to the manganese and iron complexes referred to above and presumably structurally similar with them. The ytterbium-molybdenum complex, however, could be rather more interesting than either the manganese or iron complexes since it can exist as cis or trans isomers as does the parent $Cp_2Mo_2(CO)_6$.[3] The isomerization reaction could provide us with an observable spectroscopic handle that we could use to study solution dynamic properties of these ion-pairs.

Synthetic Studies. The complexes of composition $Yb_2(C_5Me_5)_4Cp_2Mo_2(CO)_6$(I) and $Yb_2(C_5Me_5)_4(MeSiC_5H_4)_2Mo_2(CO)_6$(II) were prepared by reaction of $Yb_2(C_5Me_5)_4(OEt_2)$ and the single metal-metal bonded compound $(RC_5H_4)_2Mo_2(CO)_6$, where R is H or Me_3Si, in toluene at room temperature followed by crystallization of dark purple crystals on cooling. The C_5H_5 complex (I) also was isolated in very low yield from the reaction of

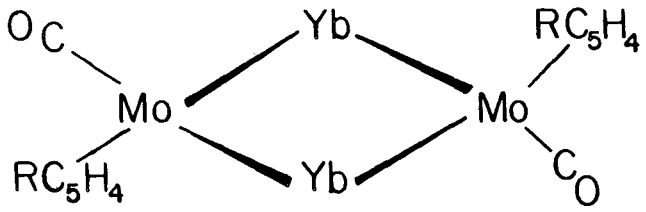
$Yb_2(C_5Me_5)_2(OEt_2)$ and the molybdenum-molybdenum triply-bonded compound $Cp_2Mo_2(CO)_4$. Methyl iodide reacts with I in toluene to give mainly $CpMo(CO)_3Me$ and a small amount (ca. 5%) of $CpMo(CO)_3I$, as judged by the infrared spectrum of the reaction product after extraction into pentane. The infrared spectra of I and II (Table I) in cyclohexane show three absorptions in the C-O stretching frequency region, one of which is at low energy, ca. 1680 cm^{-1}, indicating that Mo-CO-Yb interactions are present.[1] Theory predicts that the trans isomer (Ia or IIa) of idealized C_{2h} symmetry will have

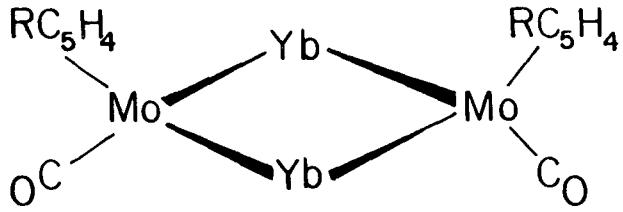
(See illustration, next page)

three infrared active CO stretches and the cis-isomer (Ib or IIb) of idealized C_{2v} symmetry will have six infrared active CO stretches. The observation of three CO-absorptions in cyclohexane or toluene is consistent with the existence of only one isomer of C_{2h} symmetry present in solution. This analysis is deceptively simple as shown by the ^{1}HNMR spectroscopic study, see below.

X-Ray Crystallographic Study of IIa. An ORTEP diagram is shown in Figure I, in which one of the trans-disposed $Me_3SiC_5H_4$ groups on a molybdenum atom has been replaced by Cp1 for clarity. Positional parameters are in Table II and crystal data are in Table IV. Thermal parameters and structure factors are in Supplementary Material. Some bond lengths and bond angles are in Table III.

The molecule crystallizes in the monoclinic crystal system with space group $P2_1/n$. The structure consists of centrosymmetric dimers. The four metal atoms (two molybdenum and two ytterbium) in the molecule are coplanar as imposed by the inversion center and the molecule has idealized C_{2h} symmetry as





Ia, R = H
b, R = $SiMe_3$

II a
II b

suggested by the solution infrared spectrum. Two of the carbonyl groups on each molybdenum atom form essentially linear Mo-CO-Yb bridges to the ytterbium atoms since the averaged Mo-C(30,31)-O(1,2) and C(30,31)-O(1,2)-Yb angles are 177.5 ± 0.1° and 172.8 ± 3.0°, respectively. The dihedral angle formed by the intersection of the Yb_2Mo_2 and YbO(1)O(2') planes is 1.6° and between the Yb_2Mo_2 and MoC(3')C(3) planes is 1.9°, indicating that the twelve-membered $Yb_2Mo_2C_4O_4$ ring is nearly planar. The angle between the centroids of the $Me_3SiC_5H_4$ rings and the Mo_2Yb_2 plane is 56°. The $Me_3SiC_5H_4$ rings are canted so that the Me_3Si group fits into the slot between the two staggered Me_5C_5 rings attached to the ytterbium atoms.

The coordination geometry about each ytterbium atom is pseudotetrahedral if the Me_5C_5 ring centroids are considered to occupy a coordination site. The centroid-Yb-centroid angle is 140° and the O(1)-Yb-O(2) angle is 88.3(1)°. The averaged ytterbium to ring centroid distance is 2.30Å, the averaged Yb-C distance is 2.58 ± 0.01Å, and the Yb-O distance is 2.245(3)Å. These parameters are similar to those of the Yb-Mn[1a] and Yb-Fe[1b] complexes described earlier.

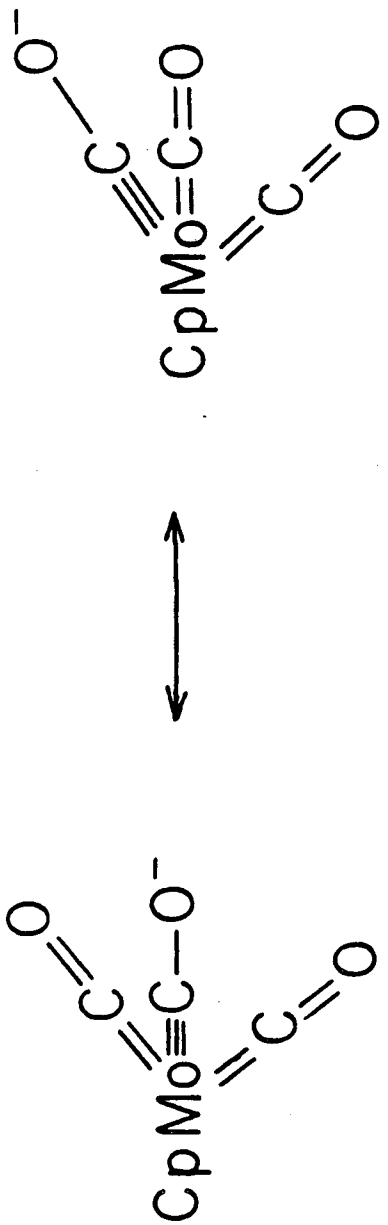
The feature of most interest in the structure of IIa is the terminal Mo-C and bridging Mo-C distances and their corresponding C-O distances. These are listed in Table V along with bond distances in related molecules. By comparing the first two entries it is apparent that reduction of the metal-metal bond in the dimer, $Cp_2Mo_2(CO)_6$, to give the separated ion-pair, $[Bn^n_4N][CpMo(CO)_3]$ shortens the Mo-C bond by 0.07 Å and lengthens the C-O bond by 0.03 Å. In molecules that contain terminal Mo-CO and bridging Mo-CO-M bonds, it is informative to compare the Mo-C distances within the same molecule. The Mo-C distance associated with the bridging carbonyl group is shortened by 0.04 to 0.10 Å and the C-O bond is lengthened by 0.03 to 0.06 Å

relative to the Mo-CO terminal bond. The molybdenum-ytterbium complex is not an exception to this trend. Thus, coordination and electron-transfer into the l.u.m.o. of a carbon monoxide ligand results in stretching the C-O bond, shrinking the Mo-C bond since the l.u.m.o. is CO antibonding and M-C bonding.[3b] This may be expressed by the valence-bond structures shown below.

(See illustration, next page)

The molybdenum-ytterbium complex can be thought of as a metallacetonyl-acetonate complex,[6] i.e., the two $[(Me_5C_5)_2Yb(III)]$ groups are bridged by the two $[(RC_5H_4)Mo(CO)(\mu\text{-}CO)_2]$ groups, affording the twelve-membered ring structure.

Solution Studies. The solution infrared spectra of I in cyclohexane and tetrahydrofuran are quite different, as shown in Table I. The number of absorptions is the same but the middle absorption increases by ca. 100 cm^{-1} and the lowest energy absorption decreases by 55 cm^{-1} on going from the hydrocarbon to the ether solvent. A similar pattern is observed in $Cp_4Ti_2(MeC_5H_4)_2Mo_2(CO)_6$, whose molecular structure and infrared spectrum in Nujol is similar to II, Table I. Further, the infrared spectrum of the titanium-molybdenum compound in tetrahydrofuran is similar to I in tetrahydrofuran. The crystal structure of the C_5H_5-titanium-molybdenum complex, crystallized from tetrahydrofuran, shows that only one of the carbonyl groups of $CpMo(CO)_3$ is bridging and the tetrahydrofuran ligand is coordinated to the titanium atom, $Cp_2Ti(thf)(\mu\text{-}OC)Mo(CO)_2Cp$.[4f] It is reasonable to postulate that a similar bridge splitting reaction occurs between I and tetrahydrofuran, i.e., the ether is a strong enough base to cleave the dimer into monomeric


O
C
C
O
C
O
CpMo
C
O
O
C
C
O
O
CpMo
C
O

units giving $(Me_5C_5)_2Yb(thf)(\mu\text{-}OC)(CO)_2MoCp$, but not strong enough to give the completely solvent-separated ion-pair, $[(Me_5C_5)_2Yb(thf)_x][CpMo(CO)_3]$. Similar cleavage reactions of ytterbium-isocarbonylmetal bonds were noted earlier.[1]

^{1}HNMR Spectroscopy. The ^{1}HNMR spectra at 25°C of I and II appear to be contradictory. The spectrum of I (C_5H_5) consists of two resonances at δ32.8 and 8.16 in area ratio 10:60 due to C_5H_5 and C_5Me_5 resonances, respectively. This is consistent with the presence of a single isomer in solution, a result that is consistent with the infrared spectrum in cyclohexane. However, the ^{1}HNMR spectrum of II($Me_3SiC_5H_4$) at 25°C indicates the presence of two complexes, tentatively identified as trans and cis isomers, IIa. and IIb, in the approximate ratio of 55:45, since each $Me_3SiC_5H_4$ group shows three broadened ($\nu_{\frac{1}{2}}$ is ca. 30 Hz) single resonances (at 250 MHz) due to the AA'BB'X_9 spin system at δ34.80, 33.50, 25.58 and 34.63, 32.05, and 29.30 in area ratio of 1.76:1.76:7.92 and 2.00:2.00:9.00, respectively. This gives the 45:55 area ratio of the two isomers. The resonances associated with the Me_5C_5 protons appear as three broadened ($\nu_{\frac{1}{2}}$ is ca. 60 Hz) singlets at δ8.98, 7.55 and 8.27 in an area ratio of 13.2:13.2:30. As the trans-isomer (IIa) has idealized C_{2h} symmetry and therefore chemically equivalent Me_5C_5 rings (assuming free rotation about the pseudo-five fold Me_5C_5-ring to ytterbium rotation axis) and the cis-isomer (IIb) has idealized C_{2v} symmetry and chemically inequivalent Me_5C_5 rings, we conclude that the isomer in greater abundance (55% at 25°C) is the trans-isomer. The isomer population does not appear to change on cooling, but on warming the resonances coalesce at 130°C (the chemical shifts are linear in T^{-1}) and $\Delta G^{\neq}$(Tc), assuming an equal population two site exchange model is valid, is ca. 20 kcal mol.$^{-1}$ The chemical shift difference, δν at Tc, is determined by plotting the chemical shift as a function of T^{-1}(K) in the slow exchange region and extrapolating to the coalescence temperature, Tc.[7] The

activation energy is not very accurate since it was assumed that the equal population two-site exchange model is valid and only one set of $Me_3SiC_5H_4$ protons could be used in determining Tc. This is due to the fact that the temperature dependence of the chemical shift for all of the other resonances in the complex is such that the difference in the chemical shift between each set of peaks decreases as the temperature is raised. Eventually the chemical shift difference for each set of protons in each pair of isomers becomes unobservable and the resonances accidentally overlap before they broaden and coalesce as expected for an exchanging system. The two $Me_3SiC_5H_4$ resonances that do broaden and coalesce due to equilibration of the trans and cis isomers do so only because their chemical shift difference increases, rather than decreases as observed for the AA'BB' protons, as the temperature is raised so that they broaden and coalesce as expected for a system undergoing chemical exchange.

The presence of two isomers in solution in the $Me_3SiC_5H_4$ complex that undergo chemical exchange with a substantial activation energy barrier caused us to examine more closely the ^{1}HNMR spectral results on the C_5H_5 system. Lowering the temperature to -58°C causes the room temperature resonance at δ32.8 to split into two new resonances at δ44.8 and 43.6, $\nu_{\frac{1}{2}}$ are ca. 50 Hz, and the Me_5C_5 resonance to move upfield to δ11.1, $\nu_{\frac{1}{2}}$ = 87 Hz. The observation of a trans $\rightleftharpoons$ cis equilibrium in II and the apparent lack of such a process in I is perplexing, since it seems unreasonable to suggest that the activation barrier's for the two complexes are so different, ca. 10 kcal mol^{-1}. The key to this apparent dicotomy is that I does not behave like a chemically exchanging system since the two C_5H_5 resonances at -58°C do not broaden and coalesce as the temperature is raised but they move into each other and move to a lower frequency due to the temperature dependence of their

chemical shifts, not because they are undergoing chemical exchange. Hence the C_5H_5 system is best rationalized by postulating that two isomers are present in solution and the chemical shift difference for the Me_5C_5 protons in the two isomers is smaller than the observed line width, $\nu_{\frac{1}{2}}$ = 87 Hz at 25°C.

The infrared spectral results, which indicate that only the trans-isomer of I and II is present in solution need to be rationalized. This is not a time scale problem since the infrared time scale is shorter than the NMR one[8], but could indicate that the frequencies of the absorptions due to the cis (six absorptions) and trans (three absorptions) isomers are very close in energy so that the absorptions are not resolved and/or some of the absorptions are weak. Similar apparent spectroscopic contradictions have been observed in the parent complex $Cp_2Mo_2(CO)_6$.[3a] In the latter case observation of the infrared spectrum in a variety of solvents of different dielectric constant helped yield an internally consistent explanation. We can not do such a study since solvents such as tetrahydrofuran cleave the dimeric units.

It is of some interest to speculate on the mechanism of trans $\rightleftarrows$ cis isomerization in II.[9] An intramolecular process in which none of the Yb-O bonds cleave, seems unlikely since the molybdenum atoms are so far apart and the Me_5C_5 groups cause considerable steric congestion above and below the molybdenum-molybdenum vector. An intermolecular process is more appealing and the high activation energy barrier is consistent with this notion. A cross-over experiment will delineate the difference between these two extreme mechanisms.[10] Equimolar quantities of I and II were stirred in toluene for 24h. Evaporation of the toluene and dissolution in benzene-d_6 gave a ^{1}HNMR spectrum at 25°C that showed resonances due to cis and trans I and II, as well as new resonances that are consistent with the cross-over products. The spectrum is very complex since there are two geometrical isomers for I, II, and for the

cross-over compound. This complexity precludes quantitative study. Further, we cannot say whether the intermolecular process leads to <u>trans</u> ⇄ <u>cis</u> isomerization, all the cross-over experiment says is that I and II undergo intermolecular exchange at room temperature during the course of 24 hours.

These studies suggested that a careful examination of the ytterbium-iron system, $(RC_5H_4)_2Fe_2(\mu\text{-}CO)_4Yb_2(C_5Me_5)_4$, might reveal some hidden exchange processes.[1] This system is relatively straight forward to study since no isomerization of the ligands is possible. Mixing equimolar amounts of $(MeC_5H_4)_2Fe_2(\mu\text{-}CO)_4\text{-}Yb_2(C_5Me_5)_4$ (III) and $(Me_3SiC_5H_4)Fe_2(\mu\text{-}CO)_4Yb_2(C_5Me_5)_4$ (IV) in PhMe-d_8 shows that statistical cross over occurs within <u>ca</u>. 10 minutes. The room temperature ^{1}HNMR spectrum is shown in Figure II. The single resonances due to the $AA'BB'X_3$ spin system of (III) appear at δ44.2, 40.3, and 38.5, respectively, and the $AA'BB'X_9$ spin system of (IV) appear at δ50.2, 32.3, and 19.5, respectively.[1] The other six singlets can be assigned to the cross-over product, $(MeC_5H_4)(Me_3SiC_5H_4)Fe_2(\mu\text{-}CO)_4Yb_2(C_5Me_5)_4$. Integration shows that the area ratio of III:IV:III/IV is 1:1:2. Heating the sample to 164° results in only one $(MeC_5H_4)Fe$ and one $(Me_3SiC_5H_4)Fe$ environment which means that the cross-over equilibrium is fast at this temperature. A simple two site exchange approximation gives values of $\Delta G^{\ddagger}$(Tc) for all six resonances that coalesce at 164°C that range from 19.0 to 19.8 kcal mol^{-1} with an averaged value of 19.4 kcal $mole^{-1}$. The similarity of the $\Delta G^{\ddagger}$(Tc) values in the iron-ytterbium case, (I) and (II), suggests but does not prove that cross-over in the latter system leads to isomerization and that these processes proceed by a common mechanism.

Two mechanistic postulates are shown in the Scheme (see next page) in which the Fe-Yb is used as a symbol for the Fe-CO-Yb unit. In pathway a, the complex completely dissociates into monomeric fragments FeYb and Fe'Yb and

then these combine to give the cross-over product. In pathway b, one Yb-O bond of the dimer breaks to give the opened dimer fragments $FeYb_2Fe$ and Fe'YbYbFe' which can then undergo cross-over. This mechanistic problem is similar to that for bridge-terminal exchange in $Me_4Al_2(\mu\text{-}Me)_2$[11]. In principal, it is possible to tell the difference between these two pathways by measuring the rate of cross-over since the method of initial rates predicts that the order for each reactant in a is 0.5 and the order for each reactant in b is 1. Unfortunately the overlapping of the resonances in the ^{1}HNMR spectrum does not allow us to determine the concentration of the species reliably. In order to separate the resonances farther apart we mixed equal molar amounts of $(Me_3SiC_5H_4)_2Fe_2(\mu\text{-}CO)_4Yb_2(C_5Me_5)_4$ and its ruthenium analogue.[1] Cross-over does indeed occur but, the low solubility at low temperature renders signal integration unreliable. This is unfortunate but the key point is that these dimers are undergoing intermolecular exchange in hydrocarbon solution. This is perhaps expected since lanthanide ions are labile ions in aqueous and non-aqueous solution.[12] Further, the transition metal carbonyl anion fragment in these lanthanide complexes can be viewed as alkoxide ligands with electron withdrawing substituents and metal alkoxides undergo rapid ligand exchange processes in solution.[13]

Experimental Section. All operations were carried out under nitrogen. Microanalyses were performed by the Microanalytical Laboratory of this department. Infrared spectra were recorded on a Perkin-Elmer 597 instrument; solid spectra were measured on Nujol mulls and solution spectra were measured in matched NaCl cells. The ^{1}HNMR spectra were measured at 250 MHz and the chemical shifts are expressed in δ-units, relative to Me_4Si at δ=0 with positive values to high frequency.

