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The Crystal Structure of the 1:2 Copper(II) Nitrate–Methyl Cyanide Complex

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The structure of $Cu(NO_3)_2.2CH_3CN$ has been solved by the heavy-atom method and refined to $R=0{\cdot}15$ by least-squares analysis based on 292 partial three-dimensional data. The complex crystallizes in the monoclinic space group $P2_1/c$ with unit-cell dimensions $a=8{\cdot}81$, $b=7{\cdot}36$, $c=14{\cdot}73$ Å, $\beta=94°$, and $Z=4$. Each copper atom in the structure is in a (4+1) tetragonal pyramidal environment and half the nitrate groups act as bridging ligands, linking tetragonal pyramids related by the twofold screw axes, to form infinite chains parallel to the *b* crystallographic axis. The remaining nitrate groups are unidentate, forming only one bond to the copper atom. Methyl cyanide molecules, coordinated to copper through their nitrogen atoms, occupy *trans* positions in the copper square plane. The structure is compared with the structures of α-cupric nitrate and its complex with nitromethane.

Introduction

The crystal structure of the 1:2 complex between anhydrous cupric nitrate and methyl cyanide has been determined in order to compare the structure of α-cupric nitrate (Wallwork & Addison, 1965) with the crystal structures of its complexes with organic ligands. It would be of interest to determine any changes in metal–nitrate bonding which may occur on complex formation and to investigate the effect of the organic ligands on the copper coordination sphere.

Experimental

Anhydrous cupric nitrate, prepared by the method of Addison & Hathaway (1958), was dissolved in freshly distilled methyl cyanide at 40 °C until a saturated solution was obtained. Deep blue crystals of the methyl cyanide adduct were deposited on standing and analysis for copper content confirmed the 1:2 composition. Because of the deliquescent nature of the complex, suitable crystals were sealed in thin-walled Pyrex capillary tubes in a dry box.

Using Cu $K\alpha$ radiation, equi-inclination multiple film Weissenberg photographs were taken of the zero levels for the crystal rotating about the *a* and *c* crystallographic axes and of the zero and first levels for the *b*-axis rotation. The intensities were measured visually using standard calibrated scales and were converted to observed structure factor values in the usual way. No correction was made for absorption. By comparing equivalent planes observed from different rotation axes, the 292 independent reflexions were placed on a common arbitrary scale.

The crystal data are as follows:

$Cu(NO_3)_2.2CH_3CN$, F.W. 269·6. Monoclinic, $a=8{\cdot}81$ (2), $b=7{\cdot}36$ (2), $c=14{\cdot}73$ (3) Å, $\beta=94$ (1)°, $U=953$ Å^3, $D_m=1{\cdot}825$ g.cm^{-3}, $Z=4$, $D_x=1{\cdot}879$ g.cm^{-3}, Cu $K\alpha$ radiation ($\lambda=1{\cdot}5418$ Å). Space group, $P2_1/c$ (no. 14).

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Table 1. *Observed and calculated structure factors*

Reflexions indicated by an asterisk were given zero weight in the least-squares refinement and excluded from the *R* calculation.

