# Crystal Structure of Nitratotetrakis(2-methylimidazole)cobalt(II) Nitrate –0·5 Ethanol

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The crystal structure of the title compound has been determined from three-dimensional $X$-ray data by Patterson and Fourier methods and refined by least-squares techniques to $R$ 0·108 for 1434 visually estimated independent reflections. The crystals are triclinic, with unit-cell dimensions $a = 8{\cdot}56(2)$, $b = 9{\cdot}35(2)$, $c = 16{\cdot}00(4)$ Å, $\alpha = 102{\cdot}75(10)$, $\beta = 108{\cdot}0(1)$, $\gamma = 91{\cdot}6(1)°$, space group is $P\bar{1}$ and $Z = 2$.

The structure contains $[\mathrm{Co}\ (2\text{-meim})_4(\mathrm{NO_3})]^+$ (2-meim = 2-methylimidazole) ions and free nitrate ions. In the complex cation one bidentate nitrate group and four 2-meim form a very distorted octahedral co-ordination about the cobalt atom. Co–O Distances are 2·115 and 2·269 Å, and Co–N in the range 1·960—2·253 Å. There is some disordered ethanol in the crystal lattice.

OXY-ANIONS such as nitrate or nitrite have provided an extensive range of metal complexes with unusual co-ordination geometries. As is evident from $X$-ray results for nitrato-complexes,[1] the inter-relationship between the mode of co-ordination of anions of this type and the stereochemical arrangement about the metal ion is intriguing, and is not yet clearly understood.

Reactions between cobalt nitrate and 2-methylimidazole (2-meim) in ethanol gave [2] two isomers of stoicheiometry $\mathrm{Co(C_4H_6N_2)_4(NO_3)_2}$. The magnetic and electronic spectral properties of the pink isomer (form $A$) suggested that it probably contained a *trans*-$\mathrm{CoN_4O_2}$ chromophore involving unidentate nitrate groups. The purple isomer (form $B$) had an electronic spectrum closely resembling that of tetrahedral $[\mathrm{Co(2\text{-}meim)_4}]\mathrm{I_2}$,[2] but, in contrast to the low magnetic moment of the iodide (4·28 B.M.) the moment of form $B$ of the nitrate was 4·99 B.M.

As Lewis and co-workers had shown [3] that some five-co-ordinate cobalt(II) complexes have electronic spectra closely fitting a tetrahedral model and yet had high magnetic moments, it was tentatively suggested [2] that form $B$ of $\mathrm{Co(2\text{-}mein)_4(NO_3)_2}$ might be five-co-ordinate, with only one anion co-ordinated. This conclusion was reinforced by the knowledge that $\mathrm{Ni(2\text{-}meim)_4Br_2}$ contains five-co-ordinate nickel.[4] An $X$-ray study has now shown that, although one anion is indeed not co-ordinated, the other is present as a chelate thus providing a very distorted six-co-ordinate geometry.

## EXPERIMENTAL

Form $B$ of nitratotetrakis(2-methylimidazole)cobalt(II) nitrate was obtained, by the addition of dichloromethane to an ethanolic solution, as purple plates containing some solvated ethanol.

*Crystal Data.*—$\mathrm{C_{16}H_{24}CoN_{10}O_6,\frac{1}{2}\text{-}C_2H_5OH}$, $M = 534{\cdot}4$, Triclinic, $a = 8{\cdot}56(2)$, $b = 9{\cdot}35(2)$, $c = 16{\cdot}00(4)$ Å, $\alpha = 102{\cdot}75(10)$, $\beta = 108{\cdot}0(1)$, $\gamma = 91{\cdot}6(1)°$, $U = 1181$ Å$^3$, $D_m$ (by flotation) $= 1{\cdot}50$, $Z = 2$, $D_c = 1{\cdot}50$, $F(000) = 556$. Space group $P\bar{1}$. Cu-$K_\alpha$ radiation, $\lambda = 1{\cdot}5418$ Å; $\mu(\text{Cu-}K_\alpha) = 57{\cdot}9\ \mathrm{cm^{-1}}$.