$\{[(Me_5C_5)_2Yb(III)][C_5H_5Mo(CO)_3]\}_2$

Bis(pentamethylcyclopentadienyl)ytterbium(II) diethyletherate (0.53g, 0.0010 mol) in toluene (30 mL) was added to a solution of $[(C_5H_5)Mo(CO)_3]_2$ (0.25g, 0.00051 mol) in toluene (10 mL). The reaction mixture turned dark purple upon mixing. After stirring for ca. 12 h the solution was filtered, concentrated to ca. 5 mL, then ca. 5 mL pentane was added. The resultant solution was then cooled to -70°C. The dark purple prisms (0.36 g, 51%) were collected and dried under reduced pressure, Mp. 335°C (dec). Anal. Calcd. for $C_{28}H_{35}MoO_3Yb$: C, 48.8; H, 5.12. Found: C, 49.0; H, 5.14. ^1H NMR (25°C) δ8.16($\nu_{\frac{1}{2}}$ = 62 Hz, 30 H) δ32.85($\nu_{\frac{1}{2}}$ = 10 Hz, 5H). Ir (Nujol): 3110brw, 2730w, 2030w, 1942vs, 1931vs, 1730brs, 1680brs, 1609s, 1165w, 1110w, 1057w, 1022w, 1005m, 783s, 725w, 640w, 615m, 584m, 503s, 482m, 470sh, 390m, 321s, 268sh cm^{-1}. Methyl iodide (0.00017 mol) was added to a solution of $\{[(Me_5C_5)_2Yb][C_5H_5Mo(CO)_3]\}_2$ (0.10g, 0.000072 mol) in toluene (30 mL). The solution was stirred for ca. 12 hr, and the solvent was removed under reduced pressure. The residue was extracted into pentane and the ir spectrum of the pentane extract showed bands attributable to $C_5H_5Mo(CO)_3Me$ and $C_5H_5Mo(CO)_3I$. The concentration of the latter was estimated to be ca. 5% on the basis of relative band area.

$\{[(Me_5C_5)_2Yb(III)][Me_3SiC_5H_4Mo(CO)_3]\}_2$

The ether complex of Bis(pentamethylcyclopentadienyl)ytterbium(II) (0.79g, 0.0015 mol) in toluene (60 ml) was added to trimethylsilylcyclopentadienylmolybdenumtricarbonyl dimer (0.48g, 0.00076 mol) in toluene (15 ml). The reaction mixture was stirred for ca. 12 hr. The purple solution was filtered, and the filtrate was concentrated under reduced pressure to ca. 20 ml. Cooling to -10°C afforded purple prisms of product. The product was

collected, and dried under reduced pressure. The mother liquors were concentrated to ca. 2 ml and cooled to -10°C, producing another crop of crystals. The combined yield was 0.87 g (76%), Mp. 300-310° (dec). Anal. Calcd. for $C_{62}H_{86}O_6Si_2Yb_2Mo_2$: C, 48.9: H, 5.70. Found: C, 48.3: H, 5.79. ^{1}HNMR (250 MHz, 25°C); δ34.8, (1.76H); 34.63, (2.0 H); 33.50, (1.76 H); 32.05, (2.0 H); 25.58, (7.92 H); 25.30, (9 H); 8.98, (13.2 H); 8.27, (30 H); 7.55, (13.2 H).

X-Ray Crystallography

Purple crystals of $[(Me_5C_5)_2Yb(Me_5SiC_5H_4)Mo(CO)_3]_2$ were obtained by slow cooling of a toluene solution to -10°C. They were mounted in thin walled quartz capillaries in an argon filled dry box, and then were flame sealed. Preliminary precession photographs indicated monoclinic (2/m) Laue symmetry and yielded preliminary cell dimensions. Examination of the 0k0, and h01 zones showed systematic absences 0k0 $h\neq 2n+1$; h01, $1+h\neq 2n+1$ consistent only with space group $P2_1/n$ (non-standard setting of $P2_1/c$).

The data crystal was then mounted on an Enraf-Nonius CAD4 automated diffractometer (for details of the CHEXRAY facility see ref. 1), and centered on the beam. Automatic peak search and indexing yielded the same unit cell as did the precession photographs, and confirmed the Laue symmetry. Accurate cell dimensions and orientation matrix were determined by a least-squares fit to the setting angles of the unresolved MoKα components of 24 symmetry related reflections with 2θ between 24 and 30°. The results are given in Table I along with the parameters used for data collection.

The 4709 raw intensity data were converted to structure factor amplitudes and their esd's by correction for scan speed, background, and Lorentz-polarization effects. Analysis of the azimuthal scan data showed a small variation in the average relative intensity (I_{min}/I_{max} = .927) curve. An

empirical absorption correction using the average relative intensity curve of the azimuthal scan data was performed because of the irregular shape of the crystal.

Rejection of systematically absent and redundant data yielded a unique set of 4293 data which were used to solve and refine the structure. Analysis of a three-dimensional Patterson map revealed the positions of the ytterbium and molybdenum atoms. The remaining atoms in the structure were found using the standard Fourier techniques, and the structure was refined using standard least-squares techniques. Hydrogen atoms were placed in idealized positions having fixed thermal parameters, and were included in structure factor calculations, but were not refined.

The final residuals for 335 variables refined against the 3327 data for which $F^2 > 3\sigma(F^2)$ were R = 2.07%, wR = 2.59%, and GOF = 1.74. The R value for all 4293 data was 4.35%.

The quantity minimized by the least-squares program was $\sum w(|F_o|-|F_c|)^2$, where w is the weight of a given observation. The p-factor, used to reduce the weight of intense reflections, was set to 0.015 in the final stages of refinement. The analytical forms for the scattering factor tables for the neutral atoms were used and all non-hydrogen scattering factors were corrected for both the real and imaginary components of anomalous dispersion.

Inspection of the residuals ordered in ranges of $\sin\theta/\lambda$, $|F_o|$, and parity and value of the individual indexes showed no unusual features or trends. There was evidence of secondary extinction in the low-angle, high-intensity data, and a correction for secondary extinction was applied. The largest peak in the final difference Fourier map had an electron density of .384 $e^-/Å^3$ near the Mo atom.

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Supplementary Material. Structure factor tables, General Temperature Expressions, Amplitudes of Thermal Vibration, and carbon-carbon bond lengths and angles (22 pages).

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Table I

Infrared Spectra of $(RC_5H_4)Mo(CO)_3X$ Complexes

Compound	Medium	νCO in cm^{-1}	Reference
$Cp_2Mo_2(CO)_6$	cyclohexane	1966s, 1922s	3a
	tetrahydrofuran	2014s, 1959m, 1916w	3a
$NaCpMo(CO)_3$	tetrahydrofuran	1899s, 1796s, 1743m	2a
$KCpMo(CO)_3$	tetrahydrofuran	1897s, 1798s, 1748m	2a
$PPNCpMo(CO)_3$	tetrahydrofuran	1896s, 1780s	2a
$Mg(thf)_4[CpMo(CO)_3]_2$	tetrahydrofuran	1912s, 1815s, 1680s	4a
$Mg(py)_4[CpMo(CO)_3]_2$	Nujol	1918s, 1828s, 1667s	4b
$Mn(py)_4[CpMo(CO)_3]_2$	Nujol	1905s, 1808s, 1650s	4c
$Cp_4Ti_2[MeC_5H_4Mo(CO)_3]_2$	Nujol	1920, 1755, 1710	4d
	tetrahydrofuran	1920s, 1830s, 1650s	4e
$(Me_5C_5)_4Ti_2[CpMo(CO)_3]_2$	Nujol	1925s, 1835s, 1610s	4e
$(Me_5C_5)_4Yb_2(CpMo(CO)_3]_2$	cyclohexane	1940s, 1730s, 1680s	this
	tetrahydrofuran	1927s, 1828s, 1625s	work
$(Me_5C_5)_4Yb_2[(Me_3SiC_5H_4)Mo(CO)_3]_2$	cyclohexane	1944s, 1730s, 1682s	this
	toluene	1935s, 1730s, 1685s	work

Table II

Positional Parameters

Atom	x	y	z	$B(A^2)$
YB1	Ø.12175(1)	Ø.ØØØ93(1)	Ø.3Ø177(1)	2.735(4)
MO1	Ø.25Ø49(3)	Ø.Ø1518(3)	Ø.62661(3)	3.83Ø(9)
SI1	Ø.3476(1)	Ø.Ø168(1)	Ø.8538(1)	5.21(4)
O1	-Ø.Ø363(2)	-Ø.ØØ33(2)	Ø.3294(2)	4.5Ø(8)
O2	Ø.1578(3)	Ø.ØØ31(2)	Ø.4434(2)	4.45(7)
O3	Ø.2652(3)	-Ø.1868(3)	Ø.6312(3)	8.4(1)
C1	Ø.2997(4)	Ø.137Ø(4)	Ø.712Ø(3)	5.8(1)
C2	Ø.3524(3)	Ø.Ø64Ø(4)	Ø.7449(3)	4.9(1)
C3	Ø.4143(4)	Ø.Ø386(5)	Ø.6794(4)	8.Ø(2)
C4	Ø.3978(5)	Ø.Ø922(6)	Ø.6Ø9Ø(4)	1Ø.6(2)
C5	Ø.3288(5)	Ø.1544(4)	Ø.6273(4)	9.1(2)
C6	Ø.3962(7)	-Ø.Ø94Ø(5)	Ø.8559(5)	14.4(3)
C7	Ø.2216(6)	Ø.Ø16Ø(6)	Ø.8854(5)	11.5(3)
C8	Ø.4192(5)	Ø.Ø854(5)	Ø.9298(4)	8.3(2)
C1Ø	Ø.2195(3)	-Ø.1423(3)	Ø.3227(3)	4.Ø(1)
C11	Ø.2351(3)	-Ø.1164(3)	Ø.241Ø(3)	4.2(1)
C12	Ø.1465(4)	-Ø.1227(3)	Ø.1915(3)	4.2(1)
C13	Ø.Ø761(4)	-Ø.1531(3)	Ø.2454(3)	4.3(1)
C14	Ø.122Ø(3)	-Ø.1647(3)	Ø.3275(3)	4.Ø(1)
C15	Ø.3ØØØ(5)	-Ø.1516(4)	Ø.3925(4)	8.Ø(2)
C16	Ø.3333(4)	-Ø.1ØØ4(4)	Ø.2Ø69(5)	8.Ø(2)
C17	Ø.13Ø5(6)	-Ø.1129(4)	Ø.Ø968(4)	8.9(2)
C18	-Ø.Ø267(4)	-Ø.1796(4)	Ø.22Ø8(5)	8.2(2)
C19	Ø.Ø751(5)	-Ø.197Ø(4)	Ø.4Ø64(4)	7.7(2)
C2Ø	Ø.2287(3)	Ø.1374(3)	Ø.2921(3)	4.3(1)
C21	Ø.1475(4)	Ø.1652(3)	Ø.3325(3)	4.6(1)
C22	Ø.Ø682(4)	Ø.1615(3)	Ø.2748(3)	4.8(1)
C23	Ø.Ø991(4)	Ø.13Ø6(3)	Ø.1964(3)	5.1(1)
C24	Ø.2Ø1Ø(4)	Ø.118Ø(3)	Ø.2Ø78(3)	4.9(1)
C25	Ø.33Ø8(5)	Ø.1363(4)	Ø.3297(5)	1Ø.2(2)
C26	Ø.1436(7)	Ø.2Ø13(4)	Ø.4218(4)	9.8(2)
C27	-Ø.Ø338(5)	Ø.1934(4)	Ø.2873(5)	1Ø.2(2)
C28	Ø.Ø387(6)	Ø.1244(5)	Ø.1133(4)	11.7(2)
C29	Ø.2664(6)	Ø.1Ø28(4)	Ø.1381(5)	11.1(2)
C3Ø	-Ø.1194(3)	-Ø.ØØ69(3)	Ø.3449(3)	3.4(1)
C31	Ø.1958(3)	Ø.ØØ65(3)	Ø.5141(3)	3.5(1)
C32	Ø.2595(4)	-Ø.11Ø6(4)	Ø.6294(4)	5.5(1)
H11	Ø.2478	Ø.1692	Ø.7422	7.5**
H31	Ø.4572	-Ø.Ø1Ø6	Ø.68Ø9	1Ø.Ø**
H41	Ø.4235	Ø.Ø941	Ø.5569	1Ø.Ø**
H51	Ø.2984	Ø.2Ø48	Ø.5964	1Ø.Ø**
H61	Ø.3971	-Ø.1216	Ø.9Ø82	15.Ø**
H62	Ø.3612	-Ø.1314	Ø.8129	15.Ø**
H63	Ø.4642	-Ø.Ø943	Ø.8366	15.Ø**
H71	Ø.2173	-Ø.ØØ58	Ø.94Ø4	12.Ø**
H72	Ø.1975	Ø.Ø768	Ø.8847	12.Ø**
H73	Ø.1813	-Ø.Ø154	Ø.8452	12.Ø**
H81	Ø.4199	Ø.Ø633	Ø.9881	8.Ø**
H82	Ø.4873	Ø.Ø894	Ø.9164	8.Ø**
H83	Ø.3956	Ø.1448	Ø.9319	8.Ø**

Table II

Positional Parameters

H151	Ø.3299	-Ø.2Ø79	Ø.3939	8.5**
H152	Ø.35Ø8	-Ø.1Ø85	Ø.388Ø	8.5**
H153	Ø.2752	-Ø.1426	Ø.4496	8.5**
H161	Ø.3615	-Ø.1535	Ø.1884	8.5**
H162	Ø.3282	-Ø.Ø6Ø7	Ø.1594	8.5**
H163	Ø.3772	-Ø.Ø748	Ø.25Ø1	8.5**
H171	Ø.1424	-Ø.1667	Ø.Ø668	8.5**
H172	Ø.Ø633	-Ø.Ø965	Ø.Ø799	8.5**
H173	Ø.1711	-Ø.Ø688	Ø.Ø741	8.5**
H181	-Ø.Ø288	-Ø.2391	Ø.2Ø14	8.5**
H182	-Ø.Ø658	-Ø.175Ø	Ø.269Ø	8.5**
H183	-Ø.Ø539	-Ø.1433	Ø.1761	8.5**
H191	Ø.Ø779	-Ø.2584	Ø.41Ø4	8.5**
H192	Ø.1Ø6Ø	-Ø.1716	Ø.4567	8.5**
H193	Ø.ØØ72	-Ø.1794	Ø.4Ø42	8.5**
H251	Ø.3627	Ø.1898	Ø.3218	1Ø.Ø**
H252	Ø.3324	Ø.1234	Ø.39Ø1	1Ø.Ø**
H253	Ø.368Ø	Ø.Ø9Ø3	Ø.3Ø37	1Ø.Ø**
H261	Ø.156Ø	Ø.263Ø	Ø.4226	1Ø.Ø**
H262	Ø.Ø84Ø	Ø.1899	Ø.4455	1Ø.Ø**
H263	Ø.1953	Ø.1746	Ø.4588	1Ø.Ø**
H271	-Ø.Ø4Ø4	Ø.2545	Ø.2764	1Ø.Ø**
H272	-Ø.Ø816	Ø.1621	Ø.2552	1Ø.Ø**
H273	-Ø.Ø479	Ø.1859	Ø.3486	1Ø.Ø**
H281	Ø.Ø378	Ø.1785	Ø.Ø819	12.Ø**
H282	Ø.Ø624	Ø.Ø798	Ø.Ø76Ø	12.Ø**
H283	-Ø.Ø286	Ø.1Ø97	Ø.122Ø	12.Ø**
H291	Ø.2868	Ø.1572	Ø.1131	12.Ø**
H292	Ø.3247	Ø.Ø718	Ø.1569	12.Ø**
H293	Ø.2348	Ø.Ø691	Ø.Ø923	12.Ø**

* -- Atoms refined with isotropic thermal parameters.
** -- Atoms included but not refined.
Anisotropically refined atoms are given in the form of the isotropic equivalent thermal parameter defined as:

$$(4/3) * [a^2*B(1,1) + b^2*B(2,2) + c^2*B(3,3) + ab(\cos \text{gamma})*B(1,2) + ac(\cos \text{beta})*B(1,3) + bc(\cos \text{alpha})*B(2,3)]$$

Table III

Bond Lengths and Bond Angles

Intramolecular Distances

ATOM 1	ATOM 2	DISTANCE
YB1	O1	2.245(3)
YB1	O2	2.245(3)
YB1	C1Ø	2.581(4)
YB1	C11	2.596(4)
YB1	C12	2.597(4)
YB1	C13	2.581(4)
YB1	C14	2.565(4)
YB1	C111	2.295(1)
YB1	C2Ø	2.565(4)
YB1	C21	2.578(4)
YB1	C22	2.592(4)
YB1	C23	2.587(4)
YB1	C24	2.6ØØ(4)
YB1	C112	2.296(1)
MO1	C1	2.369(4)
MO1	C2	2.377(4)
MO1	C3	2.383(4)
MO1	C4	2.377(6)
MO1	C5	2.387(5)
MO1	C1Ø1	2.Ø54(1)
MO1	C3Ø	1.89Ø(4)
MO1	C31	1.88Ø(4)
MO1	C32	1.928(5)
C3Ø	O1	1.185(4)
C31	O2	1.196(4)
C32	O3	1.169(5)

Intramolecular Angles

ATOM 1	ATOM 2	ATOM 3	ANGLE
O1	YB1	O2	88.26(1Ø)
O1	YB1	C111	1Ø5.Ø2(6)
O1	YB1	C112	1Ø4.89(6)
O2	YB1	C111	1Ø2.55(6)
O2	YB1	C112	1Ø3.47(6)
C111	YB1	C112	14Ø.56(1)
C3Ø	MO1	C31	83.21(15)
C3Ø	MO1	C32	89.33(17)
C3Ø	MO1	C1Ø1	129.53(1Ø)
C31	MO1	C32	88.43(17)
C31	MO1	C1Ø1	128.81(11)
C32	MO1	C1Ø1	123.84(13)
YB1	O1	C3Ø	178.8(3)
YB1	O2	C31	166.8(3)
MO1	C3Ø	O1	177.8(3)
MO1	C31	O2	177.3(3)
MO1	C32	O3	179.9(3)

Table IV

Crystal Data (25°C) for $(Me_5SiC_5H_4)_2Mo_2(CO)_2(\mu\text{-}CO)_4Yb_2(C_5Me_5)_4$