H	K	L	FO	FC
0	0	2	12.5	-10.1
0	0	4	9.8	-13.0
0	0	6	23.2	26.1
0	0	8	11.9	13.3
0	0	14	11.5	19.0
0	0	16	14.8	-17.1
1	0	-12	19.1	-17.1
1	0	-8	9.6	-6.8
1	0	-6	46.0	-44.6
1	0	-4	29.5	25.6
1	0	-2*	54.3	69.9
1	0	0*	49.9	-56.3
1	0	2	13.9	-10.9
1	0	4*	66.6	90.6
1	0	6	30.9	28.1
1	0	8	21.9	-22.1
1	0	10	14.7	14.1
1	0	14	13.4	-14.6
1	0	16	16.4	-6.4
2	0	-14	15.4	-11.2
2	0	-12	23.4	21.5
2	0	-8	54.6	-55.3
2	0	-6	19.9	21.5
2	0	-4	18.4	-10.2
2	0	-2	24.8	-17.8
2	0	0	13.3	-11.6
2	0	2	13.5	6.5
2	0	4	25.6	-26.3
2	0	6*	54.1	-68.5
2	0	8	48.1	32.8
2	0	12	31.7	-25.2
2	0	14	15.1	-6.1
3	0	-14	24.2	22.5
3	0	-12	18.9	-21.9
3	0	-10	30.8	-29.5
3	0	-8	30.5	30.0
3	0	-6	21.5	13.9
3	0	-4	19.7	-18.5
3	0	-2	25.8	-22.9
3	0	0	24.3	9.1
3	0	2	15.4	-11.5
3	0	4	8.0	-10.0
3	0	6	37.5	47.0
3	0	8	18.6	-16.8
3	0	10	44.7	-57.1
3	0	12	13.0	14.0
4	0	-14	19.4	-21.9
4	0	-12	18.4	-16.8
4	0	-10	27.4	25.6
4	0	-6	41.0	-46.3
4	0	-4	14.6	9.2
4	0	-2	33.7	31.3
4	0	0	16.1	-13.1
4	0	2	14.1	12.0
4	0	4	30.7	43.2
4	0	10	24.9	32.4
5	0	-12	19.6	21.6
5	0	-10	18.9	-19.1
5	0	-8	34.4	-35.8
5	0	-6	28.7	23.2
5	0	-4	12.6	-10.5
5	0	-2	63.6	-46.3
5	0	0	12.6	13.7
5	0	2	43.8	46.3
5	0	4	16.9	-17.6
6	0	-14	12.2	18.1
6	0	-12	14.6	-17.3
6	0	-8	22.6	19.7
6	0	-6	19.1	-14.2
6	0	-4	60.3	-40.2
6	0	-2	50.3	33.6
6	0	0	16.5	13.9
6	0	2	38.1	-39.8
6	0	6	11.7	13.8
7	0	-8	13.5	-13.9
7	0	-6	7.1	-8.1
7	0	-4	60.5	39.8
7	0	0	27.5	-28.1
7	0	2	9.1	11.9
7	0	10	15.6	18.5
8	0	-6	25.6	21.4
8	0	-4	20.2	-16.9
8	0	-2	10.0	-12.5
8	0	0	9.0	13.4
8	0	2	14.0	18.3
8	0	4	8.2	-20.5
9	0	-4	18.5	-17.4
9	0	-2	15.4	9.2
9	0	0	8.0	-10.3
9	0	2	32.7	-22.4
9	0	4	7.5	15.4
9	0	8	14.6	-13.6
10	0	-8	11.9	-8.3
10	0	-6	13.4	-13.3
10	0	-4	13.7	10.7
10	0	-2	13.8	-9.9
10	0	0	15.1	-13.9
10	0	2	11.4	11.9
10	0	4	11.2	-7.5
10	0	6	18.8	-15.2
10	0	8	4.2	0.6
0	1	1*	39.9	64.9
0	1	3	40.8	-48.5
0	1	4	42.2	-43.3
0	1	5	22.9	20.8
0	1	6	44.1	48.5
0	1	7	42.3	46.8
0	1	8	15.7	-14.7
0	1	10	12.4	10.0
0	1	11	11.0	-8.8
0	1	12	11.3	9.3
0	1	13	16.7	18.9
0	1	14	9.6	-9.9
1	1	-9	16.0	18.8
1	1	-8	27.8	-30.7
1	1	-5	38.9	-42.4
1	1	-3*	56.8	75.1
1	1	-2	16.6	-18.7
1	1	-1	28.5	26.9
1	1	0	21.9	-26.5
1	1	1*	38.6	-55.9
1	1	3	29.2	28.0
1	1	4	26.1	24.6
1	1	5	27.5	29.8
1	1	7	24.5	-25.2
1	1	11	36.3	31.6
2	1	-9	30.5	-34.4
2	1	-7	30.0	-22.8
2	1	-6	26.9	21.1
2	1	-5	32.7	33.5
2	1	-4	33.1	-33.1
2	1	-3	18.8	-19.0
2	1	-2*	57.5	-72.0
2	1	-1*	37.2	-53.5
2	1	0	21.7	17.9
2	1	1	25.3	24.4
2	1	2	44.2	-44.3
2	1	3	15.8	16.9
2	1	4	18.1	13.8
2	1	5	41.6	-42.6
2	1	6	18.1	14.0
2	1	7	17.2	-10.8
2	1	8	13.3	14.2