The unit-cell dimensions were determined from high-angle reflections on Weissenberg photographs. Although this is a reduced cell it is also the morphological unit cell with $a$ and $b$ parallel to the edges of the crystal plate.

Intensity data were collected from a crystal of dimensions *ca.* $0{\cdot}26 \times 0{\cdot}14 \times 0{\cdot}04\ \mathrm{mm^3}$, by use of Cu-$K_\alpha$ radiation and a Nonius Weissenberg camera. Equi-inclination photographs were taken to record layers 0—5$kl$ (2—3 days exposure for each photograph). Intensities were estimated visually from multiple-film exposures for a total of 1434 independent reflections. The Lorentz and polarisation corrections were applied.

*Solution and Refinement of the Structure.*—The solution and refinement of the structure were performed using the Crystal Structure Calculations 'System $X$-Ray '63' [5] on the Imperial College IBM 7094 computer, and also the least-squares program NUCLS [6] on the University of London CDC 6600 computer.

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[1] C. C. Addison, N. Logan, S. C. Wallwork, and C. D. Garner, *Quart. Rev.*, 1971, **25**, 289.

[2] D. M. L. Goodgame, M. Goodgame, and G. W. Rayner Canham, *Inorg. Chim. Acta*, 1969, **3**, 399.

[3] F. Lions, I. C. Dance, and J. Lewis, *J. Chem. Soc.* (*A*), 1967, 565.

[4] F. Akhtar, Ph.D. Thesis, University of London, 1969.

[5] '$X$-Ray '63' system of programs, J. M. Stewart, University of Maryland Report, TR 64 6.

[6] This full-matrix least-squares program is a revised and rewritten version of the Doedens–Ibers NUGLS, and is basically a highly modified version of the Martin–Busing–Levy ORFLS. It has been adapted for use on the University of London CDC 6600 computer by F. A. Stephens and D. Bright.

A three-dimensional Patterson synthesis revealed the position of the cobalt atom, and three cycles of least-squares refinement gave $R$ 0·45. Successive difference Fouriers showed the positions of the 32 expected non-hydrogen atoms, and refinement with isotropic temperature factors reduced $R$ to 0·150.

The data were now corrected for absorption according to the method of Busing and Levy[7] using an $8 \times 8 \times 8$ grid, with crystal path-lengths determined by the vector analysis procedure of Coppens *et al.*[8] This resulted in a relatively modest drop in $R$ to 0·146. A difference Fourier calculated at this stage showed four peaks of height *ca.* 2e Å$^{-3}$ astride a centre of symmetry, and forming an almost continuous band of electron density. The shape of this was consistent with ethanol solvent molecules trapped in the lattice and disordered in two orientations. To allow approximately for this, two atoms, one carbon and one oxygen, were introduced into the refinement at half occupancy, to give $R$ 0·124. Isotropic refinement was used to fix the interlayer scale factors and the cobalt atom was refined anisotropically ($R$ 0·118). All the 24 hydrogen atoms were now located from a difference Fourier and were included as a 'fixed contribution' with isotropic temperature factors of their parent atoms ($R$ 0·116).

TABLE 1

Fractional co-ordinates with estimated standard deviations in parentheses. The atoms of the 2-meim ligands are numbered (*mn*) where *m* is ligand number, and *n* is the atom number within each ligand

