Title

THE CRYSTAL AND MOLECULAR STRUCTURE OF di(TETRA-n-BUTYL AMMONIUM) COBALT (II) BIS-(MALEONITRILE DITHIOLATE) AND THE GEOMETRY OF THE DIVALENT COBALT (II) BIS-(MALEONITRILE DITHIOLATE) ION

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J. D. Forrester, Allan Zalkin and David H. Templeton

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CONTRIBUTION FROM THE LAWRENCE RADIATION LABORATORY AND DEPARTMENT OF CHEMISTRY,
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The Crystal and Molecular Structure of di-(tetra-n-butyl ammonium) cobalt (II) bis-(maleonitrile dithiolate) and the geometry of the divalent cobalt (II) bis-(maleonitrile dithiolate) ion.[1]

BY J. D. FORRESTER, ALLAN ZALKIN AND DAVID H. TEMPLETON.

The crystal and molecular structure of di-(tetra-n-butyl ammonium) cobalt (II) bis-(maleonitrile dithiolate) has been determined from an x-ray diffraction study of a single crystal specimen. A convenient triclinic cell, space group $P\bar{1}$, with $a = 10.77 \pm 0.01$, $b = 12.35 \pm 0.01$, $c = 9.81 \pm 0.01$ Å., $\alpha = 88.5 \pm 0.1$, $\beta = 114.8 \pm 0.1$ and $\gamma = 93.5 \pm 0.1^\circ$, contains one formula unit. Atomic parameters were refined by least squares methods using full three dimensional data out to $2\theta = 40^\circ$.

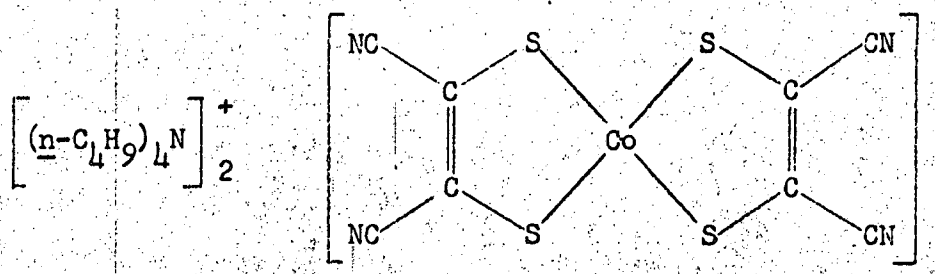
The anion is closely planar with the sulfur atoms in a square arrangement around the cobalt atom. The symmetry of the anion is mmm to a very close degree. Three of the n-butyl chains in the cation adopt the trans conformation whilst the other has the gauche conformation with a dihedral angle of 71.6°. The cobalt atoms are very well separated with the closest distance of approach as the shortest axial length of 9.81 Å. Positions of all 36 independent hydrogen atoms were determined from an electron density difference function.

Introduction

There has been considerable interest recently in the electronic energy levels of a series of compounds represented by the general formula $R'_z(M'S_4C_4R_4)^{-z}$, where $z = 0, 1, 2$; M' = Co, Ni, Cu, Pd, Pt, Zn, Rh; R = CN, CF_3, C_6H_5, etc.

and R' = $(\underline{n}\text{-}C_4H_9)_4N^+$, $(CH_3)_4N^+$, $(C_2H_5)_4N^+$, etc. Interpretation of these results however has been somewhat hampered by the lack of any detailed knowledge of the molecular structure of these compounds and certain discrepancies have arisen in the electron spin resonance measurements.

$((\underline{n}\text{-}C_4H_9)_4N)_2^+ (Co(S_2C_4N_2)_2)^{2-}$, abbreviated $((\underline{n}\text{-}Bu)_4N)_2^+ (Co(MNT)_2)^{2-}$, and shown schematically below, is a typical member of this series. The anion $(Co(MNT)_2)^{2-}$



was first prepared by Gray and co-workers[2] who found that the x-ray powder diffraction patterns for $((\underline{n}\text{-}Bu)_4N)_2^+ (M'(MNT)_2)^{2-}$ with M' = Co, Pt, Ni and later, Rh[3] were identical and differ considerably from that found with M' = Zn.

Electron spin resonance and magnetic susceptiblity measurements on these compounds have been made by Davison *et al*[4,5,6] as well as by Gray *et al*[2] and Billig *et al*[7]. Previous evidence[8,9] indicated that four co-ordinated, low spin complexes of Co were likely to be square planar. This is based on magnetic measurements and apparently the only evidence obtained by x-ray diffraction techniques is the molecular structure of Co(II)phthalocyanine where Linstead and Robertson[10,11] showed that the Co atom had a square planar environment. Little further evidence seems to be available, *e.g.* Wells[12].

An x-ray structure determination was completed very recently by Eisenberg *et al*[13] on another member of this family, *viz*, $((CH_3)_4N)_2^+ (Ni(MNT)_2)^{2-}$ and our work is in very close agreement with this.

Maki *et al*[14] have recently used the results of the present crystallographic investigation in a detailed report on the electronic structures of several members of this series of compounds.

Experimental

X-ray diffraction.—We are indebted to Dr. A.H.Maki of Harvard University for sending us some well formed crystals of the complex $(n\text{-}Bu_4N)_2^+ (CoS_4C_4(CN)_4)^{2-}$. The melting point, analysis and conductivities of these crystals are described in a paper by Davison et al[5].

X-ray photographs obtained by the Weissenberg technique and copper radiation established the diffraction symmetry of the crystal. A single crystal, in the form of a thin plate of approximate dimensions 0.24 x 0.20 x 0.10 mm and mounted about an a^* axis was used for collecting the intensity data. Intensities were measured with a General Electric XRD-5 goniostat equipped with a scintillation counter and a pulse height discriminator. MoKα radiation was used and the unit cell dimensions are based on $\lambda = 0.70926$ Å for $MoK\alpha_1$.

The 2213 independent reflections permitted by the space group in the sphere of reflection with $\sin\theta/\lambda$ less than 0.482 ($2\theta < 40^\circ$) were measured with counting times of 10 sec. each. Of these, 390 were assigned zero intensity and the maximum count was 12,350 counts/sec. for the 100 reflection. No corrections were made for either absorption or extinction. With $\mu = 5.9$ cm^{-1} for Mo radiation, μR is 0.07 or less, making the absorption effects rather small.

Calculations were made with an IBM 7094 computer using a full matrix least squares refinement program written by P.K.Gantzel, R.A.Sparks and K.N.Trueblood, with minor modifications, and Fourier and distance programs written by Zalkin (all unpublished). We minimised the function $\Sigma w(|F_o| - |F_c|)^2 / \Sigma wF_o^2$, where F_o and F_c are the observed and calculated structure factors, respectively, and w is the weighting factor.

Atomic scattering factors were taken as the values given by Ibers[15] for neutral Co, S, N, C and H. Dispersion corrections[16] of -0.4 and -0.1 electrons were added to the Co and S scattering factors respectively. The imaginary part of the dispersion correction is small and was ignored.

Results

Unit Cell and Space Group.—A convenient primitive unit cell contains one formula unit $((n\text{-}C_4H_9)_4N)_2^+ (Co(S_2C_4N_2)_2)^{2-}$ and is triclinic with dimensions :-

$$a = 10.77 \pm 0.01,\ b = 12.35 \pm 0.01,\ c = 9.81 \pm 0.01\ \text{Å}$$

$$\alpha = 88.5 \pm 0.1,\ \beta = 114.8 \pm 0.1,\ \gamma = 93.5 \pm 0.1^\circ$$

$$V = 1182.0\ \text{Å}^3.$$

With one formula unit per unit cell, the density calculated from the x-ray data is 1.16 g./cc., in comparison with the value of 1.14 g./cc. found by flotation methods using a mixture of benzene and carbon tetrachloride.