2	1	9	33.4	31.0
2	1	11	30.6	-28.5
3	1	-11	25.7	-28.6
3	1	-8	21.8	19.6
3	1	-7	38.8	38.5
3	1	-6	39.9	-41.2
3	1	-5	41.9	-39.2
3	1	-4	19.5	-18.9
3	1	-3	14.1	-12.2
3	1	0	25.4	-19.2
3	1	1	14.5	16.5
3	1	3	47.6	-54.6
3	1	4	27.5	22.0
3	1	5	15.6	15.8
3	1	6	18.3	-13.9
3	1	7	37.0	33.0
3	1	9	42.6	-37.1
4	1	-9	26.6	24.8
4	1	-7	27.9	-29.4
4	1	-3	26.0	28.8
4	1	-2	13.6	-12.2
4	1	0	7.8	-5.4
4	1	1	31.8	-30.5
4	1	2	26.7	24.4
4	1	3	30.8	34.7
4	1	4	14.5	-11.5
4	1	5	22.9	21.9
4	1	7	37.5	-35.3
5	1	-9	22.5	-29.2
5	1	-5	28.4	27.2
5	1	-3	22.6	-21.0
5	1	-1	26.1	-22.5
5	1	0	9.2	10.7
5	1	1	51.4	46.9
5	1	2	19.2	-14.3
5	1	4	18.6	-15.4
6	1	5	34.7	-36.0
6	1	-1	49.3	35.9
6	1	1	27.6	-17.1
6	1	2	24.4	-18.4
6	1	3	17.0	-16.7
6	1	5	25.0	17.5
7	1	-7	24.2	-24.1
7	1	-6	15.2	15.0
7	1	-3	25.2	22.2
7	1	-2	22.5	-18.4
7	1	-1	37.0	-25.3
7	1	0	11.5	-10.5
7	1	3	26.1	22.2
7	1	4	18.3	-15.2
7	1	7	19.3	-15.2
8	1	-5	26.4	18.5
8	1	-4	19.7	-14.8
8	1	-3	25.2	-21.1
8	1	1	20.7	19.6
8	1	5	16.2	-12.9
8	1	7	21.4	17.2
9	1	-5	20.6	-17.5
9	1	-1	20.1	14.9
9	1	1	19.8	-15.4
9	1	5	23.2	18.0
10	1	-1	18.8	-16.3
10	1	3	19.1	14.4
10	1	4	11.8	-11.4
10	1	5	14.0	-12.6
0	2	0	16.8	-20.7
0	2	1	18.8	-19.8
0	2	2	10.7	-10.3
0	2	4	9.6	-2.4
0	2	5	31.7	33.8
0	2	6	41.1	44.7
0	2	7	17.5	20.5
0	2	8	19.4	23.1
0	2	9	24.5	-25.5
0	2	10	33.9	-34.3
0	2	11	12.3	16.0
0	2	14	16.8	18.7
0	2	15	13.8	-18.9
1	2	0	7.2	-8.2
2	2	0	22.8	-21.0
3	2	0	35.3	34.3
4	2	0	19.4	-21.5
5	2	0	3.8	5.6
7	2	0	10.3	-11.9
8	2	0	12.1	16.0
0	3	2	37.7	-46.4
0	3	3	9.8	-10.3
0	3	4	20.9	20.2
0	3	6	13.0	13.5
0	3	7	10.9	11.2
0	3	8	36.9	-39.8
0	3	11	19.2	-19.6
0	3	12	16.6	20.8
0	3	13	12.8	15.6
1	3	0	12.2	-13.7
2	3	0	32.7	31.2
3	3	0	18.5	-18.1
4	3	0	9.8	7.4
5	3	0	30.1	31.7
6	3	0	15.4	-14.9
9	3	0	11.1	-14.1
0	4	0	23.6	24.2
0	4	1	24.7	-28.4
0	4	3	14.8	-15.7
0	4	5	39.5	40.4
0	4	6	8.9	-8.0
0	4	7	16,8	-17.2
0	4	9	21.5	-25.8
0	4	11	24.6	22.1
1	4	0	17.6	-15.8
2	4	0	12.3	12.9
3	4	0	5.9	-3.7
0	5	1	9.0	12.0
0	5	2	21.7	-23.1
0	5	3	16.3	16.0
0	5	4	14.8	15.2
0	5	6	26.4	27.8
0	5	8	25.2	-26.9
0	5	12	10.9	15.3
1	5	0	23.0	-21.5
2	5	0	34.9	34.4
3	5	0	10.8	-11.3
4	5	0	9.4	-8.8
6	5	0	16.0	-12.8
8	5	0	11.5	10.1
9	5	0	9.4	-11.8
0	6	0	20.4	-23.5
0	6	1	16.3	-16.5
0	6	2	13.5	13.5
0	6	4	13.5	15.8
0	6	5	20.1	22.4
0	6	8	8.9	-5.6
0	6	10	10.3	13.1
1	6	0	14.2	12.3
2	6	0	5.6	-4.9
3	6	0	14.8	-9.3
6	6	0	5.2	-7.2
7	6	0	9.4	9.4
0	7	3	18.9	21.7
0	7	5	11.6	8.9
0	7	7	14.1	-14.5
0	7	9	8.9	9.1
1	7	0	14.8	-14.3
0	8	0	14.5	-16.7
0	8	4	11.8	15.7
1	8	0	9.7	10.0
3	8	0	10.9	-14.0
4	8	0	11.5	13.9
0	9	3	9.7	10.4