| | *x* | *y* | *z* |
|---|---|---|---|
| Co | 0·3942(4) | 0·3696(3) | 0·2081(2) |
| N(21) | 0·2324(24) | 0·3490(19) | 0·0443(12) |
| O(21) | 0·1972(18) | 0·2745(14) | 0·0884(9) |
| O(22) | 0·3500(20) | 0·4429(16) | 0·0773(9) |
| O(23) | 0·1685(26) | 0·3345(21) | −0·0372(14) |
| N(31) | 0·5460(21) | 0·2104(15) | 0·1480(10) |
| C(32) | 0·6484(27) | 0·2219(20) | 0·1056(12) |
| N(33) | 0·7216(23) | 0·0934(19) | 0·0773(11) |
| C(34) | 0·6422(30) | −0·0090(24) | 0·0993(14) |
| C(35) | 0·5300(28) | 0·0609(22) | 0·1406(13) |
| C(36) | 0·7167(31) | 0·3636(24) | 0·0907(15) |
| N(41) | 0·2404(20) | 0·5363(16) | 0·2529(9) |
| C(42) | 0·2405(26) | 0·6083(20) | 0·3379(12) |
| N(43) | 0·1428(22) | 0·7157(17) | 0·3419(10) |
| C(44) | 0·0673(29) | 0·7102(23) | 0·2531(14) |
| C(45) | 0·1210(28) | 0·5998(22) | 0·2009(13) |
| C(46) | 0·3469(27) | 0·5839(22) | 0·4263(13) |
| N(51) | 0·5921(19) | 0·5020(14) | 0·2852(9) |
| C(52) | 0·6240(28) | 0·6477(21) | 0·2974(13) |
| N(53) | 0·7507(25) | 0·6935(20) | 0·3667(12) |
| C(54) | 0·8064(28) | 0·5800(23) | 0·3984(13) |
| C(55) | 0·7138(27) | 0·4619(21) | 0·3491(13) |
| C(56) | 0·5301(33) | 0·7403(26) | 0·2406(16) |
| N(61) | 0·3415(20) | 0·2411(14) | 0·2906(9) |
| C(62) | 0·2081(28) | 0·2081(20) | 0·3042(12) |
| N(63) | 0·2208(23) | 0·1307(17) | 0·3659(10) |
| C(64) | 0·3784(30) | 0·1077(21) | 0·3923(13) |
| C(65) | 0·4511(23) | 0·1723(17) | 0·3467(11) |
| C(66) | 0·0455(34) | 0·2514(26) | 0·2607(16) |
| N(11) | 0·8637(19) | 0·0648(15) | 0·4347(9) |
| O(11) | 0·7729(19) | 0·0271(15) | 0·4740(9) |
| O(12) | 0·9226(19) | 0·1931(15) | 0·4621(9) |
| O(13) | 0·9055(17) | −0·0171(14) | 0·3697(8) |
| O(71) * | 0·055(6) | 0·931(5) | 0·021(3) |
| C(72) * | 0·118(6) | 0·904(5) | 0·087(3) |

* These atoms have an occupancy factor of 0·5, and their identity is not absolutely certain.

A correction for the anomalous dispersion of cobalt was now applied using the program NUCLS. Refinement as before reduced $R$ to 0·108; further refinement was shown to be unjustified. In the final stage the Hughes weighting scheme[9] was applied, where $w = 1$ for $F < F^*$, and $\sqrt{w} = F^*/\mathrm{F}$ for $F \geqslant F^*$, with $F^* = 50$ found to be optimum. The application of the weighting scheme did not reduce $R$, but appreciably lower standard deviations resulted. The scattering factors used were taken from ref. 10 and the corrections for the real and imaginary parts of the anomalous dispersion correction for cobalt were taken from ref. 11.

Table 1 lists the final co-ordinates of the non-hydrogen atoms and Table 2 the coefficients for the anisotropic temperature factor $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + 2\beta_{12}hk + 2\beta_{13}hl + 2\beta_{23}kl)]$ of cobalt and the isotropic temperature factors of the other atoms. The co-ordinates of the hydrogen atoms are given in Table 3 and the observed and