Space Group	$P2_1/n$
a, Å	13.771(1)
b, Å	15.294(2)
c, Å	15.607(1)
β, deg	93.434(8)
V, $Å^3$	3294
z	2
fw	1520.70
d(calcd), g cm^{-3}	1.535
μ(calcd), cm^{-1}	32.5
size, mm	0.24 x 0.32 x 0.20
reflcns, collected	4709
reflcns, unique	4293
reflcns, $F_o^2 > 3\sigma(F_o^2)$	3327
R, %	2.07
R_w, %	2.59
GOF	1.74
monochromator	highly oriented graphite
radiation	MoKα (λ = 0.71073Å)
scan range, type	$3° \leq 2\theta \leq 45°$
scan speed, deg min^{-1}	0.69 - 6.7
scan width, deg	$\Delta\theta = 0.55 + 0.347 \tan\theta$

Table V

Molybdenum-Carbon and Carbon-Oxygen Bond Lengths

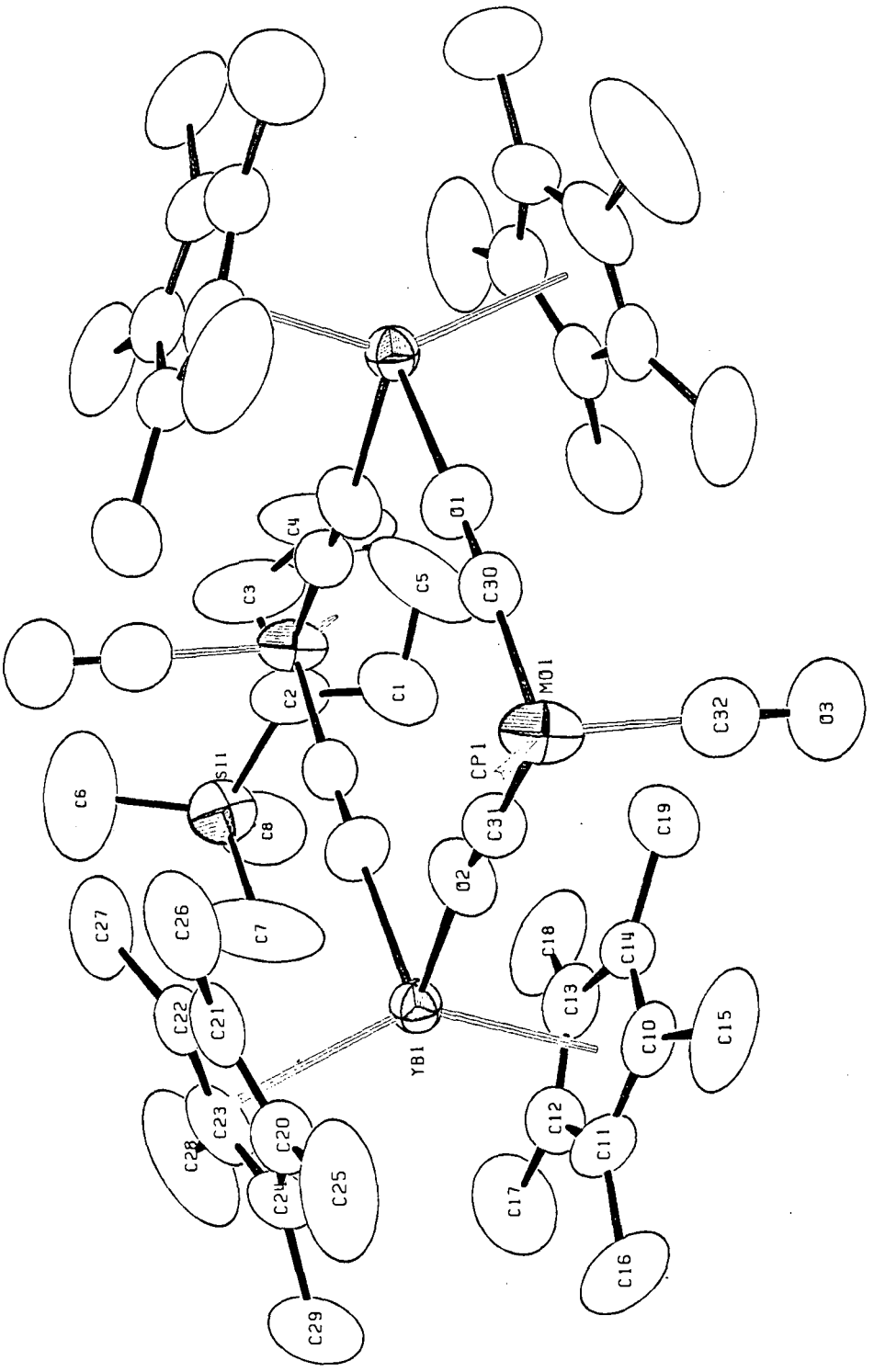
Compound	Mo-C(Å) (terminal)	Mo-C(Å) (bridging)	C-O(Å) (terminal)	C-O(Å) (bridging)	Ref.
$Cp_2Mo_2(CO)_6$	1.977(9)		1.148(2)		3a
$[Bu^n_4N][CpMo(CO)_3]$	1.909(8)		1.176(6)		5a
$[Mg(py)_4][CpMo(CO)_3]_2$	1.947(3)	1.886(2)	1.157(3)	1.189(3)	4b
$Ti(C_5Me_5)_2MeCpMo(CO)_3$	1.944(2)	1.875(4)	1.152(1)	1.212(5)	5b
$ZrCp_2MeCpMo(CO)_3$	1.93(3)	1.847(3)	1.16(1)	1.236(4)	5e
$TiCp_2(thf)CpMo(CO)_3$	1.925(5)	1.874(7)	1.152(2)	1.210(8)	4c
$Ti_2Cp_4[CpMo(CO)_3]_2$	1.92(2)	1.880(7)	1.180(5)	1.208(3)	4d
$Zr_2(NEt_2)_4(Et_2NH)_2[CpMo(CO)_3]_2$	1.96(2)	1.86(2)	1.15(2)	1.20(3)	5c

Figure I

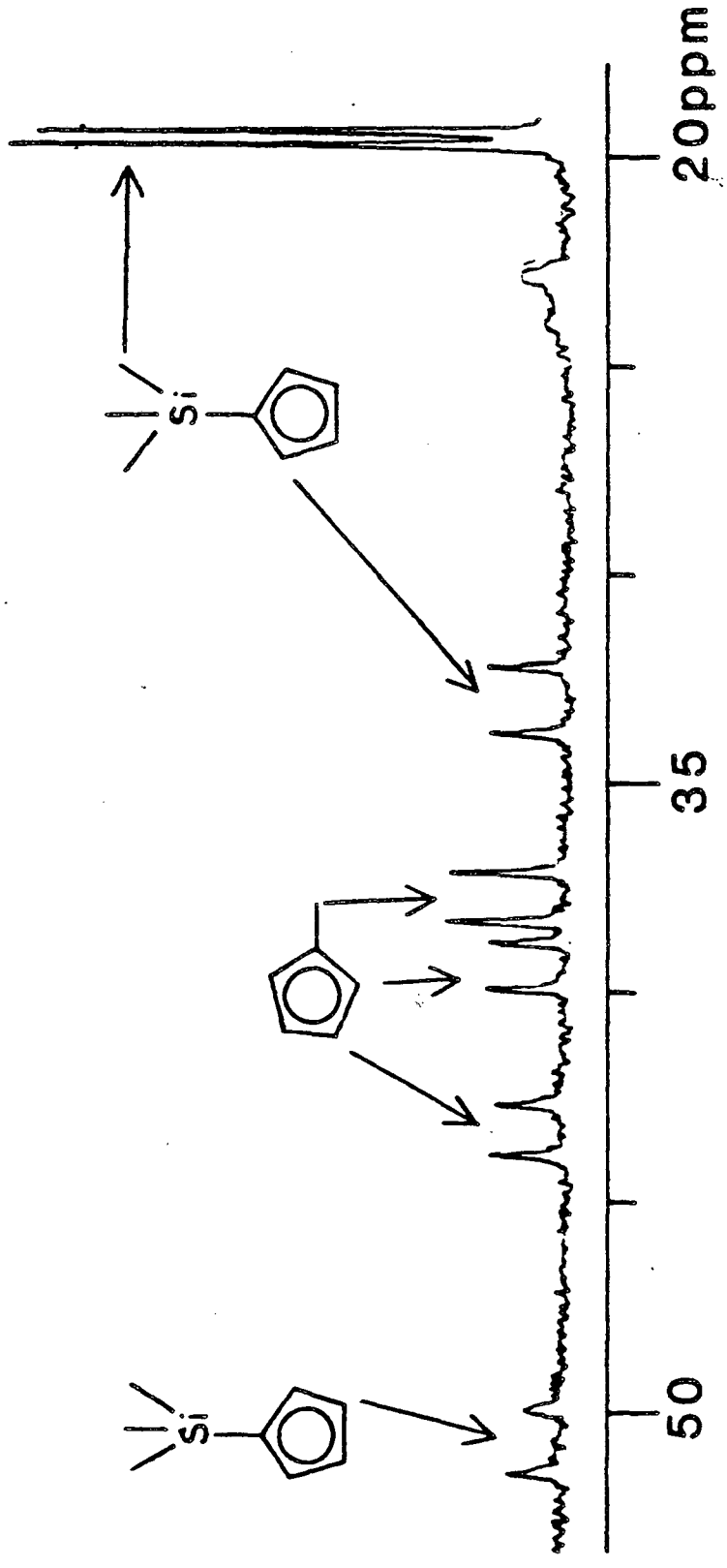
ORTEP Diagram of $(Me_5SiC_5H_4Yb_2(\mu\text{-}OC)_4Mo_2(CO)_2(C_5H_4SiMe_3)_2$. The $Me_5SiC_5H_4$ ligand on Mo(1) is removed and replaced by the symbol CP1 for clarity. The labelled atoms are related to their identical unlabelled atoms (noted by a prime, in text) by inversion.

Figure II

^{1}HNMR Spectrum of $(MeC_5H_4)_2Fe_2(\mu\text{-}CO)_4Yb_4(C_5Me_5)_4$ and $(Me_3SiC_5G_4)_2Fe_2(\mu\text{-}CO)_4Yb_4(C_5Me_5)_4$ at 25°C.



XBL 8310-11913



XBL 849-3836

Supplementary Material for Bis(Pentamethylcyclopentadienyl) Ytterbium(II) as a Lewis Acid and an Electron-Transfer Ligand; Preparation, Crystal Structure, and Solution Dynamics of $[Yb(C_5Me_5)_2(\mu\text{-}OC)_2Mo\text{-}(CO)(C_5H_4R)]_2$

James M. Boncella and Richard A. Andersen

Structure Factors, carbon-carbon bond distances and bond angles, general temperature expressions and amplitudes of thermal vibration

Table of General Temperature Factor Expressions - B's

Name	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)	Beqv
YB1	2.696(7)	2.635(7)	2.871(7)	-Ø.Ø75(8)	Ø.136(6)	Ø.Ø35(8)	2.735(4)
MO1	2.69(2)	5.75(2)	3.ØØ(2)	-Ø.77(2)	-Ø.17(1)	-Ø.Ø6(2)	3.83Ø(9)
SI1	4.81(7)	6.75(9)	3.91(6)	Ø.13(7)	-1.Ø7(6)	-Ø.1Ø(7)	5.21(4)
O1	3.1(1)	4.2(1)	6.3(2)	-Ø.2(1)	Ø.9(1)	-Ø.2(1)	4.5Ø(8)
O2	5.9(2)	3.9(1)	3.3(1)	-Ø.3(1)	-1.Ø(1)	Ø.2(1)	4.45(7)
O3	9.3(3)	7.Ø(2)	9.1(3)	2.9(2)	Ø.9(2)	1.3(2)	8.4(1)
C1	5.7(3)	6.4(3)	5.1(3)	-2.7(2)	-1.5(2)	Ø.1(2)	5.8(1)
C2	3.Ø(2)	7.9(3)	3.8(2)	-1.1(2)	-Ø.5(2)	-1.1(2)	4.9(1)
C3	2.7(2)	16.1(5)	5.1(3)	-1.8(3)	-Ø.4(2)	-2.4(3)	8.Ø(2)
C4	6.8(3)	2Ø.5(6)	4.8(3)	-7.9(3)	1.1(3)	-1.9(4)	1Ø.6(2)
C5	11.2(4)	1Ø.1(3)	5.6(3)	-8.Ø(3)	-2.5(3)	2.3(3)	9.1(2)
C6	23.6(9)	9.4(5)	9.2(5)	6.1(5)	-6.2(5)	-1.3(4)	14.4(3)
C7	6.5(4)	21.9(8)	6.1(4)	-2.6(4)	Ø.7(3)	3.8(4)	11.5(3)
C8	9.2(4)	1Ø.8(4)	4.6(3)	-2.1(4)	-1.1(3)	-1.2(3)	8.3(2)
C1Ø	4.Ø(2)	3.4(2)	4.4(2)	1.1(2)	-Ø.6(2)	-Ø.7(2)	4.Ø(1)
C11	3.6(2)	3.6(2)	5.6(3)	-Ø.Ø(2)	1.3(2)	-1.4(2)	4.2(1)
C12	5.8(3)	3.3(2)	3.6(2)	Ø.2(2)	Ø.3(2)	-Ø.6(2)	4.2(1)
C13	3.8(2)	3.1(2)	5.9(3)	Ø.Ø(2)	-Ø.9(2)	-1.2(2)	4.3(1)
C14	4.2(2)	2.8(2)	5.1(2)	Ø.3(2)	1.6(2)	Ø.1(2)	4.Ø(1)
C15	8.Ø(4)	6.4(3)	9.2(4)	3.7(3)	-3.6(3)	-2.6(3)	8.Ø(2)

Table of General Temperature Factor Expressions - B's (Continued)

Name	B(1,1)	B(2,2)	B(3,3)	B(1,2)	B(1,3)	B(2,3)	Beqv
C16	5.9(3)	5.2(3)	13.4(5)	-Ø.3(3)	4.2(3)	-2.8(3)	8.Ø(2)
C17	15.9(6)	6.5(3)	4.1(3)	Ø.3(4)	-Ø.4(4)	-1.5(3)	8.9(2)
C18	4.1(3)	5.8(3)	14.5(5)	Ø.1(2)	-1.5(3)	-3.8(3)	8.2(2)
C19	11.2(4)	4.Ø(3)	8.3(4)	Ø.7(3)	4.3(3)	1.3(3)	7.7(2)
C2Ø	3.4(2)	3.4(2)	6.1(3)	-Ø.7(2)	-Ø.Ø(2)	Ø.5(2)	4.3(1)
C21	7.2(3)	2.6(2)	3.9(2)	Ø.3(2)	-Ø.8(2)	Ø.4(2)	4.6(1)
C22	4.Ø(2)	3.Ø(2)	7.7(3)	Ø.5(2)	1.4(2)	1.7(2)	4.8(1)
C23	6.4(3)	4.1(2)	4.6(3)	-1.2(2)	-1.3(2)	1.7(2)	5.1(1)
C24	6.5(3)	3.3(2)	5.1(3)	-Ø.6(2)	2.5(2)	Ø.5(2)	4.9(1)
C25	5.7(3)	4.8(3)	19.6(7)	-1.2(3)	-3.6(4)	1.9(4)	1Ø.2(2)
C26	2Ø.2(7)	3.8(3)	5.5(3)	1.Ø(4)	2.Ø(4)	-Ø.2(3)	9.8(2)
C27	5.8(3)	5.3(3)	19.6(7)	1.6(3)	3.2(4)	4.3(4)	1Ø.2(2)
C28	17.5(6)	7.9(4)	8.7(4)	-4.2(4)	-7.7(4)	3.4(3)	11.7(2)
C29	17.Ø(5)	5.5(3)	12.Ø(4)	-1.1(4)	1Ø.4(3)	Ø.Ø(3)	11.1(2)
C3Ø	3.9(2)	3.Ø(2)	3.4(2)	-Ø.2(2)	-Ø.3(2)	-Ø.3(2)	3.4(1)
C31	3.4(2)	3.6(2)	3.6(2)	-Ø.Ø(2)	Ø.1(2)	Ø.1(2)	3.5(1)
C32	4.Ø(3)	7.2(3)	5.1(3)	1.4(2)	-Ø.2(2)	Ø.8(3)	5.5(1)

The form of the anisotropic thermal parameter is:

$$\exp[-0.25(h^2 a^{*2} B(1,1) + k^2 b^{*2} B(2,2) + l^2 c^{*2} B(3,3) + 2hka^*b^*B(1,2) + 2hla^*c^*B(1,3) + 2klb^*c^*B(2,3))]$$, where a*,b*, and c* are reciprocal lattice constants.

Table of Root-Mean-Square Amplitudes of Thermal Vibration in Angstroms.