There are no systematic extinctions and the space group could be either $P1$ (C_1) or $P\bar{1}$ (C_i). Previous evidence indicated that the Co complex was likely to be planar and we favored the space group $P\bar{1}$ (C_i) and the success of our structure determination confirms this choice.

Determination of the Structure.—After about half of the data had been collected, a three dimensional Patterson function and a three dimensional Fourier with phases based on Co placed at the origin, were calculated from the observed intensities after correction for Lorentz and polarisation effects. From these two functions and a knowledge of the molecular geometry, it was possible to determine unambiguously the positions of all the independent atoms (2S, 4C and 2N) in the anion. With the exception of the Co atom which is in a special position,

$$1\ (a)\quad 0,\ 0,\ 0$$

all the atoms are in general two fold positions,

$$2\ (i)\quad \pm(x,\ y,\ z)\ .$$

At this stage, all the data had been measured, and a second three dimensional electron density function with phases based on the whole of the anion was calculated from 1627 observed reflections (whose intensity was greater than 3 counts per sec.) after correction for Lorentz and polarisation effects. Using

this function, together with information regarding bond distances and angles and rejecting any positions which did not lead to peaks in the Patterson function, all 17 independent atoms (1N and 16C) in the tetra n-butyl ammonium ion were found in general positions.

A least squares refinement with all 26 of these atoms, each having an isotropic temperature factor of the form $\exp(-B\lambda^{-2}\sin^2\theta)$, and using the 1627 terms each with unit weight resulted in a conventional unreliability factor $R = \Sigma \left| |F_o| - |F_c| \right| / \Sigma |F_o|$ of 0.18 after 4 cycles of refinement. Interatomic distances and angles appeared at this stage to be very reasonable but there were several large discrepancies in the observed and calculated structure factors, some of the temperature factors were somewhat abnormal and we felt that the agreement should be much better. However, it was then realised that we had neglected to apply a special position factor to the Co form factor which was thus twice as large as it ought to be. Correction of this blunder and 3 cycles of refinement speedily reduced R to 0.11. Several errors in the data taking and in the card punching were corrected and the Co atom given an anisotropic temperature factor of the form $\exp(-\beta_{11}h^2 - \beta_{22}k^2 - \beta_{33}\ell^2 - 2\beta_{12}hk - 2\beta_{13}h\ell - 2\beta_{23}k\ell)$, with $4\beta_{ij} = a_i^* a_j^* B_{ij}$, a_i^* being the length of the ith reciprocal axis. With this notation, the anisotropic thermal parameters B_{ij} are in the units ($Å^2$) which are used for isotropic thermal parameters B in the temperature factors of the form $\exp(-B\lambda^{-2}\sin^2\theta)$. Four cycles of refinement with all 2213 terms included resulted in R = 0.142. The terms were weighted so that the 1823 non-zero terms were given unit weight and the 390 zero terms were given 1/4 weight.

An electron density difference function, with all the atoms except hydrogen subtracted out was calculated using the results of this refinement for the terms with $\sin\theta/\lambda < 0.4$. With the exception of several peaks due to an incorrect description of the thermal motion of the sulfur atoms, the highest peaks in this function all corresponded to reasonable positions for the 36 independent hydrogen

atoms, all in two-fold general positions. Two cycles of least squares refinement were run with the two sulfur atoms, as well as the cobalt, having anisotropic thermal parameters, and R fell to 0.126.

We now had more parameters for refinement than our program could accomodate so we ran a series of calculations refining parts of the structure separately with the remainder held fixed. First, the H atoms were included but not refined, while all the other parameters were refined and R fell to 0.103. Then all atoms except H were held fixed and the 36 H atoms, each with an isotropic temperature factor, were refined and resulted in R = 0.097. This procedure was repeated twice to give a final R factor of 0.091. In the final cycles, no heavier atom parameter moved more than 4% of a standard deviation and most moved much less than this.

The positional and thermal parameters resulting from these last cycles are listed in Tables I, II and III and the observed and calculated structure factors are compared in Table IV.

Standard deviations of the parameters of the heavy atoms were calculated assuming that the discrepancies in the structure factors represent random errors and with the neglect of the effect of the H parameters. Limitations of our computer program did not permit us to estimate the standard deviations of the hydrogen atom parameters by the method of least squares. From the results of the hydrogen bond distance calculations however, we estimate the standard deviations of the H atom positional parameters to be 0.1 to 0.2 Å.

Description of the Structure.—A projection down the b axis of the overall structure is shown in Fig.1. The planar $Co(MNT)_2^{2-}$ ion has a center of symmetry at the cobalt atom and the two tetra n-butyl ammonium ions are related to each other by a center of symmetry. The ions are interlaced to form layers in the bc plane.

The $Co(MNT)_2^{2-}$ ion.—The dimensions of the anion are illustrated in Fig.2 and compared in Table V with those found in the complex $((CH_3)_4N)_2^+ (Ni(MNT)_2)^{2-}$ by Eisenberg et al[13]. The agreement is very close, with the Co-S and Ni-S distances in the two complexes equal to well within the experimental accuracy.

The anion is very closely planar and deviations from planarity are small enough to be chemically insignificant. The three atoms Co, C(1) and C(2) define a plane of equation :-

$$-4.996\,X - 6.634\,Y + 7.975\,Z = 0 \quad .$$

The distances of the various atoms from this plane are listed in Table VI. S(1) is somewhat out of the plane of Co, S(2), C(1) and C(2) and makes the five membered ring slightly puckered and the cyanide groups are bent a small amount out of the plane. None of these deviations however is as much as 0.1 Å.

The chemically equivalent, but crystallographically non-equivalent bonds in the anion viz, S(1)-C(1) and S(2)-C(2), C(1)-C(3) and C(2)-C(4), C(3)-N(1) and C(4)-N(2) are equal to better than two standard deviations. Although the ion is required to have only a center of symmetry (C_i), the geometry is such that it does not differ significantly from mmm (D_{2h}).

The arrangement of the sulfur atoms around the cobalt atom is very close to square although the S-metal-S angle within the five membered ring is found to be somewhat greater than 91° in both the present structure determination and in that of Eisenberg et al[13].

The closest intermolecular contacts of the cobalt atom are two butyl carbon atoms from each of the cations at distances of C(9) = 3.927 ± 0.008 and C(5) = 4.179 ± 0.008 Å, together with the hydrogen atoms associated with these two carbon

atoms viz, H1C5 at 3.34, H2C5 at 4.13, H1C9 at 2.96 and H2C9 at 3.90 Å.

The cobalt atoms are very well separated as the nearest distance of approach is the shortest lattice distance, 9.81 Å.

The tetra n-butyl ammonium ion.—The configuration of this ion can be seen in Fig.1 and the important dimensions are listed in Tables VIII and IX. Three of the butyl chains adopt the trans conformation but one, (C(17)-C(20)), adopts a gauche conformation, presumably to improve the packing and to avoid too close approach to the Co atom. The dihedral angles for all the chains are listed in Table VII. The angles for the trans chains are very close to zero showing them to be very nearly planar. The dihedral angle for the gauche chain is 71.6°, in comparison with a mean dihedral angle of 61 ± 3° found by Bartell and Kohl[17] in an electron diffraction study of free hydrocarbon chains in the gas phase, and the ideal value of 60°.

The four C-N bonds are equal to within the experimental accuracy and have an average value of 1.52 ± 0.01 Å. The six tetrahedral angles at the nitrogen atom (C-N-C) average 109.5° with a spread of ± 3° and are very close to the tetrahedral angle.

In the butyl chains, the mean C-C distance is 1.515 Å. Applying a thermal correction, assuming that each carbon atom "rides" on its neighbour nearer to the central nitrogen atom, increases this distance by 0.010 Å. This assumption is reasonable as the temperature factors of the carbon atoms increase progressively along each carbon chain (see Table I). The mean value of the twelve N-C-C and C-C-C angles is 113.1°, somewhat greater than the tetrahedral angle. The four N-C-C angles all have higher than average values.