TABLE 2

Thermal parameters, anisotropic for the cobalt atom and isotropic for all other atoms

| | $10^4\beta_{11}$ | $10^4\beta_{22}$ | $10^5\beta_{33}$ | $10^4\beta_{12}$ | $10^4\beta_{13}$ | $10^4\beta_{23}$ |
|---|---|---|---|---|---|---|
| Co | 48(6) | 75(4) | 309(14) | −7(3) | −8(2) | 24(2) |

| | $B$/Å$^2$ | | $B$/Å$^2$ | | $B$/Å$^2$ |
|---|---|---|---|---|---|
| N(21) | 5·3(0·4) | N(43) | 4·5(0·4) | N(63) | 4·4(0·4) |
| O(21) | 5·0(0·3) | C(44) | 5·1(0·5) | C(64) | 4·5(0·5) |
| O(22) | 5·7(0·3) | C(45) | 4·5(0·5) | C(65) | 2·6(0·4) |
| O(23) | 10·1(0·5) | C(46) | 4·8(0·5) | C(66) | 6·7(0·6) |
| N(31) | 3·8(0·3) | N(51) | 3·0(0·3) | | |
| C(32) | 3·9(0·4) | C(52) | 4·3(0·4) | N(11) | 3·0(0·3) |
| N(33) | 5·4(0·4) | N(53) | 5·9(0·4) | O(11) | 5·6(0·3) |
| C(34) | 5·6(0·5) | C(54) | 4·8(0·5) | O(12) | 5·4(0·3) |
| C(35) | 4·8(0·5) | C(55) | 4·3(0·4) | O(13) | 4·6(0·3) |
| C(36) | 6·2(0·6) | C(56) | 6·6(0·6) | | |
| N(41) | 3·6(0·3) | N(61) | 3·0(0·3) | O(71) | 7·9(1·1) |
| C(42) | 3·5(0·4) | C(62) | 3·8(0·4) | C(72) | 9·1(1·2) |

TABLE 3

Fractional co-ordinates of the hydrogen atoms, labelled such that the first two digits are those of the carbon or the nitrogen atom to which they are attached

| | *x* | *y* | *z* |
|---|---|---|---|
| H(33) | 0·798 | 0·071 | 0·034 |
| H(34) | 0·625 | −0·109 | 0·078 |
| H(35) | 0·445 | 0·036 | 0·183 |
| H(361) | 0·741 | 0·363 | 0·022 |
| H(362) | 0·598 | 0·422 | 0·085 |
| H(363) | 0·729 | 0·246 | 0·100 |
| H(43) | 0·124 | 0·785 | 0·398 |
| H(44) | −0·037 | 0·775 | 0·238 |
| H(45) | 0·096 | 0·568 | 0·139 |
| H(461) | 0·252 | 0·528 | 0·435 |
| H(462) | 0·315 | 0·663 | 0·417 |
| H(463) | 0·420 | 0·502 | 0·413 |
| H(53) | 0·810 | 0·776 | 0·383 |
| H(54) | 0·895 | 0·590 | 0·452 |
| H(55) | 0·744 | 0·361 | 0·360 |
| H(561) | 0·512 | 0·683 | 0·183 |
| H(562) | 0·495 | 0·755 | 0·307 |
| H(563) | 0·625 | 0·811 | 0·258 |
| H(63) | 0·150 | 0·122 | 0·399 |
| H(64) | 0·441 | 0·036 | 0·420 |
| H(65) | 0·558 | 0·185 | 0·338 |
| H(661) | 0·095 | 0·296 | 0·225 |
| H(662) | −0·061 | 0·173 | 0·275 |
| H(663) | −0·008 | 0·342 | 0·303 |

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[7] W. R. Busing and H. A. Levy, *Acta Cryst.*, 1957, **10**, 180.

[8] P. Coppens, L. Leiserowitz, and D. Rabinovich, *Acta Cryst.*, 1965, **18**, 1035.

[9] E. W. Hughes, *J. Amer. Chem. Soc.*, 1941, **63**, 1737.

[10] D. T. Cromer and J. T. Waber, *Acta Cryst.*, 1965, **18**, 104.