Atom	Min.	Int'med.	Max.	Atom	Min.	Int'med.	Max.
YB1	0.181	0.186	0.191	C15	0.207	0.261	0.440
MO1	0.173	0.201	0.274	C16	0.212	0.256	0.442
SI1	0.196	0.272	0.293	C17	0.206	0.302	0.452
O1	0.192	0.230	0.285	C18	0.212	0.246	0.456
O2	0.191	0.221	0.290	C19	0.214	0.270	0.417
O3	0.249	0.334	0.384	C20	0.185	0.222	0.282
C1	0.184	0.260	0.344	C21	0.173	0.219	0.311
C2	0.169	0.231	0.325	C22	0.176	0.215	0.326
C3	0.166	0.252	0.461	C23	0.182	0.233	0.326
C4	0.199	0.241	0.554	C24	0.179	0.229	0.318
C5	0.181	0.245	0.502	C25	0.222	0.258	0.522
C6	0.276	0.320	0.606	C26	0.215	0.260	0.507
C7	0.242	0.291	0.543	C27	0.217	0.266	0.517
C8	0.219	0.334	0.394	C28	0.218	0.284	0.563
C10	0.178	0.211	0.273	C29	0.219	0.271	0.550
C11	0.181	0.213	0.288	C30	0.185	0.206	0.230
C12	0.190	0.226	0.272	C31	0.205	0.211	0.217
C13	0.179	0.211	0.295	C32	0.203	0.259	0.315
C14	0.185	0.203	0.276				

Intramolecular Distances

ATOM 1	ATOM 2	DISTANCE
YB1	O1	2.245(3)
YB1	O2	2.245(3)
YB1	C1Ø	2.581(4)
YB1	C11	2.596(4)
YB1	C12	2.597(4)
YB1	C13	2.581(4)
YB1	C14	2.565(4)
YB1	C111	2.295(1)
YB1	C2Ø	2.565(4)
YB1	C21	2.578(4)
YB1	C22	2.592(4)
YB1	C23	2.587(4)
YB1	C24	2.6ØØ(4)
YB1	C112	2.296(1)
MO1	C1	2.369(4)
MO1	C2	2.377(4)
MO1	C3	2.383(4)
MO1	C4	2.377(6)
MO1	C5	2.387(5)
MO1	C1Ø1	2.Ø54(1)
MO1	C3Ø	1.89Ø(4)
MO1	C31	1.88Ø(4)
MO1	C32	1.928(5)
C3Ø	O1	1.185(4)
C31	O2	1.196(4)
C32	O3	1.169(5)
C1	C2	1.412(6)
C1	C5	1.434(7)
C2	C3	1.426(6)
C3	C4	1.383(9)
C4	C5	1.387(9)
SI1	C2	1.858(4)
SI1	C6	1.821(6)
SI1	C7	1.834(6)
SI1	C8	1.831(5)
C1Ø	C11	1.369(5)
C1Ø	C14	1.391(5)
C11	C12	1.4Ø9(5)
C12	C13	1.4Ø3(6)
C13	C14	1.41Ø(6)
C1Ø	C15	1.517(5)
C11	C16	1.5Ø4(6)
C12	C17	1.494(6)
C13	C18	1.5ØØ(6)
C14	C19	1.512(6)
C2Ø	C21	1.385(6)
C2Ø	C24	1.385(6)
C21	C22	1.376(6)
C22	C23	1.4Ø5(6)
C23	C24	1.417(6)
C2Ø	C25	1.49Ø(6)
C21	C26	1.5Ø8(6)
C22	C27	1.511(6)
C23	C28	1.5Ø7(6)
C24	C29	1.475(6)

Intramolecular Angles

ATOM 1	ATOM 2	ATOM 3	ANGLE
C2	SI1	C6	11Ø.2(3)
C2	SI1	C7	1Ø9.71(23)
C2	SI1	C8	1Ø9.12(23)
C6	SI1	C7	11Ø.Ø(4)
C6	SI1	C8	1Ø9.8(3)
C7	SI1	C8	1ØØ.Ø(3)
SI1	C2	C1	126.6(4)
SI1	C2	C3	127.6(4)
C1	C2	C3	1Ø5.7(5)
C2	C3	C4	1Ø9.6(6)
C3	C4	C5	1ØØ.9(6)
C4	C5	C1	1Ø7.3(6)
C5	C1	C2	1ØØ.6(5)
C14	C1Ø	C11	1Ø9.1(4)
C1Ø	C11	C12	1ØØ.4(4)
C11	C12	C13	1Ø7.3(4)
C12	C13	C14	1Ø7.6(4)
C13	C14	C1Ø	1Ø7.6(4)
C15	C1Ø	C11	123.5(5)
C15	C1Ø	C14	127.2(5)
C16	C11	C1Ø	125.1(5)
C16	C11	C12	125.6(5)
C17	C12	C11	127.7(5)
C17	C12	C13	124.4(5)
C18	C13	C12	127.6(5)
C18	C13	C14	124.4(5)
C19	C14	C1Ø	125.8(5)
C19	C14	C13	126.6(5)
C2Ø	C21	C22	1ØØ.6(4)
C21	C22	C23	1ØØ.5(4)
C22	C23	C24	1Ø6.6(4)
C23	C24	C2Ø	1Ø7.8(4)
C24	C2Ø	C21	1ØØ.5(4)
C24	C2Ø	C25	125.Ø(5)
C21	C2Ø	C25	126.3(5)
C2Ø	C21	C26	127.6(5)
C22	C21	C26	123.6(5)
C21	C22	C27	127.5(6)
C23	C22	C27	123.7(5)
C22	C23	C28	126.6(6)
C24	C23	C28	126.3(6)
C23	C24	C29	124.9(6)
C2Ø	C24	C29	126.5(6)

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
0	0	2	4290	4337	23	0	4	1	762	804	8	0	7	9	347	331	8	0	11	10	273	258	12
0	0	4	2242	2171	8	0	4	2	540	587	6	0	7	11	241	240	12	0	11	11	263	253	13
0	0	6	911	940	9	0	4	3	323	349	4	0	7	13	926	923	9	0	12	0	1494	1524	13
0	0	8	652	621	6	0	4	4	548	557	6	0	7	14	140	146	22	0	12	1	215	189	13
0	0	10	1333	1310	11	0	4	5	227	235	6	0	7	15	827	827	8	0	12	2	897	897	9
0	0	12	1418	1392	13	0	4	6	1211	1219	11	0	8	0	3170	3182	12	0	12	3	257	245	11
0	0	14	287	255	10	0	4	7	222	223	7	0	8	1	618	610	6	0	12	5	268	253	11
0	0	16	743	749	7	0	4	8	700	704	7	0	8	2	1683	1681	12	0	12	6	541	556	8
0	1	1	2207	2184	20	0	4	9	254	288	8	0	8	3	526	547	6	0	12	8	682	667	7
0	1	2	147	146	4	0	4	10	889	879	8	0	8	4	158	165	11	0	12	9	235	239	14
0	1	3	3058	3033	29	0	4	12	1144	1161	11	0	8	5	673	698	7	0	12	10	592	571	8
0	1	4	175	216	7	0	4	14	345	335	9	0	8	6	916	920	9	0	13	1	549	566	7
0	1	5	1984	1927	9	0	4	16	563	562	8	0	8	7	288	259	9	0	13	2	158	153	18
0	1	6	493	524	5	0	5	1	2761	2698	9	0	8	8	854	835	8	0	13	3	1089	1107	11
0	1	7	704	737	7	0	5	2	221	232	6	0	8	9	511	492	7	0	13	5	1112	1111	12
0	1	9	644	693	6	0	5	3	2956	2978	10	0	8	10	1071	1104	11	0	13	6	340	314	10
0	1	11	198	186	12	0	5	4	140	165	10	0	8	12	991	1022	11	0	13	7	626	630	8
0	1	12	145	141	10	0	5	5	1499	1578	11	0	9	1	724	747	7	0	14	0	1086	1158	11
0	1	13	1369	1336	14	0	5	6	247	262	7	0	9	2	504	508	5	0	14	1	248	226	12
0	1	15	1051	1061	11	0	5	7	1151	1132	11	0	9	3	1171	1140	12	0	14	2	742	738	7
0	2	0	4771	4789	24	0	5	9	553	536	6	0	9	5	1125	1157	11	0	14	3	260	255	11
0	2	1	621	645	6	0	5	10	308	297	9	0	9	6	353	336	8	0	14	4	240	206	13
0	2	2	1823	1779	7	0	5	11	334	351	9	0	9	7	739	738	8	0	14	5	263	252	11
0	2	3	157	128	7	0	5	13	1054	1070	11	0	9	9	335	322	10	0	14	6	369	368	10
0	2	4	1001	1026	9	0	5	15	980	979	9	0	9	10	272	263	12	0	14	8	668	635	8
0	2	5	518	507	5	0	6	0	4414	4470	42	0	9	11	203	211	14	0	15	1	399	423	9
0	2	6	1435	1460	10	0	6	1	545	544	5	0	9	13	787	785	8	0	15	2	189	171	16
0	2	7	423	415	4	0	6	2	2112	2091	10	0	9	14	212	187	16	0	15	3	687	713	9
0	2	8	632	615	6	0	6	3	411	427	5	0	10	0	2203	2236	13	0	15	5	765	742	8
0	2	10	1019	1036	10	0	6	4	413	403	5	0	10	1	354	336	7	0	15	6	236	243	16
0	2	12	1384	1370	13	0	6	5	675	685	7	0	10	2	910	924	10	0	16	0	870	886	8
0	2	14	303	298	9	0	6	6	1179	1162	11	0	10	3	375	357	7	0	16	2	583	590	9
0	2	15	142	133	19	0	6	7	233	245	8	0	10	4	181	182	13	0	16	3	210	181	15
0	2	16	691	688	8	0	6	8	786	792	8	0	10	5	474	474	7	1	0	-15	579	580	7
0	3	1	1172	1132	7	0	6	9	464	459	7	0	10	6	509	502	7	1	0	-13	588	581	7
0	3	2	670	658	7	0	6	10	989	987	10	0	10	7	244	246	12	1	0	-9	2248	2232	12
0	3	3	1960	1929	8	0	6	12	1063	1065	10	0	10	8	735	739	7	1	0	-7	2794	2792	11
0	3	4	286	291	5	0	6	13	209	239	13	0	10	9	427	421	9	1	0	-5	230	228	5
0	3	5	2000	1954	10	0	6	14	229	225	13	0	10	10	875	865	8	1	0	-3	825	800	8
0	3	6	489	410	4	0	6	15	134	30	22	0	10	12	705	711	8	1	0	-1	171	162	3
0	3	7	1140	1100	11	0	7	1	1461	1460	11	0	11	1	750	746	9	1	0	1	2533	2535	20
0	3	9	681	686	7	0	7	2	233	240	7	0	11	2	195	186	13	1	0	3	3982	3956	29
0	3	10	252	270	8	0	7	3	2161	2140	11	0	11	3	1201	1197	12	1	0	5	3449	3418	9
0	3	11	245	241	10	0	7	4	223	220	8	0	11	5	1078	1101	12	1	0	7	1063	1059	10
0	3	13	1312	1296	13	0	7	5	1677	1659	12	0	11	6	321	302	10	1	0	9	2793	2767	12
0	3	15	1100	1100	11	0	7	6	401	387	6	0	11	7	693	675	7	1	0	11	700	730	7
0	4	0	1774	1827	8	0	7	7	762	781	8	0	11	9	243	232	12	1	0	13	215	207	13

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
1	0	15	625	601	7	1	2	11	769	769	8	1	4	6	236	230	7	1	6	3	2799	2804	11
1	1	-14	264	265	11	1	2	12	197	213	14	1	4	7	190	201	8	1	6	4	401	396	5
1	1	-12	1022	1029	10	1	2	13	610	617	7	1	4	8	380	393	6	1	6	5	2293	2244	12
1	1	-10	2248	2221	13	1	2	15	668	662	7	1	4	9	1354	1340	12	1	6	6	187	216	10
1	1	-8	981	914	10	1	3	-16	190	204	17	1	4	11	787	779	8	1	6	7	420	404	6
1	1	-7	292	304	5	1	3	-14	527	521	7	1	4	12	307	292	10	1	6	8	494	518	6
1	1	-6	1774*	1797	10	1	3	-13	156	140	17	1	4	13	755	756	7	1	6	9	1507	1499	14
1	1	-5	401	426	4	1	3	-12	1045	1066	11	1	4	15	586	613	8	1	6	11	728	736	8
1	1	-4	1872	1856	8	1	3	-10	1407	1438	14	1	4	16	191	187	17	1	6	13	462	474	8
1	1	-2	1406	1375	6	1	3	-9	205	239	9	1	5	-14	411	394	8	1	6	15	381	374	10
1	1	-1	270	201	3	1	3	-8	358	338	5	1	5	-12	936	933	9	1	7	-15	212	215	16
1	1	0	2368	2406	21	1	3	-7	106	114	12	1	5	-11	191	194	13	1	7	-14	320	333	11
1	1	1	267	265	2	1	3	-6	1185	1186	11	1	5	-10	1498	1503	15	1	7	-13	219	214	13
1	1	2	1939	1914	6	1	3	-5	265	259	5	1	5	-8	314	328	7	1	7	-12	883	857	8
1	1	3	180	169	5	1	3	-4	1483	1492	9	1	5	-7	374	381	5	1	7	-11	226	221	12
1	1	4	402	383	4	1	3	-3	343	355	4	1	5	-6	1617	1642	12	1	7	-10	1352	1329	14
1	1	5	159	171	7	1	3	-2	636	639	7	1	5	-5	287	291	5	1	7	-9	205	189	12
1	1	6	2801	2845	10	1	3	-1	595	594	6	1	5	-4	1785	1798	10	1	7	-8	599	597	6
1	1	7	219	226	6	1	3	0	618	643	6	1	5	-3	333	333	5	1	7	-7	357	364	6
1	1	8	1781	1788	12	1	3	1	142	136	7	1	5	-2	2130	2072	10	1	7	-6	967	972	9
1	1	9	176	143	10	1	3	2	467	456	4	1	5	-1	571	589	6	1	7	-5	320	330	6
1	1	10	175	163	11	1	3	3	535	529	5	1	5	0	2706	2690	9	1	7	-4	1708	1776	12
1	1	11	124	98	18	1	3	4	1112	1113	10	1	5	1	161	171	7	1	7	-3	255	272	6
1	1	12	153	144	17	1	3	6	2690	2665	10	1	5	2	668	708	7	1	7	-2	1819	1843	11
1	1	13	134	95	20	1	3	7	121	112	11	1	5	3	143	155	9	1	7	-1	400	413	5
1	1	14	219	201	12	1	3	8	1864	1875	12	1	5	4	895	853	9	1	7	0	2021	2014	11
1	1	16	633	634	8	1	3	9	299	311	7	1	5	5	404	391	5	1	7	1	192	213	7
1	2	-15	617	623	7	1	3	10	530	530	6	1	5	6	2444	2446	12	1	7	2	951	931	10
1	2	-13	512	507	7	1	3	12	224	253	13	1	5	7	230	230	8	1	7	3	182	202	8
1	2	-12	209	205	13	1	3	14	300	281	10	1	5	8	1894	1889	13	1	7	4	749	745	7
1	2	-11	318	300	8	1	3	16	701	694	8	1	5	10	255	229	10	1	7	6	2044	2041	13
1	2	-10	168	165	11	1	4	-15	551	546	8	1	5	13	245	260	11	1	7	7	165	157	12
1	2	-9	1905	1880	13	1	4	-13	522	525	7	1	5	14	213	202	13	1	7	8	1393	1356	12
1	2	-7	2125	2131	11	1	4	-10	172	134	12	1	5	15	166	156	19	1	7	9	152	138	17
1	2	-5	578	544	6	1	4	-9	1824	1817	13	1	6	-15	509	503	9	1	7	10	259	255	11
1	2	-4	231	245	5	1	4	-8	476	467	5	1	6	-13	535	531	7	1	7	11	166	153	17
1	2	-3	537	512	5	1	4	-7	2041	2025	12	1	6	-10	206	225	13	1	7	14	286	286	12
1	2	-1	1007	975	6	1	4	-6	123	119	10	1	6	-9	1565	1572	14	1	7	15	201	174	16
1	2	0	594	617	6	1	4	-5	320	324	5	1	6	-8	356	346	6	1	8	-13	344	328	10
1	2	1	668	658	6	1	4	-4	584	608	6	1	6	-7	1968	2000	13	1	8	-12	268	280	11
1	2	2	376	394	4	1	4	-3	791	733	8	1	6	-6	253	250	7	1	8	-11	309	299	9
1	2	3	3703	3724	33	1	4	-1	2190	2134	8	1	6	-5	638	638	6	1	8	-9	1226	1222	12
1	2	4	182	161	6	1	4	0	949	950	9	1	6	-4	683	668	7	1	8	-8	245	235	10
1	2	5	2928	2921	9	1	4	1	563	573	6	1	6	-3	198	201	7	1	8	-7	1455	1426	14
1	2	7	702	718	7	1	4	3	3059	3055	9	1	6	-1	178	189	7	1	8	-6	370	363	7
1	2	8	162	140	9	1	4	4	720	741	8	1	6	0	854	877	8	1	8	-5	669	667	7
1	2	9	1880	1854	12	1	4	5	2521	2507	10	1	6	1	1590	1569	10	1	8	-4	503	510	5

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
1	8	-3	333	323	6	1	10	-6	255	254	10	1	12	9	594	611	8	2	0	-6	2425	2424	10
1	8	-2	303	324	6	1	10	-5	551	526	6	1	12	11	613	582	8	2	0	-4	3656	3714	35
1	8	-1	756	770	7	1	10	-4	404	398	7	1	13	-10	510	544	9	2	0	-2	1463	1413	7
1	8	0	919	916	10	1	10	-3	292	266	8	1	13	-8	191	189	16	2	0	0	2729	2671	25
1	8	1	1478	1467	12	1	10	-2	164	170	12	1	13	-7	167	161	16	2	0	2	1304	1302	7
1	8	2	156	139	10	1	10	0	703	707	7	1	13	-6	358	388	9	2	0	4	294	239	4
1	8	3	2214	2227	12	1	10	1	1174	1163	11	1	13	-5	126	101	20	2	0	6	2039	1992	10
1	8	4	528	519	5	1	10	3	1740	1748	14	1	13	-4	1000	1028	11	2	0	8	2426	2378	12
1	8	5	1681	1713	13	1	10	4	622	612	6	1	13	-3	193	192	14	2	0	12	1615	1599	15
1	8	7	317	284	8	1	10	5	1400	1407	13	1	13	-2	1215	1197	12	2	0	14	1137	1134	11
1	8	8	585	596	7	1	10	8	335	326	10	1	13	-1	230	227	13	2	1	-15	160	165	17
1	8	9	1184	1184	12	1	10	9	892	878	8	1	13	0	821	815	8	2	1	-13	882	870	9
1	8	11	701	712	7	1	10	11	671	665	7	1	13	2	130	152	20	2	1	-11	551	534	6
1	8	12	372	378	9	1	10	12	365	381	11	1	13	4	517	513	8	2	1	-9	1068	1048	10
1	8	13	519	522	8	1	10	13	576	564	9	1	13	6	1020	1058	10	2	1	-8	155	156	10
1	9	-14	407	421	10	1	11	-12	630	631	8	1	13	8	858	842	8	2	1	-7	1938	1921	11
1	9	-13	244	253	13	1	11	-10	794	810	8	1	13	10	319	282	12	2	1	-6	329	325	5
1	9	-12	721	741	8	1	11	-8	249	256	11	1	14	-7	800	809	8	2	1	-5	918	910	9
1	9	-11	153	127	16	1	11	-7	161	163	16	1	14	-6	145	147	21	2	1	-4	115	127	10
1	9	-10	1123	1112	11	1	11	-6	656	664	6	1	14	-5	649	613	7	2	1	-3	1382	1336	8
1	9	-9	280	299	11	1	11	-5	212	198	12	1	14	-4	311	307	10	2	1	-1	4782	4906	27
1	9	-8	441	439	7	1	11	-4	954	979	10	1	14	-3	239	216	12	2	1	0	376	387	4
1	9	-7	187	188	13	1	11	-3	230	212	11	1	14	-1	318	298	10	2	1	1	2566	2562	24
1	9	-6	707	705	7	1	11	-2	1072	1043	11	1	14	0	383	377	9	2	1	2	132	128	7
1	9	-5	266	292	8	1	11	-1	377	376	8	1	14	1	879	863	9	2	1	3	441	415	4
1	9	-4	882	899	8	1	11	0	1142	1132	12	1	14	3	881	910	8	2	1	4	314	315	4
1	9	-3	337	342	6	1	11	1	201	193	12	1	14	4	266	263	12	2	1	5	1015	965	10
1	9	-2	821	830	8	1	11	2	452	468	7	1	14	5	607	633	7	2	1	6	184	174	7
1	9	-1	487	489	5	1	11	3	170	126	14	1	14	8	312	287	11	2	1	7	494	492	5
1	9	0	1241	1241	11	1	11	4	442	459	8	1	15	-6	270	296	13	2	1	9	2129	2147	13
1	9	1	266	274	7	1	11	5	145	132	19	1	15	-4	566	569	8	2	1	11	1571	1569	14
1	9	2	713	676	7	1	11	6	1305	1314	13	1	15	-3	175	154	17	2	1	13	280	284	10
1	9	3	375	388	6	1	11	8	1120	1103	11	1	15	-2	800	784	8	2	1	15	499	522	8
1	9	4	502	523	6	1	11	9	207	198	14	1	15	0	689	692	7	2	2	-16	835	840	8
1	9	6	1536	1516	15	1	11	10	370	341	9	1	15	3	185	172	16	2	2	-14	980	991	10
1	9	7	199	179	13	1	12	-9	704	702	7	1	15	4	345	334	10	2	2	-12	376	375	8
1	9	8	1208	1225	13	1	12	-7	1042	1049	10	1	15	6	665	700	8	2	2	-10	255	263	9
1	9	9	290	290	11	1	12	-6	245	258	12	1	16	-3	139	87	22	2	2	-7	198	187	7
1	9	10	458	471	8	1	12	-5	866	850	8	1	16	-1	322	287	11	2	2	-6	1988	1979	10
1	9	11	274	276	11	1	12	-4	441	426	8	1	16	0	336	314	11	2	2	-5	286	306	5
1	9	13	145	132	22	1	12	-3	431	411	8	1	16	1	659	651	8	2	2	-4	2810	2800	9
1	10	-13	258	250	13	1	12	0	428	405	8	1	16	3	640	659	8	2	2	-3	434	462	4
1	10	-12	190	209	16	1	12	1	1000	982	10	2	0	-16	844	832	9	2	2	-2	792	778	7
1	10	-11	183	199	15	1	12	3	1367	1405	14	2	0	-14	860	851	9	2	2	0	1690	1684	7
1	10	-9	1069	1068	11	1	12	4	358	358	9	2	0	-12	163	183	16	2	2	1	337	341	4
1	10	-8	203	189	13	1	12	5	1010	1013	10	2	0	-10	379	394	7	2	2	2	684	653	7
1	10	-7	1214	1234	12	1	12	8	291	255	11	2	0	-8	161	170	10	2	2	3	745	756	8