The majority of the 36 hydrogen atoms are very suitably placed with respect to both distance and angle as can be seen from Table IX. The mean C-H bond length (36 values) is 0.98 Å, somewhat smaller than the value of 1.09 Å usually taken as the standard interatomic separation. Several of the bond angles deviate largely

from tetrahedral, but the majority are very close. In particular, except for the hydrogen atoms on the terminal carbon atoms of the four n-butyl chains, all the hydrogen bond angles are within 15° of the expected value, consistent with the estimated standard deviations of the hydrogen atom positions. It is noteworthy that, unexpectedly, all the hydrogen atoms except one have calculated temperature factors less than those of the carbon atoms with which they are associated.

X-ray powder diffraction photographs of material from the sample studied in this investigation and of material used in the e.s.r. experiments (kindly supplied by Dr. N.Edelstein) are consistent but do not agree with the d-spacings reported by Davison et al[5].

We thank Prof. A.H.Maki and Dr. N.Edelstein for providing us with excellent crystals of the material and for their co-operation in and helpful discussion of the problem.

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TABLE I

FINAL CO-ORDINATES AND ISOTROPIC THERMAL PARAMETERS, TOGETHER WITH THEIR STANDARD DEVIATIONS, FOR ALL ATOMS EXCEPT HYDROGEN

Atom	x	σ(x)	y	σ(y)	z	σ(z)	B[b]	σ(B)
Co	0.0	-	0.0	-	0.0	-	a	
S(1)	0.0401	0.0002	0.1381	0.0002	0.1461	0.0002	a	
S(2)	-0.2156	0.0002	0.0303	0.0002	-0.1093	0.0002	a	
C(1)	-0.1164	0.0007	0.1930	0.0005	0.0876	0.0007	4.8	0.1
C(2)	-0.2284	0.0007	0.1462	0.0006	-0.0215	0.0008	5.1	0.2
C(3)	-0.1244	0.0008	0.2884	0.0007	0.1575	0.0009	6.2	0.2
C(4)	-0.3583	0.0010	0.1883	0.0007	-0.0717	0.0010	7.5	0.2
N(1)	-0.1273	0.0007	0.3663	0.0006	0.2173	0.0008	7.4	0.2
N(2)	-0.4644	0.0010	0.2247	0.0007	-0.1113	0.0010	10.6	0.2
N(3)	0.0867	0.0005	0.2783	0.0004	-0.2929	0.0006	4.5	0.1
C(5)	0.1928	0.0007	0.2589	0.0005	-0.1328	0.0007	4.7	0.1
C(6)	0.2939	0.0007	0.3510	0.0006	-0.0626	0.0008	5.4	0.2
C(7)	0.3797	0.0008	0.3242	0.0007	0.1022	0.0009	6.8	0.2
C(8)	0.4977	0.0010	0.4090	0.0008	0.1791	0.0011	9.3	0.3
C(9)	-0.0023	0.0007	0.1739	0.0006	-0.3417	0.0008	5.1	0.2
C(10)	-0.1166	0.0008	0.1780	0.0007	-0.5002	0.0009	7.0	0.2
C(11)	-0.2078	0.0009	0.0756	0.0008	0.4698	0.0010	8.2	0.2
C(12)	-0.3249	0.0010	0.0688	0.0008	0.3114	0.0011	8.8	0.2
C(13)	0.1539	0.0007	0.3116	0.0005	-0.3964	0.0007	5.1	0.2
C(14)	0.2348	0.0007	0.2285	0.0006	-0.4230	0.0008	5.6	0.2
C(15)	0.3224	0.0008	0.2751	0.0007	-0.5004	0.0009	6.7	0.2
C(16)	0.4075	0.0009	0.1951	0.0007	0.4737	0.0010	7.6	0.2
C(17)	0.0004	0.0007	0.3719	0.0006	-0.2930	0.0008	5.5	0.2
C(18)	-0.0670	0.0008	0.3598	0.0006	-0.1848	0.0009	6.6	0.2
C(19)	-0.1712	0.0009	0.4468	0.0007	-0.2126	0.0010	7.3	0.2
C(20)	-0.2992	0.0011	0.4290	0.0009	-0.3553	0.0012	10.6	0.3

[a] Treated anisotropically - see Table III.

[b] In $Å^2$.

TABLE II

FINAL CO-ORDINATES AND ISOTROPIC THERMAL PARAMETERS FOR THE HYDROGEN ATOMS

Atom	x	y	z	B (Å^2)	Atom	x	y	z	B (Å^2)
H1 C5	0.13	0.23	-0.08	1.1	H1 C13	0.22	0.39	-0.35	4.6
H2	0.24	0.20	-0.15	1.9	H2	0.08	0.33	-0.47	5.4
H1 C6	0.35	0.37	-0.12	1.9	H1 C14	0.29	0.20	-0.34	0.5
H2	0.25	0.42	-0.06	4.0	H2	0.18	0.17	-0.49	4.9
H1 C7	0.32	0.32	0.16	4.9	H1 C15	0.38	0.33	-0.44	3.4
H2	0.41	0.26	0.11	0.3	H2	0.26	0.31	-0.58	3.3
H1 C8	-0.43	0.42	0.12	4.6	H1 C16	0.47	0.16	0.56	5.2
H2	-0.47	0.35	0.21	1.6	H2	0.37	0.13	0.43	4.2
H3	-0.53	0.48	0.16	3.6	H3	0.46	0.24	0.43	9.9
H1 C9	-0.04	0.15	-0.25	3.4	H1 C17	-0.06	0.37	-0.40	3.1
H2	0.06	0.12	-0.34	0.9	H2	0.06	0.44	-0.28	2.9
H1 C10	-0.18	0.21	-0.48	1.0	H1 C18	0.01	0.36	-0.07	7.7
H2	-0.07	0.18	-0.57	7.9	H2	-0.12	0.29	-0.20	2.7
H1 C11	-0.25	0.08	0.55	7.0	H1 C19	-0.21	0.44	-0.12	7.0
H2	-0.14	0.05	0.45	2.9	H2	-0.14	0.52	-0.23	3.7
H1 C12	-0.38	0.11	0.33	3.5	H1 C20	-0.28	0.44	-0.44	4.4
H2	-0.27	0.04	0.26	5.3	H2	-0.33	0.37	-0.32	5.5
H3	-0.33	0.14	0.25	8.8	H3	-0.36	0.49	-0.33	22.8

TABLE III

FINAL ANISOTROPIC THERMAL PARAMETERS OF THE COBALT AND THE TWO SULFUR ATOMS.[a]

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}[b]
Co	3.5	5.1	3.8	0.1	1.1	0.0
S(1)	4.2	5.9	4.9	0.1	0.9	-0.6
S(2)	4.1	7.5	5.5	0.3	0.9	-1.8

[a] Estimated standard deviations are all approximately 0.1 $Å^2$.

[b] In $Å^2$.

TABLE IV

OBSERVED STRUCTURE FACTOR MAGNITUDES (FOBS) AND CALCULATED STRUCTURE FACTORS (FCAL), EACH MULTIPLIED BY 10

(Table in two parts, to be reproduced photographically.)

