The Crystal Structure of 1,6-Dinitrobis(ethylenediamine)-cobalt(III) Nitrate

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A preliminary report on the investigation of the crystal structure of 1,6[Co $(NO_2)_2$ $(en)_2]NO_3$ is given in this note.

$1,6[Co(NO_3)_2(en)_2]NO_3$ was prepared by oxidation of a solution of cobalt(II) nitrate, sodium nitrite, and ethylenediamine, partially neutralized by nitric acid, in a stream of air.[1] Analysis of the compound yielded 18.1 % cobalt, the theoretical value being 17.7 %.

Integrated Weissenberg photographs about the *b*-axis ($h0l-h6l$) were recorded with Cu$K\alpha$ radiation. The crystals are of monoclinic symmetry and, from the systematically absent reflections, the space group could be determined to be No. 14 — $P2_1/a$, C_{2h}^5.[2] The dimensions of the unit cell, as calculated from powder diffraction photographs, are $a=13.819$ Å, $b=9.890$ Å, $c=9.095$ Å, and $\beta=105.83°$. The cell volume is 1170.4 Å^3. Assuming a cell content of four formula units, the calculated density is 1.89 g/cm^3. From three-dimensional Patterson calculations, based on the $h0l-h6l$ intensities, the cobalt atoms were found to occupy the general four-fold position 4 (*e*), ± (x, y, z; $\frac{1}{2}+x$, $\frac{1}{2}-y$, z), with $x=0.12$, $y=0.26$, and $z=0.25$. The positions of the light atoms were then deduced from successive electron density calculations. They were all found to occupy the general position 4 (*e*). After a least squares refinement the reliability index converged to $R=0.14$. The resulting parameters are listed in Table 1. The cobalt atom is octahedrally coordinated, through nitrogen atoms, by two NO_2-groups and two $C_2H_8N_2$-groups. The bond distances are Co—N (in NO_2) 1.81 Å and 2.02 Å, and Co—N (in $C_2H_8N_2$) 1.93—1.97 Å. A more detailed presentation of the structure of $1,6[Co(NO_2)_2$ $(en)_2]NO_3$ will be published shortly in this journal.

Table 1.

Atom	x	y	z
Co	0.1196	0.2593	0.2462
N (11)	0.2672	0.2389	0.3436
O (12)	0.3246	0.3378	0.3781
O (13)	0.3106	0.1240	0.3741
N (21)	−0.0137	0.2728	0.1497
O (22)	−0.0673	0.1750	0.1082
O (23)	−0.0515	0.3935	0.1285
N (31)	0.0915	0.1251	0.3856
C (32)	0.0989	0.1762	0.5360
C (33)	0.0723	0.3331	0.5199
N (34)	0.1109	0.3901	0.4020
N (41)	0.1327	0.1206	0.0926
C (42)	0.1923	0.1825	−0.0084
C (43)	0.1538	0.3341	−0.0374
N (44)	0.1586	0.4032	0.1147
N (51)	0.3776	0.2902	0.7582
O (52)	0.4624	0.3554	0.7837
O (53)	0.3042	0.3576	0.7192
O (54)	0.3743	0.1668	0.7605

1. *Inorg. Syn.* McGraw, New York 1953, Vol. IV, p. 177.
2. *International Tables for X-ray Crystallography*, Kynoch Press, Birmingham 1952, Vol. I.

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On the Crystal Structure of 1,2-Bromidopyridinebis(ethylenediamine)cobalt(III) Nitrate

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$1,2[CoBr(C_5H_5N)(C_2H_8N_2)_2](NO_3)_2$ has been prepared and its crystal structure investigated. The preliminary results of the investigation are presented in this note.

Weissenberg photographs of the layers $h0l-h10l$ have been recorded with Cu$K\alpha$ radiation. The crystals are of monoclinic symmetry and, from the systematically absent reflections, the space group could be determined to be No. 14 — $P2_1/n$, C_{2h}^5.[1] The cell dimensions, as calculated