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
2	2	4	1052	1026	9	2	4	-1	504	508	5	2	6	-5	228	243	7	2	8	-6	1383	1378	12
2	2	5	318	328	5	2	4	0	283	299	4	2	6	-4	2618	2624	11	2	8	-5	350	315	6
2	2	6	2361	2355	10	2	4	1	290	302	5	2	6	-2	1929	1910	11	2	8	-4	1461	1466	13
2	2	7	134	133	10	2	4	2	524	524	5	2	6	-1	492	508	5	2	8	-3	330	339	6
2	2	8	2342	2281	12	2	4	3	282	303	5	2	6	0	847	853	8	2	8	-2	382	393	5
2	2	9	180	196	10	2	4	4	500	485	5	2	6	2	834	822	8	2	8	-1	599	597	6
2	2	11	131	89	18	2	4	5	304	318	5	2	6	3	601	608	6	2	8	0	917	945	9
2	2	12	1518	1502	13	2	4	6	2286	2243	11	2	6	4	547	567	5	2	8	1	314	322	6
2	2	14	1214	1190	12	2	4	7	361	385	6	2	6	5	518	537	5	2	8	2	671	658	7
2	2	16	202	187	15	2	4	8	2190	2192	13	2	6	6	1710	1716	13	2	8	3	763	782	8
2	3	-15	141	125	19	2	4	9	357	366	7	2	6	7	270	276	8	2	8	4	938	950	10
2	3	-14	123	81	20	2	4	11	149	132	17	2	6	8	1517	1500	14	2	8	5	517	515	6
2	3	-13	866	867	9	2	4	12	1315	1316	14	2	6	9	355	342	8	2	8	6	1475	1511	14
2	3	-12	190	161	14	2	4	14	1095	1119	14	2	6	10	276	192	10	2	8	7	419	434	7
2	3	-11	593	587	6	2	4	16	256	281	13	2	6	11	279	270	11	2	8	8	1136	1139	12
2	3	-10	246	231	9	2	5	-15	136	128	22	2	6	12	1084	1095	10	2	8	9	270	256	11
2	3	-9	775	777	8	2	5	-14	272	255	10	2	6	13	255	257	11	2	8	11	332	325	10
2	3	-7	1558	1600	12	2	5	-13	770	758	8	2	6	14	946	951	9	2	8	12	871	857	8
2	3	-5	732	740	7	2	5	-11	460	470	7	2	7	-14	226	219	14	2	8	13	239	246	14
2	3	-4	319	328	5	2	5	-10	337	359	8	2	7	-13	734	720	7	2	8	14	895	880	10
2	3	-3	824	856	8	2	5	-9	830	840	8	2	7	-11	757	763	8	2	9	-14	181	193	18
2	3	-2	147	113	7	2	5	-7	1683	1709	12	2	7	-10	515	527	7	2	9	-13	561	562	8
2	3	-1	1680	1677	8	2	5	-6	379	411	5	2	7	-9	885	902	9	2	9	-11	766	754	8
2	3	0	482	494	5	2	5	-5	680	694	7	2	7	-8	213	211	10	2	9	-10	426	422	8
2	3	1	1401	1376	8	2	5	-3	1167	1173	10	2	7	-7	1413	1424	14	2	9	-9	995	993	10
2	3	2	275	293	5	2	5	-2	364	386	4	2	7	-6	399	412	6	2	9	-7	983	990	10
2	3	3	1725	1667	9	2	5	-1	2534	2503	10	2	7	-5	465	474	5	2	9	-6	527	511	6
2	3	4	158	173	8	2	5	1	1305	1373	10	2	7	-3	1649	1677	12	2	9	-5	390	394	7
2	3	5	616	617	6	2	5	2	251	261	5	2	7	-2	578	578	5	2	9	-4	166	169	11
2	3	6	449	446	4	2	5	3	744	746	7	2	7	-1	2803	2806	11	2	9	-3	485	521	5
2	3	7	685	677	7	2	5	4	128	108	9	2	7	1	1528	1532	11	2	9	-2	552	554	6
2	3	9	1710	1726	13	2	5	5	484	458	5	2	7	2	313	308	5	2	9	-1	1650	1644	13
2	3	11	1494	1469	13	2	5	6	428	422	5	2	7	3	761	798	7	2	9	1	1227	1220	12
2	3	13	453	459	8	2	5	7	651	649	7	2	7	4	161	126	10	2	9	2	430	427	6
2	3	15	392	379	9	2	5	8	157	119	12	2	7	5	207	216	8	2	9	3	688	682	6
2	4	-16	831	854	9	2	5	9	1677	1685	14	2	7	6	151	177	12	2	9	5	388	392	7
2	4	-14	949	956	10	2	5	10	188	179	13	2	7	7	738	751	7	2	9	6	344	333	8
2	4	-12	516	516	7	2	5	11	1296	1306	13	2	7	9	1590	1584	15	2	9	7	475	481	7
2	4	-10	488	484	6	2	5	13	389	380	8	2	7	10	250	229	12	2	9	9	1378	1369	15
2	4	-9	212	194	9	2	5	14	197	153	14	2	7	11	1226	1235	13	2	9	10	150	151	10
2	4	-8	336	337	6	2	6	-14	807	803	8	2	7	13	340	313	9	2	9	11	1104	1105	10
2	4	-7	218	200	8	2	6	-13	233	222	12	2	8	-14	745	740	7	2	9	13	370	368	10
2	4	-6	1842	1860	11	2	6	-12	375	373	9	2	8	-12	293	298	10	2	10	-12	358	357	10
2	4	-5	242	254	6	2	6	-10	369	375	8	2	8	-11	128	115	20	2	10	-10	207	209	13
2	4	-4	2382	2426	10	2	6	-9	231	232	11	2	8	-9	346	331	9	2	10	-9	224	218	12
2	4	-3	209	185	6	2	6	-8	264	282	8	2	8	-8	315	318	9	2	10	-8	330	325	9
2	4	-2	2400	2372	9	2	6	-6	1905	1913	12	2	8	-7	236	252	10	2	10	-7	128	143	21

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
2	10	-6	1122	1153	11	2	12	8	648	665	7	3	0	5	2240	2240	10	3	2	7	821	806	8
2	10	-5	272	281	9	2	12	9	259	256	13	3	0	7	543	531	5	3	2	8	323	352	6
2	10	-4	1223	1234	13	2	13	-10	301	281	12	3	0	9	297	297	7	3	2	9	724	711	7
2	10	-3	165	171	13	2	13	-9	589	589	8	3	0	11	1301	1273	13	3	2	11	1320	1291	13
2	10	-2	861	853	8	2	13	-7	544	564	8	3	0	13	411	412	8	3	2	12	189	199	15
2	10	-1	510	522	6	2	13	-3	693	689	7	3	0	15	915	907	10	3	2	13	282	280	10
2	10	0	305	268	8	2	13	-2	165	163	17	3	1	-16	885	884	9	3	2	15	947	943	10
2	10	1	267	259	8	2	13	-1	1106	1145	12	3	1	-14	1081	1070	11	3	3	-16	823	821	9
2	10	2	610	612	6	2	13	0	133	135	20	3	1	-12	245	228	12	3	3	-14	1003	1003	10
2	10	3	476	475	6	2	13	1	913	912	9	3	1	-10	1889	1896	14	3	3	-11	129	151	19
2	10	4	791	771	8	2	13	2	376	381	9	3	1	-8	1934	1908	12	3	3	-10	1552	1549	14
2	10	5	339	327	9	2	13	3	640	625	7	3	1	-7	358	348	5	3	3	-9	100	137	17
2	10	6	1228	1258	13	2	13	6	270	256	11	3	1	-6	714	696	7	3	3	-8	1365	1363	13
2	10	7	330	336	10	2	13	7	532	522	8	3	1	-5	460	434	5	3	3	-6	645	657	6
2	10	8	1109	1108	11	2	13	9	709	702	8	3	1	-4	555	552	5	3	3	-4	801	811	7
2	10	9	302	297	10	2	14	-8	432	409	9	3	1	-3	169	176	7	3	3	-3	246	255	5
2	10	12	684	688	8	2	14	-6	744	755	8	3	1	-2	1835	1822	8	3	3	-2	725	725	7
2	11	-11	496	495	8	2	14	-4	721	759	7	3	1	-1	97	73	10	3	3	-1	111	83	10
2	11	-10	258	242	11	2	14	-2	590	609	7	3	1	0	1091	1076	8	3	3	0	2032	1993	9
2	11	-9	809	790	8	2	14	-1	320	295	9	3	1	1	415	414	4	3	3	1	289	290	5
2	11	-7	859	867	8	2	14	1	130	85	19	3	1	2	2703	2725	8	3	3	2	2400	2424	9
2	11	-6	275	291	10	2	14	2	475	470	8	3	1	3	264	270	5	3	3	3	707	730	7
2	11	-5	340	352	9	2	14	3	361	351	9	3	1	4	2232	2221	9	3	3	4	1775	1831	10
2	11	-3	351	322	8	2	14	4	768	734	7	3	1	6	188	87	7	3	3	5	159	164	8
2	11	-2	178	182	13	2	14	5	306	272	11	3	1	8	968	924	10	3	3	6	579	534	6
2	11	-1	1266	1263	13	2	14	6	769	771	8	3	1	10	393	393	7	3	3	8	122	127	13
2	11	1	1056	1063	11	2	14	8	413	450	10	3	1	12	796	801	8	3	3	10	480	480	6
2	11	2	302	266	9	2	15	-3	400	415	9	3	1	14	1092	1103	11	3	3	11	183	152	14
2	11	3	600	565	6	2	15	-2	198	195	16	3	1	16	345	345	10	3	3	12	1255	1265	12
2	11	5	217	212	13	2	15	-1	780	810	8	3	2	-15	289	277	11	3	3	14	1155	1158	12
2	11	6	223	216	13	2	15	1	726	718	7	3	2	-13	1269	1283	13	3	4	-15	303	307	11
2	11	7	428	437	8	2	15	2	270	235	12	3	2	-11	1560	1549	15	3	4	-13	1169	1199	11
2	11	9	913	934	9	2	15	3	434	421	9	3	2	-9	423	419	6	3	4	-12	180	191	16
2	11	10	166	177	18	2	15	6	195	200	17	3	2	-7	445	448	5	3	4	-11	1388	1421	14
2	11	11	741	751	8	2	16	-2	412	375	10	3	2	-6	239	252	6	3	4	-9	340	326	7
2	12	-10	152	143	19	2	16	-1	184	194	17	3	2	-5	868	861	8	3	4	-8	283	291	7
2	12	-8	336	319	9	2	16	2	370	361	10	3	2	-4	481	504	5	3	4	-7	745	718	8
2	12	-6	1000	1097	12	2	16	3	161	168	20	3	2	-3	1635	1608	9	3	4	-6	276	267	6
2	12	-4	1433	1462	14	3	0	-13	1190	1153	11	3	2	-2	284	288	5	3	4	-5	751	766	8
2	12	-2	1090	1072	10	3	0	-11	1694	1710	15	3	2	-1	2777	2777	8	3	4	-4	651	692	7
2	12	-1	324	331	10	3	0	-9	811	833	8	3	2	0	200	177	6	3	4	-3	1178	1194	10
2	12	2	584	574	7	3	0	-7	657	663	7	3	2	1	866	909	8	3	4	-1	3190	3205	9
2	12	3	306	309	10	3	0	-5	933	914	9	3	2	2	517	525	5	3	4	0	161	183	7
2	12	4	970	960	10	3	0	-3	817	773	8	3	2	3	1032	988	9	3	4	1	990	1001	10
2	12	5	222	210	13	3	0	-1	3213	3152	27	3	2	4	451	480	4	3	4	2	245	243	5
2	12	6	1020	1030	10	3	0	1	1656	1615	8	3	2	5	1841	1835	10	3	4	3	1290	1312	10
2	12	7	230	234	12	3	0	3	1262	1293	9	3	2	6	318	312	5	3	4	4	402	397	4

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
3	4	5	1683	1655	11	3	6	4	569	578	6	3	8	1	842	870	9	3	10	3	470	503	7
3	4	7	1031	1031	10	3	6	5	1609	1596	12	3	8	2	190	208	9	3	10	4	330	340	9
3	4	8	478	467	6	3	6	6	294	311	7	3	8	3	342	333	6	3	10	5	1032	1007	11
3	4	9	782	799	7	3	6	7	902	928	8	3	8	4	288	287	7	3	10	6	209	198	13
3	4	11	998	1013	10	3	6	8	454	466	7	3	8	5	1130	1093	11	3	10	7	965	931	9
3	4	12	278	293	11	3	6	9	453	478	7	3	8	6	323	311	8	3	10	8	509	496	8
3	4	13	209	198	13	3	6	11	730	730	7	3	8	7	862	860	9	3	10	9	744	765	7
3	4	15	862	868	8	3	6	12	257	242	11	3	8	8	562	562	7	3	10	11	605	611	8
3	5	-14	852	865	9	3	6	13	196	194	14	3	8	9	717	700	7	3	10	12	329	342	11
3	5	-11	368	379	9	3	6	15	695	695	8	3	8	11	785	786	9	3	11	-10	579	598	7
3	5	-10	1228	1223	12	3	7	-15	148	141	21	3	8	12	320	307	10	3	11	-9	155	169	17
3	5	-9	255	265	9	3	7	-14	748	762	7	3	9	-13	198	199	16	3	11	-8	939	948	9
3	5	-8	1553	1587	14	3	7	-13	136	109	19	3	9	-11	234	253	13	3	11	-7	304	298	10
3	5	-7	465	464	5	3	7	-11	341	333	9	3	9	-10	953	975	10	3	11	-6	878	851	9
3	5	-6	772	799	8	3	7	-10	1170	1163	12	3	9	-9	274	269	10	3	11	-5	288	294	10
3	5	-5	579	599	6	3	7	-9	270	276	10	3	9	-8	1083	1118	12	3	11	-4	707	705	7
3	5	-4	726	699	7	3	7	-8	1385	1396	13	3	9	-7	409	407	8	3	11	-3	164	162	15
3	5	-3	244	241	5	3	7	-7	419	425	6	3	9	-6	644	638	7	3	11	-2	512	522	7
3	5	-2	1291	1252	10	3	7	-6	987	982	10	3	9	-5	402	413	7	3	11	-1	285	276	10
3	5	-1	547	578	5	3	7	-5	543	556	6	3	9	-4	410	404	6	3	11	0	835	825	8
3	5	0	1432	1425	10	3	7	-4	491	465	5	3	9	-3	331	325	7	3	11	1	162	154	15
3	5	1	183	196	7	3	7	-3	219	196	7	3	9	-2	298	281	7	3	11	2	1429	1436	13
3	5	2	2496	2514	10	3	7	-2	131	121	11	3	9	-1	403	429	6	3	11	3	187	185	15
3	5	4	1694	1707	11	3	7	-1	609	657	7	3	9	0	1111	1124	12	3	11	4	1189	1171	11
3	5	5	338	340	6	3	7	0	1273	1288	12	3	9	1	234	216	8	3	11	5	221	230	13
3	5	6	221	210	8	3	7	1	171	179	8	3	9	2	1681	1684	13	3	11	6	410	402	8
3	5	7	288	289	7	3	7	2	2008	2028	12	3	9	3	344	347	7	3	11	7	164	158	17
3	5	8	281	263	8	3	7	3	506	515	5	3	9	4	1420	1409	14	3	11	8	196	168	14
3	5	10	373	377	8	3	7	4	1009	1033	13	3	9	5	206	208	12	3	11	9	240	220	12
3	5	12	1032	1041	10	3	7	5	247	232	8	3	9	6	454	437	7	3	11	10	441	405	9
3	5	14	957	959	10	3	7	6	232	220	9	3	9	7	347	331	9	3	11	11	171	171	19
3	6	-15	197	199	16	3	7	7	430	423	7	3	9	8	234	232	13	3	12	-11	710	735	8
3	6	-13	991	988	10	3	7	8	477	489	7	3	9	10	454	440	8	3	12	-9	418	414	9
3	6	-12	166	143	16	3	7	9	174	160	15	3	9	11	300	295	11	3	12	-8	218	228	13
3	6	-11	1313	1303	13	3	7	10	406	400	8	3	9	12	748	756	8	3	12	-5	833	838	9
3	6	-10	156	147	16	3	7	12	782	771	7	3	10	-13	668	679	8	3	12	-4	288	283	10
3	6	-9	520	533	6	3	7	14	754	749	8	3	10	-12	161	150	18	3	12	-3	1266	1267	13
3	6	-8	368	341	7	3	8	-13	836	840	8	3	10	-11	873	887	9	3	12	-1	1309	1330	12
3	6	-7	496	505	5	3	8	-11	1060	1072	11	3	10	-9	494	499	7	3	12	0	216	220	13
3	6	-5	929	930	9	3	8	-9	516	520	7	3	10	-8	170	185	15	3	12	1	591	582	7
3	6	-4	377	387	5	3	8	-8	313	304	9	3	10	-7	213	195	12	3	12	2	176	174	16
3	6	-3	1308	1290	11	3	8	-7	164	171	14	3	10	-5	517	523	7	3	12	3	152	177	18
3	6	-1	2976	2938	11	3	8	-5	673	676	7	3	10	-4	323	344	8	3	12	4	373	371	9
3	6	0	332	334	5	3	8	-4	311	317	7	3	10	-3	782	764	8	3	12	5	869	882	10
3	6	1	1500	1464	11	3	8	-3	1056	1076	11	3	10	-1	1476	1507	14	3	12	7	868	863	10
3	6	2	426	416	5	3	8	-1	1799	1803	12	3	10	0	323	312	8	3	12	8	294	267	11
3	6	3	765	773	8	3	8	0	356	339	6	3	10	1	590	604	6	3	12	9	529	495	8