H,K= 0, 0			
L	FOBS	FCAL	
1	590	551	-5
2	315	302	-4
3	377	-379	-3
4	186	-171	-2
5	185	-160	-1
6	157	158	0
7	136	131	1
8	90	99	2
			3
H,K= 0, 1			4
L	FOBS	FCAL	5
-8	114	109	6
-7	160	152	
-6	63	79	H,K= 0, 8
-5	180	-176	L
-4	242	-244	-5
-3	446	455	-4
-2	1001	1005	-3
-1	52	21	-2
0	473	415	-1
1	631	587	0
2	337	306	1
3	255	236	2
4	265	261	3
5	22	-16	4
6	175	171	5
7	120	131	6
8	131	137	7
			8
H,K= 0, 2			
L	FOBS	FCAL	
-8	122	129	
-7	92	91	
-6	0	-23	
-5	138	136	
-4	136	142	
-3	356	344	
-2	233	-240	
-1	673	655	
0	472	-486	
1	45	19	
2	99	89	
3	286	271	
4	217	198	
5	232	216	
6	155	146	
7	0	9	
8	0	3	
H,K= 0, 3			
L	FOBS	FCAL	
-8	97	83	
-7	89	85	
-6	78	-81	
-5	50	58	
-4	0	8	
-3	145	161	
-2	43	-38	
-1	507	503	
0	245	231	
1	143	137	
2	0	2	
3	205	207	
4	197	192	
5	126	115	
6	35	23	
7	27	25	
8	0	-13	
H,K= 0, 4			
L	FOBS	FCAL	
-8	42	48	
-7	120	110	
-6	44	46	
-5	0	-1	
-4	96	106	
-3	51	60	
-2	148	157	
-1	180	184	
0	0	-14	
1	40	29	
2	520	509	
3	180	196	
4	0	38	
5	57	-49	
6	98	-99	
7	0	-12	
8	111	91	
H,K= 0, 5			
L	FOBS	FCAL	
-7	63	69	
-6	143	133	
-5	146	143	
-4	205	195	
-3	51	31	
-2	91	-80	
-1	0	21	
0	368	369	
1	506	501	
2	581	572	
3	224	239	
4	0	-11	
5	103	-93	
6	108	-118	
7	116	-111	
H,K= 0, 6			
L	FOBS	FCAL	
-7	0	37	
-6	138	137	
-5	170	190	
-4	53	56	
-3	70	-80	
-2	21	-36	
-1	136	157	
0	313	308	
1	419	433	
2	517	519	
3	312	301	
4	0	45	
5	84	-76	
6	61	-53	
7	0	-7	
H,K= 0, 7			
L	FOBS	FCAL	
-6	105	96	
-5	92	108	
-4	0	20	
-3	0	19	
-2	0	17	
-1	112	126	
0	191	192	
1	282	264	
2	109	107	
3	85	90	
4	0	1	
5	0	35	
6	162	151	
H,K= 0, 8			
L	FOBS	FCAL	
-5	97	93	
-4	39	-37	
-3	0	-43	
-2	0	39	
-1	34	50	
0	189	202	
1	93	85	
2	237	226	
3	54	-37	
4	25	39	
5	166	151	
6	103	96	
7	51	42	
H,K= 0, 9			
L	FOBS	FCAL	
-5	50	53	
-4	0	-27	
-3	0	8	
-2	45	43	
-1	71	75	
0	0	6	
1	133	137	
2	152	160	
3	145	123	
4	92	88	
5	142	144	
H,K= 0, 10			
L	FOBS	FCAL	
-4	82	81	
-3	28	33	
-2	82	88	
-1	0	14	
0	0	-16	
1	0	-36	
2	82	78	
3	143	140	
4	29	52	
H,K= 0, 11			
L	FOBS	FCAL	
5	87	95	
6	26	20	
7	69	63	
H,K= 0, 12			
L	FOBS	FCAL	
0	40	41	
1	0	8	
2	71	80	
H,K= 1, -11			
L	FOBS	FCAL	
-4	349	356	
-3	391	383	
-2	388	376	
-1	337	337	
0	509	-524	
1	372	369	
2	84	-101	
3	226	229	
4	184	165	
5	239	231	
6	81	70	
7	111	104	
H,K= 1, -10			
L	FOBS	FCAL	
-8	0	-17	
-7	36	-39	
-6	118	128	
-5	294	286	
-4	238	246	
-3	41	52	
-2	216	-225	
-1	189	185	
0	277	-317	
1	156	140	
2	258	260	
3	101	-97	
4	112	97	
5	191	196	
6	50	63	
7	123	122	
8	107	118	
H,K= 1, -9			
L	FOBS	FCAL	
-7	103	102	
-6	130	131	
-5	0	-13	
-4	102	103	
-3	56	63	
-2	97	101	
-1	80	67	
0	15		
1	42	36	
H,K= 1, -8			
L	FOBS	FCAL	
-8	100	93	
-7	128	125	
-6	99	91	
-5	109	97	
-4	0	8	
-3	42	44	
-2	107	-112	
-1	33	38	
0	119	111	
1	71	77	
2	24	34	
3	0	20	
4	0	27	
5	28	25	
H,K= 1, -7			
L	FOBS	FCAL	
8	102	108	
H,K= 1, 0			
L	FOBS	FCAL	
2	61	39	
3	24	33	
4	68	97	
5	101	95	
6	82	74	
H,K= 1, -6			
L	FOBS	FCAL	
0	191	192	
1	282	264	
2	109	107	
3	85	90	
4	52	58	
-3	266	257	
-2	256	271	
-1	238	238	
0	117	112	
1	79	-58	
2	37	-50	
3	51	75	
4	196	174	
5	285	279	
6	238	228	
H,K= 1, -5			
L	FOBS	FCAL	
0	68	-72	
1	153	-158	
2	0	18	
3	159	170	
4	300	282	
5	172	177	
6	145	152	
7	0	36	
H,K= 1, -4			
L	FOBS	FCAL	
-6	50	-40	
-7	142	-129	
-6	60	-58	
-5	82	81	
-4	82	88	
-3	593	572	
-2	576	553	
-1	329	328	
0	0	19	
1	80	78	
2	106	93	
3	246	241	
4	50	57	
5	87	95	
6	26	20	
7	69	63	
H,K= 1, -3			
L	FOBS	FCAL	
0	847	859	
1	73	61	
2	122	121	
3	73	62	
4	227	199	
5	151	160	
6	126	127	
7	158	149	
H,K= 1, 4			
L	FOBS	FCAL	
2	84	73	
H,K= 1, -2			
L	FOBS	FCAL	
-1	44	-16	
0	188	-181	
1	215	218	
2	195	178	
3	270	264	
4	140	133	
5	0	-5	
6	0	-26	
7	70	69	
H,K= 1, 5			
L	FOBS	FCAL	
-8	0	17	
-7	0	9	
-6	26	35	
-5	0	7	
-4	66	97	
-3	210	216	
-2	55	-43	
-1	183	174	
0	255	233	
1	187	180	
2	356	338	
3	119	122	
4	74	-68	
5	56	-52	
6	27	-8	
7	0	4	
H,K= 1, 6			
L	FOBS	FCAL	
2	61	77	
3	0	2	
4	28	24	
5	0	4	
H,K= 1, -7			
L	FOBS	FCAL	
7	145	145	
H,K= 1, 7			
L	FOBS	FCAL	
3	86	92	
4	115	121	
5	125	125	
6	42	41	
H,K= 2, -8			
L	FOBS	FCAL	
4	126	113	
5	196	206	
6	206	189	
7	90	100	
H,K= 2, -7			
L	FOBS	FCAL	
3	236	233	
4	133	148	
5	195	206	
6	206	189	
7	122	129	
H,K= 2, -6			
L	FOBS	FCAL	
2	281	-299	
3	256	233	
4	133	148	
5	195	206	
6	206	189	
7	90	100	
H,K= 2, -5			
L	FOBS	FCAL	
-9	88	88	
-8	152	139	
-7	97	-102	
-6	121	126	
-5	74	71	
-4	203	218	
-3	204	196	
-2	738	746	
-1	431	418	
0	261	266	
1	244	-234	
2	69	64	
3	292	-288	
4	301	290	
5	289	296	
6	196	207	
7	0	26	
H,K= 2, 2			
L	FOBS	FCAL	
-1	0	-20	
0	290	284	
1	88	87	
2	76	64	
3	213	211	
4	239	223	
5	119	118	
6	84	81	
H,K= 2, 3			
L	FOBS	FCAL	
-5	50	57	
-4	0	28	
-3	26	36	
-2	121	117	
-1	183	168	
0	0	-0	
1	44	22	
2	37	46	
3	86	85	
4	90	100	
5	136	137	
H,K= 2, 4			
L	FOBS	FCAL	