[11] D. T. Cromer, *Acta Cryst.*, 1965, **18**, 17.

calculated structure amplitudes are listed in Supplementary Publication No. SUP 20350 (5 pp., 1 microfiche).[*]

The possibility that the true space group is $P1$ and that the ethanol is ordered was tested. Refinement gave only a marginal drop in $R$ to 0·107 and much worse standard deviations. The possibility was therefore rejected.

## DESCRIPTION OF THE STRUCTURE AND DISCUSSION

The structure contains complex cations $[Co(2\text{-meim})_4NO_3]^+$ and free nitrate ions; there is also some disordered ethanol in the lattice. The complex cation has been shown to contain a bidentate nitrate group, and the very distorted octahedral co-ordination is completed by four donor nitrogen atoms from the 2-meim ligands. The shape of the cation is shown in Figure 1, and the more important bond lengths and angles are given in Table 4. The two Co–O distances are 2·115 and 2·269 Å, and this difference seems to be significant: thus the nitrate group is to a slight extent asymmetrically bidentate. This seemed unusual since when asymmetry is present it is generally much more marked (see Table 10 in ref. 1). In a recent preliminary note,[12] however, the structure of methyltin trinitrate is described. There, all three ligand nitrate groups show a very similar degree of asymmetry in bonding, *ca.* 0·15 Å, to that observed in the cobalt complex. The four Co–N distances range from 1·960 to 2·253 Å. This represents a spread from ' rather short ' to ' rather long ' for this type of bond, although it is hard to rationalise why one particular distance, to N(51), is appreciably shorter than the others.

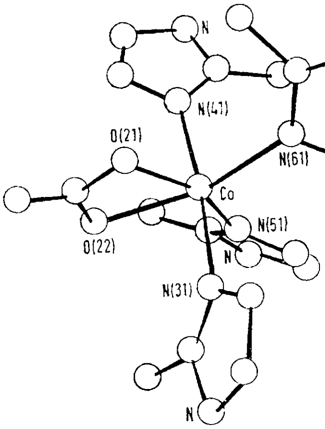

FIGURE 1 The $[Co(2\text{-meim})_4NO_3]^+$ ion

Although the cobalt atom is six-co-ordinate the co-ordination geometry is severely distorted from an octahedron. Indeed, as far as the donor nitrogen atoms of the imidazole rings are concerned the co-ordination geometry is slightly closer to a trigonal bipyramid than to an octahedron. Various workers have suggested [13-17] that in some cases a bidentate group may be considered as occupying one co-ordination site about a metal ion. Although such a concept has its limitations, the assumption of a pseudo-trigonal bipyramidal geometry for $[Co(2\text{-meim})_4NO_3]^+$ correlates well with the observed spectral and magnetic properties.

TABLE 4

Bond lengths (Å) and angles (°) with standard deviations in parentheses

| | | | |
|---|---|---|---|
| (*a*) Distances | | | |
| Co–O(21) | 2·115(12) | Co–O(22) | 2·269(16) |
| Co–N(31) | 2·253(17) | Co–N(41) | 2·209(17) |
| Co–N(51) | 1·960(13) | Co–N(61) | 2·105(17) |
| N(11)–O(11) | 1·23(3) | N(21)–O(21) | 1·21(2) |
| N(11)–O(12) | 1·22(2) | N(21)–O(22) | 1·19(2) |
| N(11)–O(13) | 1·30(2) | N(21)–O(23) | 1·23(3) |
| Mean N(*m*1)–C(*m*2) | 1·32(3) | Mean C(*m*4)–C(*m*5) | 1·35(3) |
| Mean C(*m*2)–N(*m*3) | 1·34(3) | Mean C(*m*5)–N(*m*1) | 1·36(2) |
| Mean N(*m*3)–C(*m*4) | 1·33(3) | Mean C(*m*2)–C(*m*6) | 1·49(3) |
| (*b*) Angles | | | |
| O(21)–Co–O(22) | 56·8(6) | N(51)–Co–N(61) | 105·5(6) |
| O(21)–Co–N(61) | 97·7(6) | O(22)–Co–N(51) | 99·9(6) |
| N(31)–Co–O(21) | 85·3(5) | N(31)–Co–O(22) | 82·7(6) |
| N(31)–Co–N(51) | 91·7(6) | N(31)–Co–N(61) | 96·4(6) |
| N(41)–Co–O(21) | 91·3(5) | N(41)–Co–O(22) | 90·5(6) |
| N(41)–Co–N(51) | 89·2(6) | N(41)–Co–N(61) | 89·8(6) |
| O(21)–Co–N(51) | 156·8(7) | O(22)–Co–N(61) | 154·5(5) |
| N(31)–Co–N(41) | 173·3(6) | | |
| O(11)–N(11)–O(12) | 115·0(1·5) | O(21)–N(21)–O(22) | 121·7(1·7) |
| O(11)–N(11)–O(13) | 127·4(1·4) | O(21)–N(21)–O(23) | 123·8(1·8) |
| O(12)–N(11)–O(13) | 117·5(1·7) | O(22)–N(21)–O(23) | 114·5(2·2) |