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
3	13	-9	138	62	20	4	1	-13	526	538	7	4	3	-7	1944	1958	12	4	5	-11	1210	1225	13
3	13	-8	767	770	7	4	1	-11	1232	1231	12	4	3	-6	257	227	6	4	5	-10	417	435	8
3	13	-7	321	328	11	4	1	-9	336	349	7	4	3	-5	2516	2503	11	4	5	-9	374	372	8
3	13	-6	868	858	9	4	1	-7	2209	2244	12	4	3	-3	1342	1311	10	4	5	-7	2047	2027	13
3	13	-5	360	338	9	4	1	-6	223	221	7	4	3	-2	660	647	7	4	5	-6	292	293	7
3	13	-4	466	468	8	4	1	-5	2626	2643	10	4	3	-1	135	124	8	4	5	-5	2638	2588	12
3	13	-3	138	106	18	4	1	-3	507	508	5	4	3	0	127	137	9	4	5	-4	122	128	11
3	13	-1	283	260	10	4	1	-2	342	360	4	4	3	1	107	77	10	4	5	-3	1292	1279	11
3	13	0	682	677	7	4	1	-1	148	155	7	4	3	2	233	247	6	4	5	-2	485	467	5
3	13	2	918	934	9	4	1	0	133	146	8	4	3	3	518	499	5	4	5	-1	120	104	10
3	13	4	882	902	9	4	1	1	154	184	7	4	3	4	186	182	7	4	5	0	240	238	6
3	13	5	142	123	19	4	1	2	240	218	5	4	3	5	2515	2509	11	4	5	1	425	402	4
3	13	6	354	339	9	4	1	3	917	857	9	4	3	7	2384	2365	12	4	5	2	511	496	5
3	13	8	158	106	20	4	1	4	263	261	5	4	3	9	250	209	9	4	5	3	510	507	5
3	14	-8	242	227	14	4	1	5	2202	2338	11	4	3	11	624	638	6	4	5	5	2030	2044	12
3	14	-5	599	603	8	4	1	6	211	200	7	4	3	13	701	704	7	4	5	6	412	422	6
3	14	-4	259	229	12	4	1	7	1996	2062	12	4	3	15	494	495	9	4	5	7	1944	1907	13
3	14	-3	828	817	8	4	1	10	117	107	18	4	4	-14	203	218	14	4	5	10	160	169	16
3	14	-1	868	892	9	4	1	11	751	747	8	4	4	-13	145	137	18	4	5	11	648	635	7
3	14	0	141	156	19	4	1	13	700	711	7	4	4	-12	207	323	11	4	5	13	670	657	7
3	14	1	400	426	8	4	1	15	392	391	9	4	4	-11	134	131	20	4	5	14	220	208	15
3	14	4	166	181	17	4	2	-14	168	145	16	4	4	-10	1137	1113	11	4	5	15	477	482	9
3	14	5	471	486	9	4	2	-12	275	275	11	4	4	-9	120	115	18	4	6	-14	158	168	20
3	14	7	680	664	8	4	2	-10	1283	1284	13	4	4	-8	1806	1799	13	4	6	-12	302	307	10
3	15	-6	564	542	8	4	2	-8	1975	1994	13	4	4	-6	600	640	6	4	6	-11	302	284	10
3	15	-5	213	214	15	4	2	-7	308	309	6	4	4	-5	249	240	6	4	6	-10	1077	1061	11
3	15	-4	186	176	16	4	2	-6	753	746	8	4	4	-4	1041	1043	10	4	6	-8	1825	1828	14
3	15	-1	229	208	14	4	2	-5	226	210	6	4	4	-3	181	199	7	4	6	-7	315	331	7
3	15	0	566	550	8	4	2	-4	1144	1154	10	4	4	-2	1430	1437	10	4	6	-6	864	852	9
3	15	2	632	646	8	4	2	-3	340	354	5	4	4	0	1248	1261	10	4	6	-4	898	887	9
3	15	4	557	557	8	4	2	-2	2033	2008	9	4	4	1	95	130	12	4	6	-3	247	265	7
3	15	5	139	130	23	4	2	0	1717	1665	9	4	4	2	1831	1826	10	4	6	-2	1395	1382	12
3	16	-1	580	587	8	4	2	1	556	566	6	4	4	3	367	376	5	4	6	-1	460	500	5
3	16	1	273	288	13	4	2	2	2010	2002	9	4	4	4	1656	1661	11	4	6	0	1245	1229	12
4	0	-10	1370	1405	12	4	2	3	150	145	8	4	4	5	360	358	5	4	6	1	112	114	12
4	0	-8	2712	2685	12	4	2	4	1908	1900	10	4	4	6	560	543	5	4	6	2	1440	1438	12
4	0	-6	857	806	9	4	2	5	324	327	5	4	4	7	382	358	6	4	6	3	671	691	7
4	0	-4	1478	1373	10	4	2	6	651	660	7	4	4	8	1824	1803	13	4	6	4	1099	1061	11
4	0	-2	1996	1993	9	4	2	8	2127	2111	13	4	4	9	183	169	12	4	6	5	308	318	7
4	0	0	1706	1731	9	4	2	10	1032	1018	10	4	4	10	881	916	9	4	6	6	623	633	7
4	0	2	1493	1403	9	4	2	12	341	347	9	4	4	11	319	316	9	4	6	7	316	311	8
4	0	4	1667	1593	10	4	2	14	213	190	13	4	4	12	363	377	9	4	6	8	1617	1634	15
4	0	6	805	780	8	4	3	-15	541	535	8	4	4	13	168	164	16	4	6	10	879	890	8
4	0	8	2460	2431	12	4	3	-13	741	754	7	4	4	14	236	226	13	4	6	11	379	393	9
4	0	10	1066	1054	10	4	3	-11	1237	1225	12	4	5	-15	508	501	8	4	6	12	306	319	10
4	0	12	194	193	13	4	3	-10	231	200	11	4	5	-14	256	230	12	4	6	13	249	264	13
4	1	-15	381	385	10	4	3	-9	233	218	9	4	5	-13	573	590	7	4	7	-14	294	282	12

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
4	7	-13	509	517	8	4	9	-7	1154	1147	11	4	11	5	1240	1253	13	4	15	4	174	129	18
4	7	-11	755	750	8	4	9	-6	451	451	7	4	11	6	204	191	14	5	0	-15	958	1008	9
4	7	-10	327	338	9	4	9	-5	1376	1361	13	4	11	7	1082	1082	11	5	0	-11	890	899	9
4	7	-9	121	81	19	4	9	-3	719	729	7	4	11	9	219	212	14	5	0	-9	1110	1130	13
4	7	-7	1468	1467	14	4	9	-2	745	737	8	4	11	11	263	304	14	5	0	-7	1716	1657	12
4	7	-6	418	430	6	4	9	0	262	276	8	4	12	-10	668	677	8	5	0	-5	2073	2030	11
4	7	-5	2026	2031	13	4	9	1	232	221	8	4	12	-8	908	912	9	5	0	-3	1929	1901	10
4	7	-3	1108	1115	11	4	9	2	572	562	6	4	12	-6	506	496	7	5	0	-1	1753	1723	10
4	7	-2	588	592	6	4	9	3	628	619	7	4	12	-4	343	353	9	5	0	1	3243	3243	10
4	7	1	239	229	7	4	9	4	327	338	9	4	12	-2	988	1006	10	5	0	3	1246	1247	10
4	7	2	428	441	5	4	9	5	1431	1417	13	4	12	-1	321	312	9	5	0	5	269	254	6
4	7	3	553	545	6	4	9	6	310	300	10	4	12	0	1118	1093	11	5	0	7	389	404	6
4	7	5	1519	1494	13	4	9	7	1243	1247	13	4	12	2	858	852	8	5	0	9	372	379	7
4	7	6	416	437	6	4	9	10	303	319	11	4	12	4	426	455	8	5	0	11	1292	1251	12
4	7	7	1188	1183	12	4	9	11	332	329	10	4	12	6	261	255	11	5	0	13	1185	1174	11
4	7	10	257	269	11	4	9	13	538	540	8	4	12	7	234	229	12	5	0	15	198	168	14
4	7	11	482	479	8	4	10	-12	309	297	11	4	12	8	650	690	8	5	1	-16	239	228	14
4	7	13	626	615	8	4	10	-11	138	108	21	4	12	10	560	548	9	5	1	-14	1071	1079	10
4	8	-14	159	114	18	4	10	-10	961	947	9	4	13	-7	641	656	7	5	1	-12	850	847	8
4	8	-13	138	161	22	4	10	-8	1260	1258	13	4	13	-6	190	161	14	5	1	-10	436	427	7
4	8	-12	420	421	8	4	10	-6	453	464	7	4	13	-5	1055	1076	10	5	1	-8	964	943	10
4	8	-11	292	284	10	4	10	-5	183	175	14	4	13	-3	985	978	9	5	1	-6	644	620	6
4	8	-10	1083	1090	11	4	10	-4	391	419	8	4	13	-2	372	345	9	5	1	-5	205	189	7
4	8	-8	1369	1375	13	4	10	-3	170	173	14	4	13	-1	419	410	8	5	1	-4	1649	1641	11
4	8	-7	176	179	14	4	10	-2	929	949	10	4	13	1	236	194	11	5	1	-3	421	431	4
4	8	-6	594	591	6	4	10	-1	348	330	8	4	13	2	345	332	9	5	1	-2	3915	4018	10
4	8	-5	236	233	9	4	10	0	1084	1078	11	4	13	3	627	612	7	5	1	-1	467	485	5
4	8	-4	529	523	6	4	10	1	220	226	11	4	13	5	825	824	8	5	1	0	1446	1427	10
4	8	-3	320	321	7	4	10	2	883	892	9	4	13	6	204	195	15	5	1	1	654	664	7
4	8	-2	1172	1177	12	4	10	4	647	665	7	4	13	7	620	606	8	5	1	2	1028	1023	9
4	8	-1	462	475	5	4	10	6	270	275	11	4	14	-6	181	193	17	5	1	3	400	411	4
4	8	0	1231	1240	11	4	10	7	220	225	13	4	14	-4	251	270	12	5	1	4	1100	1080	11
4	8	1	349	351	6	4	10	8	1124	1119	11	4	14	-2	717	715	7	5	1	6	353	365	5
4	8	2	1194	1207	12	4	10	10	822	824	8	4	14	-1	198	214	15	5	1	7	122	134	13
4	8	3	302	296	7	4	10	11	215	192	15	4	14	0	878	872	8	5	1	8	956	974	10
4	8	4	824	816	8	4	10	12	450	447	9	4	14	1	213	206	14	5	1	10	1400	1432	13
4	8	5	241	242	10	4	11	-11	530	549	8	4	14	2	660	654	7	5	1	11	162	152	16
4	8	6	502	515	7	4	11	-10	255	255	12	4	14	4	273	278	12	5	1	12	453	425	7
4	8	7	286	260	10	4	11	-7	938	936	10	4	14	6	241	239	14	5	1	14	763	780	8
4	8	8	1445	1442	14	4	11	-6	301	294	10	4	14	7	205	170	16	5	2	-15	997	990	10
4	8	10	972	961	9	4	11	-5	1401	1420	14	4	15	-5	531	552	9	5	2	-12	233	228	13
4	8	11	298	291	11	4	11	-3	1015	1003	10	4	15	-3	501	481	9	5	2	-11	803	814	8
4	8	12	447	445	9	4	11	-2	502	492	7	4	15	-2	322	310	11	5	2	-10	223	184	11
4	9	-13	513	488	8	4	11	-1	311	291	9	4	15	-1	226	198	14	5	2	-9	878	861	9
4	9	-11	560	553	7	4	11	1	304	289	9	4	15	1	278	261	12	5	2	-8	148	147	12
4	9	-10	273	266	10	4	11	2	439	441	8	4	15	2	219	216	15	5	2	-7	1237	1242	11
4	9	-8	179	170	15	4	11	3	774	750	8	4	15	3	529	514	9	5	2	-5	1785	1811	11

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
5	2	-3	1452	1413	11	5	4	3	1400	1405	12	5	6	8	327	309	9	5	8	12	262	264	13
5	2	-1	1596	1577	10	5	4	4	775	779	8	5	6	9	200	228	13	5	8	13	821	831	9
5	2	1	2019	2029	10	5	4	5	1047	1035	11	5	6	11	1043	1041	11	5	9	-12	627	638	8
5	2	2	170	158	7	5	4	7	855	840	8	5	6	13	969	968	10	5	9	-11	307	294	10
5	2	3	1054	1094	9	5	4	9	266	273	10	5	7	-14	719	718	8	5	9	-10	447	467	8
5	2	4	103	115	12	5	4	11	1339	1355	14	5	7	-12	782	776	8	5	9	-9	265	294	11
5	2	5	906	865	8	5	4	13	1158	1154	12	5	7	-11	347	345	9	5	9	-8	425	431	8
5	2	6	235	249	7	5	5	-15	151	140	21	5	7	-10	566	578	7	5	9	-7	134	131	19
5	2	7	715	702	7	5	5	-14	919	910	9	5	7	-9	228	263	12	5	9	-5	239	235	10
5	2	9	394	401	7	5	5	-13	124	115	20	5	7	-8	584	574	7	5	9	-4	910	914	9
5	2	10	238	249	11	5	5	-12	865	880	8	5	7	-7	334	320	8	5	9	-3	378	361	7
5	2	11	1392	1391	14	5	5	-11	249	245	12	5	7	-5	270	275	8	5	9	-2	1878	1886	14
5	2	13	1190	1200	11	5	5	-10	660	663	7	5	7	-4	1196	1203	12	5	9	-1	347	351	8
5	3	-14	1056	1069	10	5	5	-8	627	621	7	5	7	-3	376	387	6	5	9	0	910	925	9
5	3	-12	947	964	10	5	5	-7	556	550	6	5	7	-2	2590	2570	13	5	9	1	444	430	7
5	3	-10	478	489	7	5	5	-5	362	386	6	5	7	-1	290	295	7	5	9	2	186	200	13
5	3	-8	633	660	7	5	5	-4	1518	1496	12	5	7	0	1493	1472	13	5	9	3	411	410	7
5	3	-7	192	205	9	5	5	-3	644	673	6	5	7	1	531	527	6	5	9	4	565	570	6
5	3	-4	1803	1796	11	5	5	-2	3179	3155	11	5	7	2	191	187	9	5	9	5	388	374	8
5	3	-3	272	308	6	5	5	-1	291	292	6	5	7	3	635	616	6	5	9	6	747	739	7
5	3	-2	3315	3317	10	5	5	0	1558	1552	11	5	7	4	742	735	7	5	9	7	407	415	8
5	3	0	905	913	9	5	5	1	794	777	8	5	7	5	289	286	8	5	9	8	1014	1011	9
5	3	1	149	172	8	5	5	2	841	818	8	5	7	6	637	635	6	5	9	10	898	906	10
5	3	2	744	718	7	5	5	3	606	623	6	5	7	7	442	419	7	5	9	11	268	257	12
5	3	3	100	86	12	5	5	4	1179	1173	11	5	7	8	893	893	8	5	9	12	265	256	13
5	3	4	857	871	9	5	5	5	266	266	7	5	7	10	942	944	9	5	10	-12	208	236	16
5	3	5	181	178	8	5	5	6	758	733	7	5	7	12	289	304	11	5	10	-11	290	315	12
5	3	6	861	876	9	5	5	7	402	421	7	5	8	-13	137	157	22	5	10	-9	617	623	7
5	3	7	243	255	8	5	5	8	1044	1016	11	5	8	-12	222	220	13	5	10	-8	274	279	11
5	3	8	1327	1341	12	5	5	10	996	1006	10	5	8	-11	501	516	8	5	10	-7	935	923	10
5	3	10	1309	1292	13	5	5	12	258	259	11	5	8	-9	758	781	8	5	10	-5	935	920	9
5	3	11	199	202	14	5	5	14	654	652	8	5	8	-8	243	240	11	5	10	-4	272	277	10
5	3	12	288	292	10	5	6	-13	179	170	15	5	8	-7	1075	1051	10	5	10	-3	542	552	7
5	3	14	771	772	7	5	6	-12	200	185	13	5	8	-6	199	148	12	5	10	-1	869	861	8
5	4	-15	897	880	9	5	6	-11	494	478	7	5	8	-5	1213	1217	13	5	10	0	287	260	10
5	4	-11	561	535	7	5	6	-9	727	734	8	5	8	-4	214	208	9	5	10	1	1396	1404	13
5	4	-9	647	642	7	5	6	-8	335	319	8	5	8	-3	815	817	8	5	10	2	138	129	18
5	4	-8	246	262	9	5	6	-7	1172	1151	11	5	8	-1	857	841	8	5	10	3	1150	1165	11
5	4	-7	989	1000	10	5	6	-5	1402	1478	13	5	8	0	244	254	8	5	10	4	381	369	8
5	4	-6	102	74	14	5	6	-4	165	173	10	5	8	1	1333	1343	12	5	10	5	818	805	7
5	4	-5	1428	1416	12	5	6	-3	1216	1226	11	5	8	3	1194	1178	11	5	10	7	355	358	9
5	4	-4	433	456	5	5	6	-1	1083	1072	11	5	8	4	269	294	9	5	10	8	274	278	11
5	4	-3	1093	1122	10	5	6	1	2129	2145	12	5	8	5	793	777	8	5	10	9	339	312	9
5	4	-1	1608	1568	11	5	6	3	1572	1549	13	5	8	7	357	331	9	5	10	11	738	731	8
5	4	0	538	538	5	5	6	4	355	357	6	5	8	8	346	346	10	5	11	-11	240	220	14
5	4	1	2181	2186	11	5	6	5	652	670	6	5	8	9	338	333	9	5	11	-10	539	523	8
5	4	2	538	528	5	5	6	7	420	420	7	5	8	11	871	878	9	5	11	-8	400	383	8