-8	0	-15	
-7	45	29	
-6	148	144	
-5	311	301	
-4	337	344	
-3	378	394	
-2	93	92	
-1	161	-175	
0	241	-232	
1	61	-66	
2	418	409	
3	545	531	
4	423	425	
5	72	71	
6	0	0	
7	29	-30	
H,K= 2, -3			
L	FOBS	FCAL	
0	77	-76	
1	140	146	
2	128	104	
3	205	223	
4	257	245	
5	0	30	
6	0	47	
7	65	75	
H,K= 2, 4			
L	FOBS	FCAL	
-4	0	17	
-3	48	-69	
-2	0	-20	
-1	0	4	
0	107	94	
1	233	221	
2	119	126	
3	42	54	
H,K= 2, 5			
L	FOBS	FCAL	
1	555	546	
2	293	294	
3	243	244	
4	85	92	
5	95	100	
6	0	14	
7	98	86	
H,K= 2, 6			
L	FOBS	FCAL	
2	171	167	
3	57	51	
4	30	-24	
H,K= 2, 7			
L	FOBS	FCAL	
1	78	-52	
2	253	263	
3	32	34	
4	120	121	
5	142	137	
6	123	138	
H,K= 2, 8			
L	FOBS	FCAL	
-6	40	32	
-5	0	2	
-4	0	34	
-3	168	184	
-2	255	265	
-1	169	181	
0	128	141	
1	122	-124	
2	210	202	
3	141	-133	
4	0	35	
5	102	97	
H,K= 2, 9			
L	FOBS	FCAL	
5	49	49	
-4	78	72	
-3	143	132	
-2	210	202	
-1	191	197	
0	0	35	
1	26	9	
2	47	-48	
3	0	11	
4	58	56	
H,K= 2, 10			
L	FOBS	FCAL	
-3	584	599	
-2	1128	1173	
-1	220	197	
0	305	-321	
1	755	-739	
2	31	39	
3	90	96	
4	263	264	
5	264	253	
6	238	222	
7	99	104	
H,K= 2, 11			
L	FOBS	FCAL	
-4	571	595	
-3	544	585	
-2	375	411	
-1	236	236	
0	77	-76	
1	140	140	
2	128	104	
3	205	223	
4	257	245	
5	0	30	
6	0	47	
7	65	75	
H,K= 2, -2			
L	FOBS	FCAL	
-9	51	-50	
-8	82	-83	
-7	44	56	
-6	165	181	
-5	444	438	
-4	354	357	
-3	236	213	
-2	21	20	
-1	927	931	
0	107	106	
1	102	110	
2	40	38	
3	64	-59	
4	58	57	
5	218	205	
6	99	89	
7	107	110	
H,K= 2, -1			
L	FOBS	FCAL	
-9	29	-24	
-8	27	34	
-7	152	162	
-6	72	72	
-5	171	166	
-4	162	169	
-3	322	326	
-2	370	-389	
-1	292	279	
0	238	-247	
1	59	54	
2	211	197	
3	638	628	
4	155	-156	
5	256	240	
6	155	155	
7	145	145	
H,K= 2, 0			
L	FOBS	FCAL	
4	0	-25	
5	0	8	
6	127	131	
H,K= 2, 7			
L	FOBS	FCAL	
-4	0	3	
-3	41	44	
-2	240	257	
-1	185	169	
0	298	287	
1	133	127	
2	64	-65	
3	107	-106	
4	0	-30	
5	49	-41	
H,K= 2, 8			
L	FOBS	FCAL	
0	126	141	
1	138	149	
2	122	-124	
3	168	184	
4	0	35	
5	102	97	
H,K= 2, 9			
L	FOBS	FCAL	
-1	169	181	
0	128	141	
1	0	-19	
2	122	-124	
3	141	-133	
4	0	34	
5	102	97	
H,K= 2, 10			
L	FOBS	FCAL	
-2	202	200	
-1	309	-326	
0	59	-41	
1	229	229	
2	349	358	
3	297	296	
4	323	321	
5	0	-33	
6	57	-53	
H,K= 2, -3			
L	FOBS	FCAL	
-8	61	57	
-7	132	132	
-6	214	232	
-5	145	160	
-4	230	248	
-3	0	24	
-2	280	278	
-1	86	71	
0	343	327	
1	373	340	
2	487	485	
3	308	315	
4	108	109	
5	98	-46	
6	0	-37	
H,K= 2, -2			
L	FOBS	FCAL	
-5	78	65	
-4	0	-0	
-3	48	-59	
-2	0	-20	
-1	0	4	
0	107	94	
1	233	221	
2	119	126	
3	42	54	
H,K= 2, -9			
L	FOBS	FCAL	
0	449	421	
1	159	174	
2	459	453	
3	233	226	
4	0	14	
5	61	85	
6	28	34	
H,K= 2, -8			
L	FOBS	FCAL	
0	186	208	
1	130	122	
2	199	200	
3	171	167	
4	57	51	
5	71	73	
6	30	-24	
H,K= 2, -7			
L	FOBS	FCAL	
-9	0	29	
-8	71	60	
-7	325	319	
-6	344	345	
-5	304	312	
-4	203	197	
-3	146	130	
-2	492	-498	
-1	202	209	
0	190	193	
1	144	150	
2	171	167	
3	370	356	
4	136	130	
5	102	101	
6	110	104	
7	30	49	
H,K= 2, -6			
L	FOBS	FCAL	
-8	0	41	
-7	86	83	
-6	60	63	
-5	25	-28	
-4	0	-7	
-3	42	-71	
-2	194	208	
-1	0	1	
0	178	184	
1	162	164	
2	55	64	
3	0	-11	
4	19	42	
5	39	21	
6	105	96	
H,K= 2, -5			
L	FOBS	FCAL	
-4	125	114	
-3	61	49	
-2	107	118	
-1	121	112	
0	82	98	
1	111	108	
2	0	9	
3	375	380	
4	0	9	
5	280	286	
6	159	-152	
7	0	-8	
8	0	0	
H,K= 2, -4			
L	FOBS	FCAL	
-8	0	0	
-7	6	-8	
-6	248	244	
-5	280	286	
-4	159	-152	
-3	0	-8	
-2	207	-209	
-1	330	332	
0	265	253	
1	228	204	
2	0	-1	
3	60	51	
4	270	286	
5	316	313	
6	146	141	
7	0	7	
H,K= 2, -3			
L	FOBS	FCAL	
3	271	262	
4	228	221	
5	72	74	
6	0	12	
H,K= 2, -2			
L	FOBS	FCAL	
-1	120	133	
0	175	-176	
1	229	-227	
2	126	126	
3	530	526	
4	152	160	
5	155	136	
6	0	30	
H,K= 2, -1			
L	FOBS	FCAL	
0	30	37	
H,K= 2, 0			
L	FOBS	FCAL	
0	0	-4	
1	309	-326	
2	59	-41	
3	68	71	
4	93	93	
5	233	248	
6	0	30	
H,K= 2, 1			
L	FOBS	FCAL	
0	59	-41	
1	229	229	
2	349	358	
3	297	296	
4	323	321	
5	0	-33	
6	57	-53	
H,K= 2, 2			
L	FOBS	FCAL	
0	343	327	
1	373	340	
2	487	485	
3	308	315	
4	108	109	
5	98	-46	
6	0	-37	
H,K= 2, 3			
L	FOBS	FCAL	
-2	280	278	
-1	86	71	
0	343	327	
1	373	340	
2	487	485	
3	308	315	
4	108	109	
5	98	-46	
6	0	-37	
H,K= 2, 4			
L	FOBS	FCAL	
-1	0	-29	
0	320	-323	
1	91	78	
2	322	346	
3	135	139	
4	238	233	
5	225	203	
6	64	58	
H,K= 2, 5			
L	FOBS	FCAL	
-6	0	14	
-5	108	-103	
-4	26	-33	
-3	0	3	
-2	205	214	
-1	210	201	
0	278	268	
1	101	95	
2	0	18	
3	0	-9	
4	30	23	
H,K= 2, -7			
L	FOBS	FCAL	
-7	0	20	
-6	38	-31	
-5	58	-63	
-4	43	44	
-3	165	171	
-2	247	256	
-1	344	358	
0	170	159	
1	175	165	
2	0	-45	
3	77	-66	
4	0	-16	
H,K= 2, -6			
L	FOBS	FCAL	
-1	129	157	
0	358	379	
1	318	316	
2	41	45	
3	76	94	
4	0	12	
5	118	111	
H,K= 2, 7			
L	FOBS	FCAL	
0	0	-14	
1	0	9	
2	89	73	
3	169	173	
4	28	36	
5	59	65	
H,K= 2, -5			
L	FOBS	FCAL	
-1	0	8	
0	248	255	
1	55	64	