If N(21) is taken to be the effective centre of the ligand nitrate group, and geometrical calculations are carried out on the basis of this concept, it is found that Co, N(21), N(51), and N(61) form a very good plane (maximum deviation *ca.* 0·012 Å) and the remaining two donor nitrogen atoms are *ca.* 2·22 Å above and below this plane. The angles within the plane are: N(51)–Co–N(61) 105·5(6)°, N(51)–Co–N(21) 128·2(7)°, and N(21)–Co–N(61) 126·3(6)°; the axial Co–N bonds are longer than the equatorial ones.[†]

Both nitrate groups are planar and as is often found show slight deviations from perfect $\bar{6}2m$ symmetry. The accuracy of the bond lengths and angles, however, is such that it is doubtful whether these small differences could be profitably discussed. Table 4 also contains mean values for the various C–N and C–C bonds in the 2-meim ligands. These distances seem reasonable, but here again the accuracy is not sufficient for a detailed discussion of the bonding.

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[*] For details of Supplementary Publications see Notice to Authors No. 7 in *J. Chem. Soc.* (*A*), 1970, Issue No. 20 (items less than 10 pp. are supplied as full size copies).

[†] *Note added in proof:* A recent preliminary communication, W. Harrison, N. L. Paddock, J. Trotter, and J. N. Wingfield, *J.C.S. Chem. Comm.*, 1972, 23, shows that in the distorted trigonal-bipyramidal cation $[N_6P_6(NMe_2)_{12}CoCl]^+$ a similar effect is observed, with the axial Co–N bonds longer than the equatorial ones by *ca.* 0·19 Å.

[12] G. S. Brownlee, A. Walker, S. C. Nyburg, and J. T. Szymanski, *Chem. Comm.*, 1971, 1073.

[13] F. A. Cotton, D. M. L. Goodgame, and R. H. Soderberg, *Inorg. Chem.*, 1963, **2**, 1162.

[14] J. G. Bergman and F. A. Cotton, *Inorg. Chem.*, 1966, **5**, 1208.

[15] C. D. Garner and S. C. Wallwork, *J. Chem. Soc.* (*A*), 1966, 1496.

[16] J. C. Taylor, M. H. Mueller, and R. L. Hitterman, *Acta Cryst.*, 1966, **20**, 842.

[17] D. Britton and J. D. Dunitz, *Acta Cryst.*, 1965, **19**, 815.