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
5	11	-7	347	327	9	5	14	-5	533	525	8	6	2	-14	785	797	8	6	4	-8	1042	1042	11
5	11	-6	155	131	17	5	14	-3	327	329	10	6	2	-12	1345	1327	13	6	4	-7	211	203	10
5	11	-5	209	214	13	5	14	-1	289	292	11	6	2	-11	194	188	15	6	4	-6	1566	1582	13
5	11	-4	864	848	8	5	14	0	198	182	14	6	2	-10	370	394	8	6	4	-5	196	185	8
5	11	-3	210	192	13	5	14	1	645	661	7	6	2	-8	1257	1255	12	6	4	-4	1010	1013	10
5	11	-2	1551	1557	14	5	14	3	709	705	8	6	2	-6	1664	1669	13	6	4	-3	278	290	6
5	11	0	919	926	9	5	14	4	221	216	15	6	2	-4	851	837	9	6	4	-2	1243	1275	12
5	11	1	235	238	12	5	14	5	478	452	9	6	2	-3	239	239	6	6	4	-1	145	151	10
5	11	3	228	230	13	5	15	-4	474	473	9	6	2	-2	1217	1207	11	6	4	0	599	609	6
5	11	4	650	641	7	5	15	-3	163	152	20	6	2	-1	125	109	10	6	4	1	115	130	12
5	11	5	238	224	12	5	15	-2	739	744	8	6	2	0	862	883	9	6	4	2	876	853	9
5	11	6	773	757	7	5	15	0	550	538	8	6	2	2	779	785	8	6	4	3	286	295	7
5	11	7	368	343	9	5	15	1	162	176	20	6	2	4	2529	2500	12	6	4	4	2507	2503	12
5	11	8	755	759	8	5	15	2	153	146	21	6	2	5	189	176	9	6	4	5	209	216	9
5	11	10	582	567	8	5	15	3	205	195	16	6	2	6	1831	1838	13	6	4	6	1912	1941	14
5	12	-9	520	517	8	6	0	-14	733	724	8	6	2	7	148	146	13	6	4	7	145	150	15
5	12	-8	303	293	11	6	0	-12	1359	1361	15	6	2	8	334	349	8	6	4	8	348	345	8
5	12	-7	856	848	8	6	0	-10	471	464	7	6	2	12	175	198	15	6	4	11	252	248	11
5	12	-5	838	848	9	6	0	-8	1464	1473	14	6	2	14	768	778	7	6	4	12	189	214	14
5	12	-4	170	164	15	6	0	-6	2006	1953	12	6	3	-15	410	409	10	6	4	13	209	179	14
5	12	-3	517	535	7	6	0	-4	715	706	7	6	3	-14	145	146	21	6	4	14	746	770	8
5	12	-1	487	482	7	6	0	-2	1275	1236	11	6	3	-13	176	195	15	6	5	-14	171	158	18
5	12	1	1053	1069	11	6	0	0	1285	1298	11	6	3	-11	1374	1367	14	6	5	-13	216	195	13
5	12	3	1064	1054	12	6	0	2	586	611	6	6	3	-10	188	195	14	6	5	-11	1243	1231	12
5	12	4	273	264	11	6	0	4	2203	2215	11	6	3	-9	1437	1450	13	6	5	-10	215	230	13
5	12	5	616	613	7	6	0	6	1449	1469	13	6	3	-8	236	203	10	6	5	-9	1555	1550	15
5	12	8	205	166	15	6	0	8	155	131	13	6	3	-7	320	336	7	6	5	-7	632	622	6
5	12	9	299	303	12	6	0	12	204	214	13	6	3	-6	386	373	6	6	5	-6	393	411	6
5	13	-8	208	227	15	6	0	14	726	726	8	6	3	-5	316	311	6	6	5	-5	361	357	6
5	13	-7	226	226	14	6	1	-15	505	511	9	6	3	-4	387	358	5	6	5	-3	243	214	7
5	13	-6	295	274	11	6	1	-11	1322	1335	14	6	3	-2	439	457	5	6	5	-2	495	510	5
5	13	-5	237	234	13	6	1	-9	1766	1725	14	6	3	-1	1391	1358	11	6	5	-1	1327	1342	12
5	13	-4	741	756	7	6	1	-7	555	533	5	6	3	0	321	304	5	6	5	1	2536	2524	12
5	13	-3	191	179	14	6	1	-4	226	209	7	6	3	1	2659	2648	11	6	5	2	585	612	5
5	13	-2	1163	1174	12	6	1	-3	652	635	7	6	3	2	419	428	5	6	5	3	1998	1958	13
5	13	-1	169	138	16	6	1	-2	228	250	6	6	3	3	2227	2211	12	6	5	5	286	289	7
5	13	0	804	816	9	6	1	-1	1374	1372	11	6	3	5	413	437	5	6	5	6	543	564	6
5	13	1	280	268	10	6	1	0	207	224	6	6	3	6	185	195	10	6	5	7	1418	1413	13
5	13	2	244	245	11	6	1	1	2882	2911	11	6	3	7	1636	1634	14	6	5	9	756	746	8
5	13	3	241	259	12	6	1	2	208	201	7	6	3	9	752	744	8	6	5	10	481	502	7
5	13	4	362	366	9	6	1	3	2140	2184	11	6	3	11	566	589	7	6	5	11	492	495	7
5	13	5	169	141	17	6	1	5	558	556	5	6	3	13	669	675	7	6	5	13	540	526	8
5	13	6	649	641	8	6	1	7	1713	1762	13	6	4	-14	745	764	8	6	6	-14	655	649	8
5	13	7	229	209	14	6	1	9	692	711	7	6	4	-13	128	130	21	6	6	-12	1064	1069	11
5	13	8	607	592	8	6	1	10	216	196	12	6	4	-12	1230	1257	12	6	6	-11	317	305	10
5	14	-7	666	646	8	6	1	11	503	497	7	6	4	-10	548	533	7	6	6	-10	475	474	8
5	14	-6	160	158	19	6	1	13	665	657	7	6	4	-9	155	147	16	6	6	-8	859	839	8

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
6	6	-7	153	176	16	6	8	0	422	396	6	6	11	-10	191	197	17	7	0	-11	517	535	7
6	6	-6	1463	1440	14	6	8	1	300	285	8	6	11	-9	959	967	9	7	0	-9	1417	1375	13
6	6	-5	218	215	9	6	8	2	434	424	7	6	11	-7	621	628	7	7	0	-7	876	883	8
6	6	-4	1192	1199	12	6	8	4	1288	1281	13	6	11	-6	267	254	11	7	0	-5	1485	1437	13
6	6	-3	425	423	6	6	8	5	218	185	12	6	11	-4	127	83	20	7	0	-3	3112	3160	12
6	6	-2	1387	1379	13	6	8	6	1069	1092	10	6	11	-3	379	366	9	7	0	-1	1627	1599	12
6	6	-1	242	236	7	6	8	7	152	131	17	6	11	-2	477	478	8	7	0	1	307	273	5
6	6	0	619	610	6	6	8	8	300	319	10	6	11	-1	1000	987	10	7	0	3	641	616	6
6	6	1	355	357	6	6	8	12	277	294	12	6	11	1	1295	1307	13	7	0	5	164	171	10
6	6	2	487	476	5	6	9	-11	846	835	8	6	11	2	349	326	9	7	0	7	1748	1711	14
6	6	3	275	247	8	6	9	-10	165	176	17	6	11	3	1017	1019	10	7	0	9	1438	1415	13
6	6	4	1562	1557	14	6	9	-9	1091	1085	10	6	11	6	339	323	10	7	0	11	329	317	9
6	6	5	269	282	9	6	9	-8	264	263	11	6	11	7	695	723	7	7	0	13	433	424	9
6	6	6	1220	1255	11	6	9	-7	561	560	7	6	11	9	631	616	8	7	1	-14	238	207	13
6	6	8	199	199	14	6	9	-6	398	393	8	6	11	10	261	244	13	7	1	-13	147	89	17
6	6	11	198	230	14	6	9	-4	225	185	11	6	12	-8	349	375	10	7	1	-12	258	257	12
6	6	12	302	304	11	6	9	-3	173	156	14	6	12	-6	869	888	9	7	1	-8	1665	1629	14
6	6	13	139	139	23	6	9	-2	519	512	7	6	12	-4	914	887	8	7	1	-6	2617	2556	13
6	7	-11	1056	1041	11	6	9	-1	986	958	10	6	12	-3	291	267	10	7	1	-4	1370	1313	13
6	7	-9	1311	1302	13	6	9	1	1456	1445	13	6	12	-2	731	742	7	7	1	-2	735	750	8
6	7	-8	193	211	14	6	9	2	344	359	8	6	12	1	139	150	19	7	1	0	826	831	9
6	7	-7	721	728	7	6	9	3	1089	1113	11	6	12	2	447	454	8	7	1	2	321	329	6
6	7	-6	318	345	8	6	9	5	172	164	15	6	12	4	970	976	9	7	1	3	137	120	11
6	7	-5	134	135	16	6	9	6	366	346	9	6	12	6	893	882	8	7	1	4	1391	1429	12
6	7	-2	468	470	6	6	9	7	991	997	10	6	12	7	290	270	12	7	1	5	143	147	11
6	7	-1	1039	1079	10	6	9	9	721	719	7	6	12	8	341	318	11	7	1	6	1704	1721	13
6	7	1	1667	1698	14	6	9	10	225	209	14	6	13	-7	533	534	8	7	1	7	156	128	14
6	7	2	512	513	6	6	9	11	559	565	8	6	13	-6	270	243	12	7	1	8	286	314	9
6	7	3	1194	1179	11	6	10	-10	191	193	16	6	13	-5	141	113	20	7	1	9	305	310	9
6	7	5	290	275	9	6	10	-9	215	238	13	6	13	-3	331	333	10	7	1	10	1389	1401	14
6	7	6	426	428	7	6	10	-8	744	744	7	6	13	-2	312	321	10	7	1	11	156	172	15
6	7	7	1156	1139	11	6	10	-7	212	202	13	6	13	-1	823	820	8	7	1	12	1068	1066	11
6	7	9	761	769	8	6	10	-6	1149	1146	12	6	13	1	785	814	8	7	1	14	230	214	14
6	7	10	370	371	9	6	10	-5	217	201	12	6	13	2	253	246	12	7	2	-15	521	538	9
6	7	11	522	543	8	6	10	-4	748	758	7	6	13	3	580	582	7	7	2	-13	436	433	8
6	7	13	439	443	9	6	10	-3	329	331	9	6	13	6	304	285	12	7	2	-12	209	224	13
6	8	-12	820	803	9	6	10	-2	690	702	7	6	13	7	474	477	9	7	2	-11	608	617	7
6	8	-11	158	148	17	6	10	-1	124	99	20	6	14	-6	575	582	9	7	2	-10	233	213	12
6	8	-9	265	265	11	6	10	0	250	296	11	6	14	-5	157	143	20	7	2	-9	1186	1210	12
6	8	-8	855	820	8	6	10	1	257	270	11	6	14	-4	691	687	8	7	2	-7	615	613	6
6	8	-7	221	225	12	6	10	2	590	592	7	6	14	-3	192	159	16	7	2	-5	1248	1241	11
6	8	-6	1139	1161	11	6	10	4	1464	1486	14	6	14	-2	605	599	8	7	2	-4	191	205	8
6	8	-5	325	323	8	6	10	6	1251	1232	12	6	14	2	313	307	11	7	2	-3	2509	2515	12
6	8	-4	961	966	10	6	10	7	266	278	12	6	14	4	605	616	8	7	2	-1	1246	1258	12
6	8	-3	315	332	8	6	10	8	360	359	10	6	15	-1	615	603	8	7	2	1	125	103	11
6	8	-2	1037	1026	10	6	10	9	179	188	17	7	0	-15	557	547	9	7	2	2	214	204	7
6	8	-1	265	265	9	6	10	11	148	133	21	7	0	-13	354	358	10	7	2	3	150	148	10

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
7	2	5	520	496	5	7	5	-14	228	238	15	7	7	-6	1552	1544	13	7	9	1	296	297	10
7	2	7	1653	1674	14	7	5	-12	229	225	12	7	7	-4	932	904	9	7	9	2	789	800	8
7	2	9	1316	1316	13	7	5	-11	233	226	12	7	7	-3	486	489	7	7	9	3	235	217	12
7	2	11	302	301	9	7	5	-8	1255	1261	14	7	7	-2	387	367	7	7	9	4	1175	1194	12
7	2	13	435	441	9	7	5	-7	303	297	9	7	7	-1	115	135	17	7	9	5	343	338	9
7	3	-14	247	232	13	7	5	-6	1729	1712	14	7	7	0	692	701	7	7	9	6	1046	1036	11
7	3	-12	208	215	14	7	5	-4	768	787	8	7	7	1	423	420	7	7	9	7	248	239	12
7	3	-10	172	184	16	7	5	-3	404	399	6	7	7	2	741	734	7	7	9	9	289	271	11
7	3	-8	1385	1409	13	7	5	-2	761	764	8	7	7	3	261	295	10	7	9	10	695	689	7
7	3	-7	235	266	10	7	5	-1	112	112	14	7	7	4	1200	1200	12	7	9	11	239	247	14
7	3	-6	1790	1805	14	7	5	0	1024	1040	10	7	7	5	193	195	13	7	10	-11	493	486	9
7	3	-5	212	194	9	7	5	1	591	600	6	7	7	6	1088	1106	10	7	10	-9	638	635	8
7	3	-4	644	638	6	7	5	2	978	961	10	7	7	7	209	190	13	7	10	-8	255	232	11
7	3	-2	1033	1011	10	7	5	3	562	556	6	7	7	9	183	182	14	7	10	-7	177	180	14
7	3	-1	150	132	10	7	5	4	1467	1457	14	7	7	10	897	896	9	7	10	-5	731	729	8
7	3	0	1052	1016	11	7	5	6	1311	1319	13	7	7	11	218	201	14	7	10	-4	310	298	10
7	3	1	263	239	7	7	5	7	240	238	11	7	7	12	871	870	10	7	10	-3	1360	1351	13
7	3	2	951	932	9	7	5	8	138	154	19	7	8	-12	240	258	14	7	10	-1	968	971	9
7	3	3	264	269	7	7	5	10	1081	1083	11	7	8	-11	512	517	8	7	10	0	359	371	9
7	3	4	1802	1792	13	7	5	12	985	978	9	7	8	-9	784	779	8	7	10	1	385	376	9
7	3	5	295	316	8	7	6	-13	400	399	10	7	8	-8	181	188	15	7	10	4	299	284	10
7	3	6	1639	1618	14	7	6	-11	649	661	7	7	8	-7	307	289	10	7	10	5	456	453	8
7	3	8	165	173	15	7	6	-9	1200	1189	12	7	8	-5	819	806	8	7	10	6	159	114	16
7	3	9	380	380	8	7	6	-8	337	347	10	7	8	-4	294	299	9	7	10	7	969	963	9
7	3	10	1193	1214	12	7	6	-7	648	651	7	7	8	-3	1555	1563	15	7	10	9	787	793	7
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7	3	12	1042	1031	10	7	6	-4	402	403	7	7	8	0	292	280	9	7	11	-7	194	189	15
7	4	-13	458	455	8	7	6	-3	2065	2062	14	7	8	1	428	441	7	7	11	-6	1018	1033	10
7	4	-11	713	706	7	7	6	-1	1526	1504	14	7	8	2	133	147	18	7	11	-4	700	702	7
7	4	-9	1283	1273	14	7	6	0	451	473	6	7	8	3	231	224	11	7	11	-3	402	406	8
7	4	-8	280	256	10	7	6	1	440	455	6	7	8	4	265	273	11	7	11	-2	193	214	14
7	4	-7	615	612	7	7	6	2	238	245	8	7	8	5	488	494	7	7	11	-1	172	167	15
7	4	-5	1076	1062	11	7	6	4	220	222	11	7	8	7	1302	1297	13	7	11	0	794	790	8
7	4	-4	439	448	6	7	6	5	437	462	7	7	8	8	308	306	10	7	11	1	324	317	9
7	4	-3	2248	2221	13	7	6	6	127	139	20	7	8	9	1036	1031	10	7	11	2	868	855	9
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7	4	0	541	556	5	7	6	8	148	136	19	7	9	-12	144	148	22	7	11	4	844	838	8
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7	4	4	287	272	7	7	6	11	345	339	9	7	9	-7	224	215	12	7	12	-8	234	238	14
7	4	5	577	602	5	7	6	12	219	230	15	7	9	-6	1292	1294	13	7	12	-7	171	205	18
7	4	6	197	184	12	7	6	13	260	263	13	7	9	-5	179	154	15	7	12	-5	417	417	8
7	4	7	1516	1519	15	7	7	-12	194	189	15	7	9	-4	722	710	7	7	12	-4	249	254	12
7	4	9	1130	1132	12	7	7	-11	207	202	13	7	9	-3	385	396	8	7	12	-3	1008	1033	10
7	4	11	292	278	10	7	7	-10	219	211	13	7	9	-2	377	379	8	7	12	-1	903	918	9
7	4	12	138	151	20	7	7	-8	1121	1123	11	7	9	-1	297	278	9	7	12	0	287	284	10
7	4	13	392	391	10	7	7	-7	181	157	15	7	9	0	725	704	7	7	12	1	386	352	8