H,K= 0, 1
L FOBS FCAL
-8 41 47
-7 108 93
-6 38 -41
-5 58 61
-4 0 16
-3 65 74
-2 95 112
-1 146 152
0 112 117

H,K= 0, 2
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 0, 3
L FOBS FCAL
-8 51 34
-7 0 30
-6 102 90
-5 176 176
-4 161 164
-3 68 76
-2 52 53
-1 110 128
0 103 80
1 127 114
2 145 145

H,K= 0, 4
L FOBS FCAL
-8 42 47
-7 108 93
-6 38 41
-5 58 61
-4 0 16
-3 62 55
-2 51 51
-1 116 111
0 85 83
1 0 28
2 117 92

H,K= 0, 5
L FOBS FCAL
-8 41 47
-7 108 93
-6 38 41
-5 58 61
-4 0 16
-3 62 55
-2 51 51
-1 116 111
0 85 83
1 0 28
2 117 92

H,K= 0, 6
L FOBS FCAL
-8 41 47
-7 108 93
-6 38 41
-5 58 61
-4 0 16
-3 62 55
-2 51 51
-1 116 111
0 85 83
1 0 28
2 117 92

H,K= 0, 7
L FOBS FCAL
-8 41 47
-7 108 93
-6 38 41
-5 58 61
-4 0 16
-3 62 55
-2 51 51
-1 116 111
0 85 83
1 0 28
2 117 92

H,K= 0, 8
L FOBS FCAL
-8 41 47
-7 108 93
-6 38 41
-5 58 61
-4 0 16
-3 62 55
-2 51 51
-1 116 111
0 85 83
1 0 28
2 117 92

H,K= 0, 9
L FOBS FCAL
-8 41 47
-7 108 93
-6 38 41
-5 58 61
-4 0 16
-3 62 55
-2 51 51
-1 116 111
0 85 83
1 0 28
2 117 92

H,K= 0, 10
L FOBS FCAL
-8 41 47
-7 108 93
-6 38 41
-5 58 61
-4 0 16
-3 62 55
-2 51 51
-1 116 111
0 85 83
1 0 28
2 117 92

H,K= 0, 11
L FOBS FCAL
-8 41 47
-7 108 93
-6 38 41
-5 58 61
-4 0 16
-3 62 55
-2 51 51
-1 116 111
0 85 83
1 0 28
2 117 92

H,K= 0, 12
L FOBS FCAL
-8 41 47
-7 108 93
-6 38 41
-5 58 61
-4 0 16
-3 62 55
-2 51 51
-1 116 111
0 85 83
1 0 28
2 117 92

H,K= 0, 13
L FOBS FCAL
-8 41 47
-7 108 93
-6 38 41
-5 58 61
-4 0 16
-3 62 55
-2 51 51
-1 116 111
0 85 83
1 0 28
2 117 92

H,K= 0, 14
L FOBS FCAL
-8 41 47
-7 108 93
-6 38 41
-5 58 61
-4 0 16
-3 62 55
-2 51 51
-1 116 111
0 85 83
1 0 28
2 117 92

H,K= 0, 15
L FOBS FCAL
-8 41 47
-7 108 93
-6 38 41
-5 58 61
-4 0 16
-3 62 55
-2 51 51
-1 116 111
0 85 83
1 0 28
2 117 92

H,K= 0, 16
L FOBS FCAL
-8 41 47
-7 108 93
-6 38 41
-5 58 61
-4 0 16
-3 62 55
-2 51 51
-1 116 111
0 85 83
1 0 28
2 117 92

H,K= 0, 17
L FOBS FCAL
-8 41 47
-7 108 93
-6 38 41
-5 58 61
-4 0 16
-3 62 55
-2 51 51
-1 116 111
0 85 83
1 0 28
2 117 92

H,K= 0, 18
L FOBS FCAL
-8 41 47
-7 108 93
-6 38 41
-5 58 61
-4 0 16
-3 62 55
-2 51 51
-1 116 111
0 85 83
1 0 28
2 117 92

H,K= 1, 0
L FOBS FCAL
-8 41 47
-7 108 93
-6 38 41
-5 58 61
-4 0 16
-3 62 55
-2 51 51
-1 116 111
0 85 83
1 0 28
2 117 92

H,K= 1, 1
L FOBS FCAL
-8 41 47
-7 108 93
-6 38 41
-5 58 61
-4 0 16
-3 62 55
-2 51 51
-1 116 111
0 85 83
1 0 28
2 117 92

H,K= 1, 2
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 1, 3
L FOBS FCAL
-8 51 34
-7 0 30
-6 102 90
-5 176 176
-4 161 164
-3 68 76
-2 52 53
-1 110 128
0 103 80
1 127 114
2 145 145

H,K= 1, 4
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 1, 5
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 1, 6
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 1, 7
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 1, 8
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 1, 9
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 1, 10
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 1, 11
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 1, 12
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 1, 13
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 1, 14
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 1, 15
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 1, 16
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 1, 17
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
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-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 1, 18
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 2, 0
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 2, 1
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 2, 2
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 2, 3
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 2, 4
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 2, 5
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 2, 6
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 2, 7
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 2, 8
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 2, 9
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 2, 10
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 2, 11
L FOBS FCAL
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-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 2, 12
L FOBS FCAL
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-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 2, 13
L FOBS FCAL
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-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 2, 14
L FOBS FCAL
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-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 2, 15
L FOBS FCAL
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-6 60 64
-5 91 88
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-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 2, 16
L FOBS FCAL
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-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 2, 17
L FOBS FCAL
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-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 2, 18
L FOBS FCAL
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-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 3, 0
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 3, 1
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 3, 2
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 3, 3
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 3, 4
L FOBS FCAL
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-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 3, 5
L FOBS FCAL
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-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 3, 6
L FOBS FCAL
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-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 3, 7
L FOBS FCAL
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-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 3, 8
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 3, 9
L FOBS FCAL
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-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 3, 10
L FOBS FCAL
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-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 3, 11
L FOBS FCAL
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-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 3, 12
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 3, 13
L FOBS FCAL
-8 51 36
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-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 3, 14
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 3, 15
L FOBS FCAL
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-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 3, 16
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 3, 17
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 3, 18
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 4, 0
L FOBS FCAL
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-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 4, 1
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 4, 2
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 4, 3
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 4, 4
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 4, 5
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 4, 6
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 4, 7
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 4, 8
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 4, 9
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 4, 10
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 4, 11
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 4, 12
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 4, 13
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 4, 14
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 4, 15
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 4, 16
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 4, 17
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 4, 18
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 5, 0
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 5, 1
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 5, 2
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 5, 3
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 5, 4
L FOBS FCAL
-8 51 36
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-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 5, 5
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 5, 6
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 5, 7
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 5, 8
L FOBS FCAL
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-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 5, 9
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 5, 10
L FOBS FCAL
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-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 6, 0
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 6, 1
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 6, 2
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 6, 3
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 6, 4
L FOBS FCAL
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-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 6, 5
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 6, 6
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 6, 7
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 6, 8
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 6, 9
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 6, 10
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 7, 0
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 7, 1
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 7, 2
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 7, 3
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 7, 4
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 7, 5
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 7, 6
L FOBS FCAL
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-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 7, 7
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 7, 8
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 8, 0
L FOBS FCAL
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-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 8, 1
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 8, 2
L FOBS FCAL
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-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 8, 3
L FOBS FCAL
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-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 8, 4
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-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 8, 5
L FOBS FCAL
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-6 60 64
-5 91 88
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-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 8, 6
L FOBS FCAL
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-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 8, 7
L FOBS FCAL
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-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 8, 8
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 9, 0
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 9, 1
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 9, 2
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 9, 3
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 9, 4
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 9, 5
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 9, 6
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 9, 7
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 9, 8
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 10, 0
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 10, 1
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