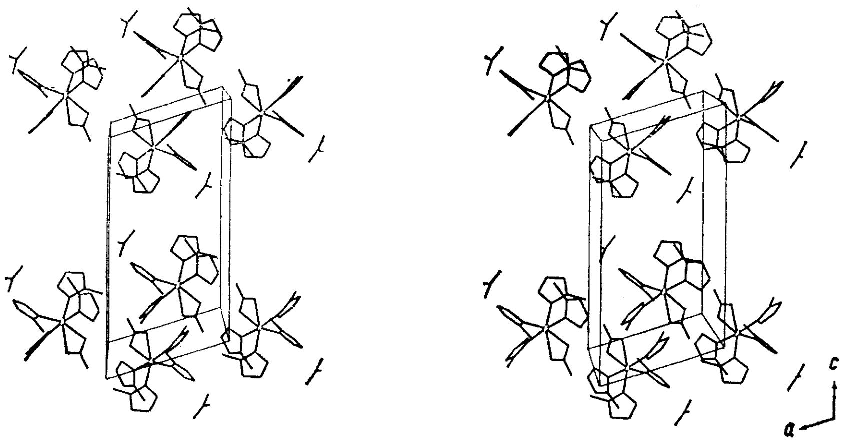

FIGURE 2 A stereoscopic view showing the packing of $[Co(2\text{-meim})_4NO_3]^+$ and $NO_3^-$ ions

A stereoscopic view[18] of the structure is shown in Figure 2 and Table 5 lists the shortest 'intermolecular' distances. These show first that all oxygen atoms of the free nitrate group are at short distances from the non-donor nitrogen atoms of 2-meim ligands, and secondly, although the position of the disordered ethanol is not well defined, it does seem likely that its hydroxy-group takes part in hydrogen bonding.

TABLE 5

Some short non-bonded distances

| | | | |
|---|---|---|---|
| $O(11) \cdots O(13^{I})$ | 3·115 | $O(12) \cdots N(53^{IV})$ | 3·205 |
| $O(11) \cdots N(43^{II})$ | 3·232 | $O(12) \cdots C(54^{IV})$ | 3·050 |
| $O(11) \cdots N(63^{III})$ | 3·214 | $O(12) \cdots N(43^{II})$ | 3·287 |
| $O(13) \cdots N(63^{V})$ | 3·021 | $O(23) \cdots C(45^{VII})$ | 3·188 |
| $O(13) \cdots N(53^{VI})$ | 2·964 | $N(11) \cdots N(11^{VIII})$ | 3·089 |
| $O(71) \cdots O(21^{VII})$ | 2·715 | $N(33) \cdots O(71^{IX})$ | 2·818 |

Roman numerals as superscripts refer to atoms in the following positions, relative to the reference molecule at $x, y, z$:

I $2 - x, -y, 1 - z$
II $1 - x, 1 - y, 1 - z$
III $1 - x, -y, 1 - z$
IV $2 - x, 1 - y, 1 - z$
V $1 + x, y, z$
VI $x, y - 1, z$
VII $-x, 1 - y, -z$
VIII $2 - x, -y, 1 - z$
IX $1 - x, 1 - y, -z$

Least-squares calculations have shown that the 2-meim ligands and the nitrate groups are satisfactorily planar (Table 6), although the cobalt atom in some cases deviates quite significantly from the planes of the ligands. This is particularly striking in the case of 2-meim ligand (5*n*) where the deviation of the cobalt atom from the least-squares plane (metal atom not included in calculation) is almost 0·4 Å.

TABLE 6

Planarity of the 2-meim ligands and of the nitrate groups, distances in Å

| Planar group | Mean devn. | Maximum devn. | Distance Co to plane |
|---|---|---|---|
| Free nitrate (1*n*) | 0·004 | 0·008 | |
| Bonded nitrate (2*n*) | 0·002 | 0·003 | 0·159(17) |
| Ring (3*n*) | 0·020 | 0·037 | 0·011(26) |
| Ring (4*n*) | 0·017 | 0·031 | 0·232(21) |
| Ring (5*n*) | 0·019 | 0·028 | 0·385(22) |
| Ring (6*n*) | 0·009 | 0·016 | 0·115(11) |

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[1/2147 *Received*, 15*th November*, 1971]

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[18] C. K. Johnson, ORTEP thermal ellipsoid plotting program, Oak Ridge National Laboratory Report, 1965, ORNL 3794.