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
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7	12	5	462	455	9	8	2	-9	164	181	17	8	4	5	200	222	11	8	6	12	762	763	8
7	12	7	694	705	8	8	2	-8	366	361	8	8	4	6	409	429	8	8	7	-11	253	273	13
7	13	-6	701	722	8	8	2	-6	404	403	7	8	4	7	204	219	13	8	7	-10	188	162	14
7	13	-4	590	589	8	8	2	-4	889	881	8	8	4	8	407	412	8	8	7	-9	154	134	16
7	13	-3	212	217	15	8	2	-2	962	966	10	8	4	9	247	254	11	8	7	-7	429	432	8
7	13	0	517	533	8	8	2	0	2403	2421	13	8	4	10	766	772	8	8	7	-6	257	268	12
7	13	1	269	245	12	8	2	1	102	81	16	8	4	12	911	899	10	8	7	-5	922	920	9
7	13	2	716	685	7	8	2	2	1840	1822	13	8	5	-13	770	769	8	8	7	-3	1743	1753	15
7	13	3	247	242	13	8	2	4	117	94	15	8	5	-11	230	239	13	8	7	-2	312	306	9
7	13	4	640	642	8	8	2	6	523	505	6	8	5	-9	165	174	16	8	7	-1	934	927	10
7	13	6	388	407	10	8	2	8	350	358	9	8	5	-7	406	386	8	8	7	1	310	316	9
7	14	-4	209	191	15	8	2	10	826	821	8	8	5	-6	321	311	9	8	7	2	252	264	10
7	14	-3	715	729	8	8	2	12	1028	1044	10	8	5	-5	854	870	8	8	7	3	944	917	10
7	14	-1	705	692	8	8	3	-13	840	829	8	8	5	-3	1890	1903	14	8	7	5	784	780	8
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8	0	-12	870	865	9	8	3	-7	473	434	7	8	5	1	680	661	7	8	7	8	178	175	14
8	0	-10	850	842	8	8	3	-6	236	271	10	8	5	2	422	416	7	8	7	9	561	550	7
8	0	-8	380	363	8	8	3	-5	763	765	7	8	5	3	1310	1297	13	8	7	10	316	307	10
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8	0	10	805	812	8	8	3	6	266	265	9	8	6	-13	266	245	13	8	8	-4	470	486	8
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8	1	-11	281	291	11	8	3	11	232	226	12	8	6	-9	291	283	10	8	8	0	1573	1585	16
8	1	-8	127	100	19	8	3	13	854	878	9	8	6	-8	713	729	7	8	8	1	291	268	9
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8	1	-5	951	945	9	8	4	-10	906	913	9	8	6	-6	753	744	8	8	8	3	170	174	16
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8	1	5	820	822	8	8	4	-4	680	652	7	8	6	2	1402	1384	13	8	8	10	675	678	8
8	1	7	676	677	7	8	4	-3	369	368	7	8	6	3	168	153	14	8	9	-11	237	235	14
8	1	9	937	943	9	8	4	-2	1019	991	10	8	6	4	170	157	14	8	9	-10	231	243	13
8	1	11	253	261	11	8	4	0	2180	2166	13	8	6	5	377	360	8	8	9	-9	231	201	13
8	1	13	863	861	9	8	4	1	269	283	8	8	6	6	446	455	8	8	9	-7	527	528	7
8	2	-12	919	938	10	8	4	2	1589	1614	14	8	6	8	570	566	7	8	9	-6	343	341	9
8	2	-11	149	155	17	8	4	3	111	98	17	8	6	9	240	230	12	8	9	-5	762	769	8

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8	9	-2	276	267	11	8	12	2	744	739	8	9	2	9	784	780	8	9	5	10	276	272	11
8	9	-1	760	753	7	8	12	3	185	170	16	9	2	11	623	623	7	9	6	-9	909	917	9
8	9	0	158	174	17	8	12	5	235	214	14	9	3	-12	832	814	9	9	6	-8	207	226	13
8	9	1	346	326	9	8	12	6	331	310	11	9	3	-10	1085	1084	11	9	6	-7	1352	1378	13
8	9	2	304	297	10	8	13	-5	600	584	8	9	3	-8	260	254	11	9	6	-5	674	693	7
8	9	3	996	991	10	8	13	-3	748	764	8	9	3	-6	745	754	8	9	6	-4	295	310	10
8	9	4	219	170	12	8	13	-2	261	246	12	9	3	-4	739	731	8	9	6	-3	122	158	20
8	9	5	791	789	7	8	13	-1	356	384	10	9	3	-3	163	172	14	9	6	0	467	472	7
8	9	6	418	425	9	8	13	2	174	170	18	9	3	-2	877	870	9	9	6	1	383	381	8
8	9	7	545	529	7	8	13	3	616	600	8	9	3	0	1203	1208	13	9	6	2	177	181	14
8	9	9	479	465	9	9	0	-13	662	660	8	9	3	2	993	958	10	9	6	3	1463	1469	14
8	10	-10	628	635	8	9	0	-11	156	158	17	9	3	4	374	365	7	9	6	4	197	171	13
8	10	-9	253	239	12	9	0	-9	1159	1167	12	9	3	6	1376	1387	14	9	6	5	1343	1332	14
8	10	-8	473	453	8	9	0	-7	1664	1693	15	9	3	8	815	800	8	9	6	8	161	169	16
8	10	-7	211	210	13	9	0	-5	655	645	6	9	3	9	246	236	11	9	6	9	606	608	7
8	10	-6	259	233	11	9	0	-3	111	59	17	9	3	10	236	226	11	9	6	11	585	589	8
8	10	-5	263	265	11	9	0	-1	191	228	10	9	4	-13	507	505	9	9	7	-10	896	904	10
8	10	-4	192	192	14	9	0	1	202	198	9	9	4	-9	1144	1166	12	9	7	-8	347	354	9
8	10	-3	328	351	9	9	0	3	1710	1705	14	9	4	-8	234	243	13	9	7	-7	224	211	13
8	10	-2	686	675	7	9	0	5	1754	1780	15	9	4	-7	1473	1481	14	9	7	-6	519	516	7
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8	10	1	240	214	12	9	0	9	998	1006	10	9	4	-4	352	359	8	9	7	-4	761	746	7
8	10	2	1087	1082	11	9	0	11	647	655	7	9	4	0	228	239	10	9	7	-3	216	194	12
8	10	3	198	203	14	9	1	-12	832	838	8	9	4	1	333	322	8	9	7	-2	886	898	9
8	10	4	171	166	15	9	1	-10	1305	1266	12	9	4	2	209	204	11	9	7	0	1058	1084	11
8	10	6	340	338	10	9	1	-8	466	456	8	9	4	3	1515	1533	15	9	7	1	264	243	10
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8	10	8	404	384	10	9	1	-4	1051	1075	11	9	4	9	595	598	7	9	7	4	489	476	7
8	10	9	217	198	16	9	1	-2	960	995	10	9	4	11	563	578	8	9	7	5	412	409	8
8	11	-7	469	474	9	9	1	0	1409	1424	14	9	5	-12	692	708	8	9	7	6	1454	1425	15
8	11	-6	195	205	16	9	1	1	159	151	12	9	5	-11	183	200	16	9	7	7	243	233	11
8	11	-5	684	670	7	9	1	2	1328	1327	12	9	5	-10	1006	1008	10	9	7	8	882	882	9
8	11	-3	968	982	10	9	1	4	547	559	6	9	5	-8	390	399	8	9	7	9	227	191	13
8	11	-1	574	568	7	9	1	5	178	148	13	9	5	-7	159	180	18	9	7	10	341	348	11
8	11	0	151	138	17	9	1	6	1857	1869	15	9	5	-6	527	525	7	9	8	-9	761	751	7
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8	11	2	270	257	11	9	1	10	165	189	16	9	5	-4	654	660	7	9	8	-7	1020	1036	11
8	11	3	870	882	9	9	2	-13	584	578	8	9	5	-3	160	161	15	9	8	-5	492	489	7
8	11	4	138	145	20	9	2	-9	1246	1257	12	9	5	-2	776	743	8	9	8	-4	349	346	9
8	11	5	771	756	8	9	2	-7	1551	1557	15	9	5	0	975	983	10	9	8	0	461	472	8
8	11	6	502	478	9	9	2	-5	466	458	7	9	5	1	162	168	14	9	8	1	595	605	7
8	11	7	413	415	10	9	2	-3	116	94	17	9	5	2	745	772	7	9	8	2	124	29	20
8	12	-7	224	218	15	9	2	1	413	431	6	9	5	4	474	472	7	9	8	3	1403	1410	15
8	12	-6	361	369	11	9	2	3	1743	1727	14	9	5	5	169	152	16	9	8	4	334	345	9
8	12	-2	579	575	8	9	2	4	190	168	12	9	5	6	1448	1420	14	9	8	5	1262	1281	14
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9	8	9	494	491	8	10	0	-6	896	898	9	10	3	4	173	196	15	10	6	-2	837	845	8
9	9	-10	714	722	8	10	0	-4	1976	1957	15	10	3	5	809	794	7	10	6	-1	272	250	10
9	9	-8	262	249	12	10	0	-2	882	850	9	10	3	6	166	214	16	10	6	0	313	293	9
9	9	-7	196	202	14	10	0	0	711	695	7	10	3	7	150	142	16	10	6	1	155	184	17
9	9	-6	505	510	8	10	0	2	832	809	8	10	3	9	1010	1000	10	10	6	2	535	546	7
9	9	-4	771	754	8	10	0	4	371	365	8	10	3	11	947	961	11	10	6	3	259	262	11
9	9	-3	403	405	8	10	0	6	975	979	10	10	4	-12	271	271	13	10	6	4	457	470	8
9	9	-2	814	810	8	10	0	8	1218	1250	12	10	4	-10	215	205	13	10	6	5	164	185	16
9	9	-1	267	265	10	10	0	10	415	416	9	10	4	-9	167	140	15	10	6	6	840	832	8
9	9	0	852	877	9	10	1	-13	393	398	11	10	4	-6	931	922	9	10	6	7	257	248	11
9	9	2	773	757	8	10	1	-11	423	437	9	10	4	-4	1613	1665	16	10	6	8	832	848	9
9	9	5	260	251	11	10	1	-9	739	726	7	10	4	-2	720	729	7	10	6	9	241	240	14
9	9	6	984	992	10	10	1	-7	1057	1071	10	10	4	-1	353	365	8	10	6	10	276	247	12
9	9	8	776	778	7	10	1	-6	167	182	16	10	4	0	449	428	7	10	7	-9	696	699	8
9	9	9	275	272	13	10	1	-5	675	675	7	10	4	1	297	295	10	10	7	-7	818	821	8
9	10	-9	573	563	8	10	1	-3	928	946	9	10	4	2	402	400	8	10	7	-6	162	161	16
9	10	-8	213	215	15	10	1	-2	141	133	17	10	4	3	221	227	12	10	7	-5	483	480	8
9	10	-7	818	823	8	10	1	-1	1473	1456	15	10	4	4	213	230	13	10	7	-3	610	614	7
9	10	-5	471	461	8	10	1	1	866	864	9	10	4	5	300	305	9	10	7	-2	140	173	19
9	10	-4	472	469	8	10	1	2	186	182	13	10	4	6	858	855	8	10	7	-1	1167	1165	12
9	10	-1	176	199	15	10	1	3	580	580	6	10	4	8	1020	1011	10	10	7	0	184	171	15
9	10	0	273	264	10	10	1	4	215	215	12	10	4	9	158	163	18	10	7	1	887	873	9
9	10	1	441	429	8	10	1	5	578	572	7	10	4	10	311	310	11	10	7	2	267	281	11
9	10	3	912	917	9	10	1	7	199	236	13	10	5	-11	434	423	9	10	7	3	477	473	8
9	10	4	289	287	11	10	1	9	1077	1078	11	10	5	-10	189	185	16	10	7	5	312	323	10
9	10	5	963	972	10	10	1	11	1095	1094	11	10	5	-9	610	642	7	10	7	7	303	284	10
9	11	-6	261	241	12	10	2	-12	287	295	12	10	5	-8	147	137	17	10	7	9	801	823	8
9	11	-4	619	615	8	10	2	-10	328	331	10	10	5	-7	917	927	9	10	8	-10	250	228	13
9	11	-3	249	261	12	10	2	-6	928	927	9	10	5	-5	605	581	7	10	8	-9	203	178	15
9	11	-2	696	685	7	10	2	-4	1770	1767	15	10	5	-4	188	189	15	10	8	-8	132	112	21
9	11	-1	172	193	16	10	2	-2	809	804	7	10	5	-3	690	677	6	10	8	-6	740	730	7
9	11	0	552	547	7	10	2	0	530	533	6	10	5	-2	269	277	10	10	8	-5	267	283	11
9	11	2	368	383	9	10	2	2	563	552	6	10	5	-1	1071	1055	12	10	8	-4	1331	1336	14
9	11	3	152	123	19	10	2	4	210	220	13	10	5	1	620	624	6	10	8	-3	236	233	12
9	11	6	659	674	8	10	2	6	904	923	9	10	5	2	310	325	9	10	8	-2	754	784	9
9	12	-5	581	574	8	10	2	7	128	93	18	10	5	3	442	449	8	10	8	-1	209	215	13
9	12	-4	337	322	10	10	2	8	1160	1188	13	10	5	5	498	488	7	10	8	0	148	162	17
9	12	-1	181	157	16	10	2	10	381	373	9	10	5	6	148	163	18	10	8	2	457	460	8
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9	12	3	668	672	8	10	3	-7	869	869	8	10	6	-10	306	292	11	10	8	5	253	240	12
9	12	4	186	194	19	10	3	-6	173	154	15	10	6	-9	176	179	16	10	8	6	699	710	7
9	13	-2	655	636	8	10	3	-5	478	466	7	10	6	-7	131	132	20	10	8	8	747	738	8
9	13	0	530	539	9	10	3	-3	863	879	8	10	6	-6	927	898	9	10	9	-9	603	590	8
10	0	-12	299	333	12	10	3	-1	1212	1252	13	10	6	-5	299	286	10	10	9	-7	546	555	8
10	0	-10	482	480	8	10	3	1	727	742	7	10	6	-4	1663	1659	16	10	9	-6	188	205	15

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
10	9	-5	293	284	10	11	1	1	136	142	18	11	5	-7	152	179	17	11	9	-4	426	411	9
10	9	-3	559	565	7	11	1	2	1531	1566	14	11	5	-6	599	621	7	11	9	-1	152	154	19
10	9	-1	1035	1033	11	11	1	4	963	967	10	11	5	-5	214	241	13	11	9	0	432	424	9
10	9	1	808	810	8	11	1	10	133	144	21	11	5	-4	651	667	7	11	9	2	916	902	8
10	9	2	288	279	10	11	2	-11	943	924	9	11	5	-2	334	336	9	11	9	4	797	813	8
10	9	3	482	486	8	11	2	-9	385	382	9	11	5	0	478	482	8	11	9	5	245	234	14
10	9	5	347	357	10	11	2	-7	184	204	15	11	5	2	1264	1249	12	11	10	-5	261	252	13
10	9	6	348	323	10	11	2	-6	211	216	12	11	5	4	920	915	9	11	10	-4	274	292	12
10	9	7	153	132	19	11	2	-5	146	158	18	11	5	5	213	234	13	11	10	-3	563	573	8
10	10	-7	158	162	19	11	2	-4	187	194	14	11	5	6	152	165	17	11	10	-1	747	742	8
10	10	-6	532	515	8	11	2	-3	853	860	9	11	6	-9	449	454	9	11	10	1	634	640	8
10	10	-4	922	926	9	11	2	-1	1618	1629	16	11	6	-5	193	189	14	12	0	-10	713	717	8
10	10	-2	558	550	7	11	2	1	1192	1194	11	11	6	-3	733	726	7	12	0	-8	1191	1212	12
10	10	-1	343	343	9	11	2	3	362	351	9	11	6	-2	174	181	15	12	0	-6	561	575	7
10	10	1	274	271	11	11	2	4	146	143	17	11	6	-1	1207	1206	12	12	0	-4	513	530	7
10	10	2	356	367	10	11	2	5	1026	1021	9	11	6	0	317	329	10	12	0	-2	714	711	7
10	10	3	273	261	11	11	2	7	458	454	8	11	6	1	779	790	7	12	0	0	451	447	7
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10	11	-5	282	276	12	11	3	-8	970	985	10	11	6	7	539	537	8	12	0	8	991	982	10
10	11	-3	352	347	10	11	3	-6	594	596	7	11	6	8	250	239	13	12	1	-9	427	405	9
10	11	-2	135	139	22	11	3	-4	735	758	7	11	7	-8	779	783	7	12	1	-7	780	760	7
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10	11	1	610	614	8	11	3	-2	471	475	7	11	7	-6	559	567	8	12	1	-3	647	650	7
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11	1	-6	569	578	7	11	4	5	876	857	8	11	8	3	214	220	13	12	2	6	152	160	18
11	1	-5	196	211	14	11	4	7	474	465	8	11	8	4	364	382	10	12	2	8	888	897	9
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11	1	-3	200	189	13	11	4	9	311	327	11	11	8	7	518	540	9	12	3	-7	700	726	7
11	1	-2	404	398	8	11	5	-10	546	541	9	11	9	-6	492	483	8	12	3	-6	183	166	15
11	1	0	773	776	8	11	5	-8	854	866	9	11	9	-5	221	209	15	12	3	-5	1226	1236	13
																		12	3	-3	759	765	8

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
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12	3	-1	299	288	9	12	7	3	372	375	10	13	4	-5	982	1013	10	14	4	0	541	546	8
12	3	1	221	232	12	12	7	5	846	849	8	13	4	-3	635	634	8	14	4	2	195	186	16
12	3	3	250	230	11	12	8	-6	468	458	9	13	4	-1	306	338	11	14	5	-1	326	335	11
12	3	5	1016	1031	11	12	8	-5	152	160	22	13	4	1	925	905	9	14	5	1	875	890	9
12	3	7	806	801	8	12	8	-4	252	222	12	13	4	3	659	647	8						
12	4	-8	972	983	10	12	8	-2	560	559	8	13	4	4	160	178	19						
12	4	-6	489	485	8	12	8	-1	176	157	16	13	4	5	472	466	9						
12	4	-5	245	259	12	12	8	0	563	549	8	13	5	-6	301	305	12						
12	4	-4	353	367	9	12	8	2	607	609	8	13	5	-4	509	530	9						
12	4	-2	602	612	7	12	8	3	212	200	15	13	5	-2	1220	1210	12						
12	4	-1	238	255	11	12	8	4	561	567	8	13	5	-1	211	184	14						
12	4	0	579	570	7	12	9	-3	672	664	8	13	5	0	896	904	9						
12	4	1	200	217	13	12	9	-2	161	210	20	13	5	4	269	274	12						
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12	4	4	978	961	9	12	9	2	188	161	16	13	6	-3	504	492	8						
12	4	6	163	135	17	13	0	-7	484	469	8	13	6	-1	374	365	10						
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12	5	-9	259	270	14	13	0	-3	697	702	7	13	6	1	857	856	9						
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12	5	-5	1174	1177	12	13	0	1	1039	1063	11	13	6	4	178	222	18						
12	5	-3	753	770	8	13	0	3	525	538	8	13	7	-4	408	401	10						
12	5	-2	330	323	9	13	0	5	380	347	9	13	7	-3	150	169	21						
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12	5	7	720	718	8	13	1	-2	1455	1436	14	14	0	-4	332	355	11						
12	6	-8	955	941	9	13	1	0	995	975	11	14	0	-2	508	528	8						
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12	6	-2	660	675	8	13	2	-4	168	191	16	14	1	-1	195	186	15						
12	6	-1	265	234	10	13	2	-3	694	709	7	14	1	1	989	964	10						
12	6	0	637	638	7	13	2	-1	382	388	9	14	1	3	981	971	10						
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12	6	2	740	742	8	13	2	3	570	572	7	14	2	-4	403	401	9						
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12	6	5	137	117	22	13	3	-8	296	302	12	14	2	2	239	222	13						
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12	7	-7	565	550	8	13	3	-4	585	572	7	14	3	-2	167	161	18						
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12	7	-1	170	172	16	13	3	6	338	335	10	14	4	-4	493	494	9						

LAWRENCE BERKELEY LABORATORY
TECHNICAL INFORMATION DEPARTMENT
UNIVERSITY OF CALIFORNIA
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