H,K= 10, 2
L FOBS FCAL
-8 51 36
-7 56 54
-6 60 64
-5 91 88
-4 99 99
-3 142 149
-2 85 99
-1 101 107
0 54 48

TABLE V

A COMPARISON OF INTERATOMIC DISTANCES AND ANGLES IN THE TWO IONS $Co(MNT)_2^{2-}$ AND $Ni(MNT)_2^{2-}$

		$Co(MNT)_2^{2-}$		$Ni(MNT)_2^{2-}$	
	Atoms	Distance	e.s.d.	Distance	e.s.d.
Ni or Co	-S(1)	2.159	0.003	2.16	0.008 Å
	-S(2)	2.163	0.003	2.16	0.008
	S(1)-C(1)	1.715	0.007	1.75	a
	S(2)-C(2)	1.731	0.007	1.75	a
	C(1)-C(3)	1.40	0.010	1.44	a
	C(2)-C(4)	1.40	0.010	1.42	a
	C(1)-C(2)	1.34	0.010	1.30	0.02
	C(3)-N(1)	1.15	0.010	1.13	0.02
	C(4)-N(2)	1.16	0.010	1.13	0.02

Atoms	Angles	e.s.d.	Angles[b]
S(1)-Co/Ni-S(2)	91.4°	0.1°	91.7°
Co/Ni-S(1)-C(1)	103.8	0.3	103
S(1)-C(1)-C(2)	121.1	0.5	123
C(1)-C(2)-S(2)	120.0	0.6	120
Co/Ni-S(2)-C(2)	103.7	0.3	103
S(2)-C(2)-C(4)	117.2	0.6	-
S(1)-C(1)-C(3)	118.1	0.5	-
C(2)-C(1)-C(3)	120.8	0.7	120
C(1)-C(3)-N(1)	178.2	0.8	179 ~~181~~
C(1)-C(2)-C(4)	122.8	0.7	124
C(2)-C(4)-N(2)	178.7	1.0	177 ~~183~~

[a] Intermediate between ± 0.008 and ± 0.02 [b] e.s.d. all approximately ± 1.0°

TABLE VI

DISTANCES OF THE VARIOUS ATOMS IN THE $Co(MNT)_2^{2-}$ ION FROM THE PLANE THROUGH ATOMS Co, C(1) AND C(2)

Atom	Distance from plane	e.s.d. of the atomic position	e.s.d. of the plane at a particular atom
Co	0	0	0
S(1)	+0.049 Å	0.002 Å	0.004 Å
S(2)	+0.004	0.002	0.004
C(1)	0	0.007	0.007
C(2)	0	0.007	0.007
C(3)	-0.035	0.008	0.010
C(4)	-0.031	0.009	0.010
N(1)	-0.062	0.007	0.012
N(2)	-0.058	0.009	0.012

TABLE VII

THE DIHEDRAL ANGLES FOR THE FOUR BUTYL CHAINS IN THE TETRA n-BUTYL-AMMONIUM ION

Plane (1) Defined by atoms	Plane (2) Defined by atoms	Dihedral angle
C(5) C(6) C(7)	C(6) C(7) C(8)	6.5°
C(9) C(10) C(11)	C(10) C(11) C(12)	1.6
C(13) C(14) C(15)	C(14) C(15) C(16)	1.3
C(17) C(18) C(19)	C(18) C(19) C(20)	71.6

TABLE VIII

DISTANCES AND ANGLES INVOLVING THE CARBON AND NITROGEN ATOMS IN THE TETRA n-BUTYL AMMONIUM GROUP

A) C-N Distances and Angles

Atoms	Distance[a]	Atoms	Angles[b]
N(3)-C(5)	1.53 Å	C(5) -N(3)-C(9)	106.3°
-C(9)	1.52	-C(13)	111.7
-C(13)	1.51	-C(17)	109.4
-C(17)	1.53	C(9) -N(3)-C(13)	112.9
		-C(17)	110.3
		C(13)-N(3)-C(17)	106.3
Mean C-N distance -	1.52 Å	Mean C-N-C angle -	109.5°

[a] estimated standard deviations all ± 0.01 Å

[b] estimated standard deviations all ± 0.5°

TABLE VIII (Contd.)

B) C-N Distances and Angles

Atoms	Distance[d]	Distance[c]	Atoms	Angles	e.s.d.
C(5) -C(6)	1.49 Å	1.49 Å	N(3) -C(5) -C(6)	115.6°	0.5°
C(6) -C(7)	1.53	1.54	C(5) -C(6) -C(7)	108.9	0.6
C(7) -C(8)	1.53	1.56	C(6) -C(7) -C(8)	112.5	0.7
C(9) -C(10)	1.53	1.54	N(3) -C(9) -C(10)	114.0	0.6
C(10)-C(11)	1.51	1.52	C(9) -C(10)-C(11)	109.5	0.7
C(11)-C(12)	1.54	1.54	C(10)-C(11)-C(12)	114.3	0.8
C(13)-C(14)	1.48	1.49	N(3) -C(13)-C(14)	115.7	0.6
C(14)-C(15)	1.52	1.53	C(13)-C(14)-C(15)	112.4	0.6
C(15)-C(16)	1.48	1.49	C(14)-C(15)-C(16)	114.2	0.7
C(17)-C(18)	1.52	1.53	N(3) -C(17)-C(18)	115.3	0.6
C(18)-C(19)	1.54	1.54	C(17)-C(18)-C(19)	111.4	0.7
C(19)-C(20)	1.51	1.53	C(18)-C(19)-C(20)	113.3	0.8
Mean C-C distance -	1.515	1.525	Mean angle -	113.1	

[c]Corrected for thermal vibration assuming that atom C(n+1) "rides" on atom C(n)

[d]estimated standard deviations all ± 0.01 Å

TABLE IX

CARBON-HYDROGEN DISTANCES IN THE TETRA n-BUTYL AMMONIUM GROUP

Atoms	Distances[a]	Atoms	Distances[a]
C(5) -H(1)C(5)	1.04 Å	C(13)-H(1)C(13)	1.08 Å
-H(2)	1.02	-H(2)	0.83
C(6) -H(1)C(6)	0.99	C(14)-H(1)C(14)	0.88
-H(2)	0.96	-H(2)	0.96
C(7) -H(1)C(7)	1.04	C(15)-H(1)C(15)	0.97
-H(2)	0.91	-H(2)	0.94
C(8) -H(1)C(8)	1.10	C(16)-H(1)C(16)	0.97
-H(2)	0.77	-H(2)	0.89
-H(3)	0.96	-H(3)	0.97
C(9) -H(1)C(9)	1.11	C(17)-H(1)C(17)	0.96
-H(2)	0.93	-H(2)	1.05
C(10)-H(1)C(10)	0.86	C(18)-H(1)C(18)	1.09
-H(2)	1.04	-H(2)	0.95
C(11)-H(1)C(11)	1.10	C(19)-H(1)C(19)	1.14
-H(2)	0.88	-H(2)	1.00
C(12)-H(1)C(12)	0.83	C(20)-H(1)C(20)	0.94
-H(2)	0.94	-H(2)	0.89
-H(3)	1.06	-H(3)	1.13

Mean carbon-hydrogen distance - 0.98 Å

[a]estimated standard deviations of all distances ± 0.1 Å

Figure Captions

Fig. 1.—Projection of the structure of $((\underline{n}\text{-}C_4H_9)_4N)_2^+ Co(S_2C_4N_2)_2^{2-}$ down the b axis. The small black circles represent examples of each type of hydrogen atom.

Fig. 2.—Dimensions of the $Co(MNT)_2^{2-}$ ion. See Table V for the estimated standard deviations.

$((C_4H_9)_4N)_2\ Co(S_2C_4N_2)_2$

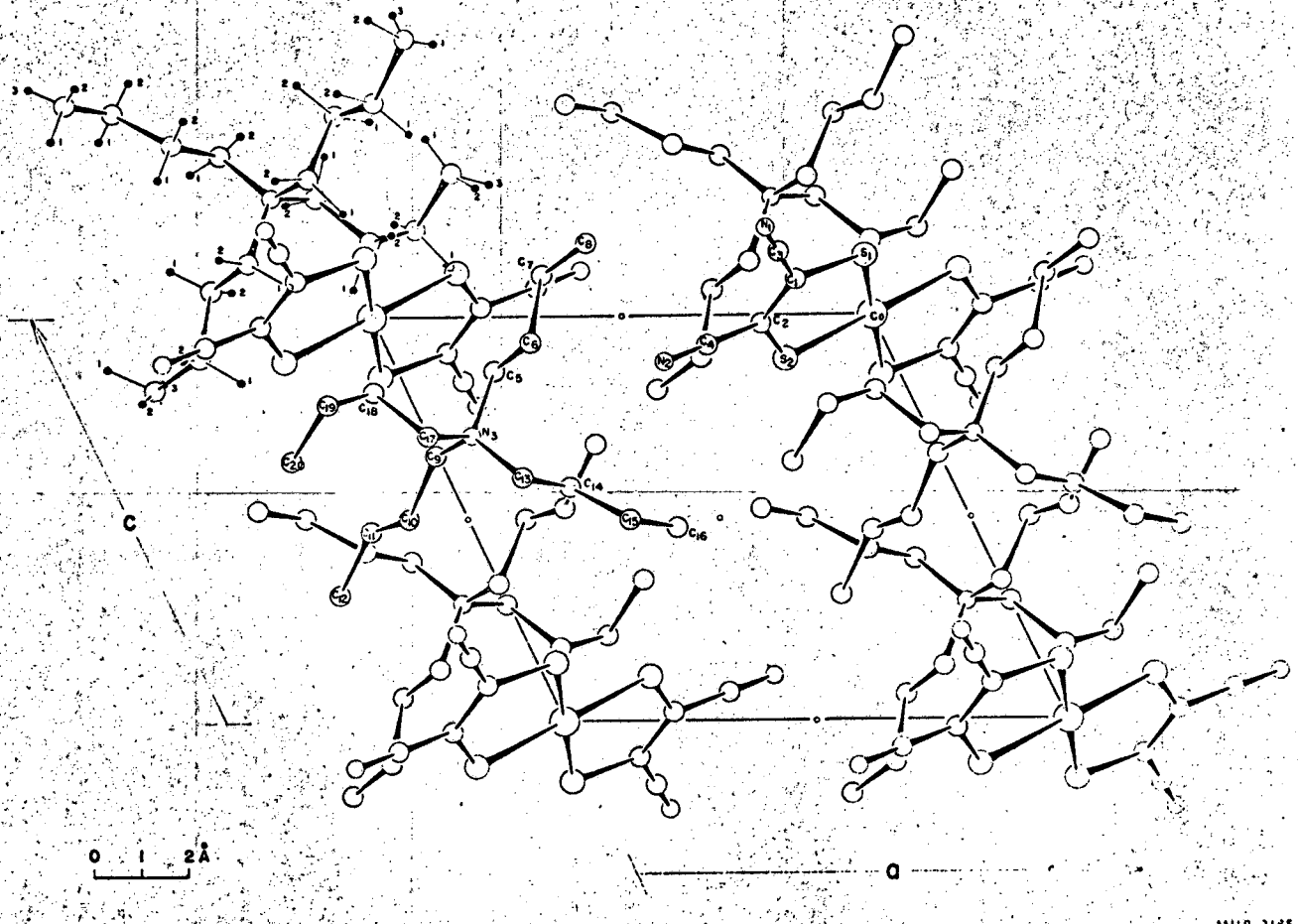

Fig. 1

$((C_4H_9)_4N)_2\ Co(S_2C_4N_2)_2$

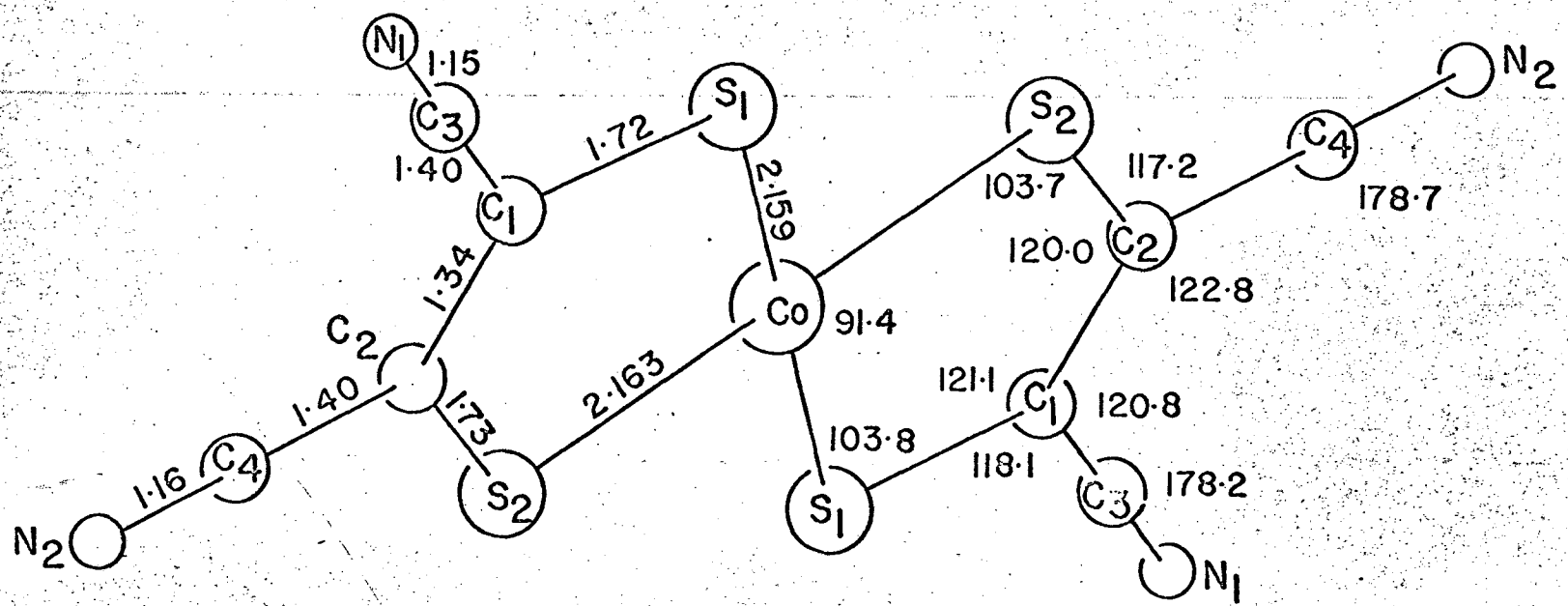

Fig. 2

MU-32324