Structure determination and refinement

The structure determination commenced by examination of the three two-dimensional zones. The position of the copper atom in the asymmetric unit was determined from the Patterson projections and a three-dimensional vector map, calculated with use of all the available data, confirmed the copper coordinates. A structure factor calculation based on the copper position alone, and applying the scattering factor curve listed in *International Tables for X-ray Crystallography* (1962, p.204) with an assumed isotropic temperature factor of $B=1{\cdot}0$ Å^2, gave a reliability index R of 0·39 for the 292 observed planes.

A three-dimensional copper-phased Fourier synthesis was calculated from all the observed data and the electron-density map confirmed the copper coordinates and indicated the positions of seven 'lighter' atoms, four of which were at a distance of approximately 2 Å from the copper atom and occupied square planar positions with respect to copper. The data were

Table 2. *Final atomic parameters and their standard deviations*

	x/a	y/b	z/c	B	$\sigma(x/a)$	$\sigma(y/b)$	$\sigma(z/c)$	$\sigma(B)$
Cu	0·638	0·561	0·353	1·6	0·001	0·001	0·001	0·2
O(1)	0·805	0·692	0·409	2·4	0·004	0·006	0·002	0·8
O(2)	0·749	0·517	0·514	3·6	0·004	0·009	0·003	0·9
O(3)	0·953	0·711	0·539	2·2	0·003	0·006	0·002	0·8
O(4)	0·452	0·451	0·284	3·5	0·004	0·008	0·003	0·9
O(5)	0·485	0·260	0·395	4·3	0·004	0·011	0·003	1·2
O(6)	0·313	0·210	0·280	2·1	0·004	0·006	0·002	0·8
N(1)	0·490	0·727	0·396	2·3	0·004	0·010	0·003	1·1
N(2)	0·757	0·367	0·311	1·4	0·004	0·008	0·003	0·9
N(3)	0·418	0·290	0·321	2·5	0·006	0·009	0·004	1·1
N(4)	0·844	0·642	0·493	2·3	0·005	0·008	0·003	0·9
C(1)	0·408	0·805	0·424	2·4	0·006	0·010	0·004	1·2
C(2)	0·269	0·901	0·459	2·5	0·006	0·010	0·004	1·2
C(3)	0·828	0·264	0·292	1·0	0·005	0·010	0·003	1·0
C(4)	0·925	0·090	0·268	3·5	0·006	0·011	0·004	1·4

placed on an absolute scale by Wilson's (1942) method and after four cycles of electron-density syntheses, all the atoms in the asymmetric unit, apart from hydrogen, had been located and R was 0·20.

Refinement continued by the method of least squares using the full-matrix program of Busing, Martin & Levy (1962) with individual scale factors for each layer. Two cycles of refinement, using unit weights and refining the individual atom coordinates, isotropic temperature factors and scale factors, reduced the reliability index to 0·17. A weighting scheme was now applied which was based on the agreement between observed and calculated structure factors for different regions of sin θ, and two further cycles of refinement reduced R to 0·15.

At this stage the shifts in parameters were less than their standard deviations and the refinement was terminated. The observed and calculated structure factors are given in Table 1, and the final set of atomic parameters and their standard deviations are shown in Table 2.

Discussion

The main interatomic bond distances and angles are given in Table 3 and are shown in Fig. 1. Figs. 2 and 3 show the a- and b-axis projections of the structure respectively.

Table 3. *Interatomic distances and angles and their standard deviations* (*in parentheses*)

	Length
Cu —O(1)	1·89 (4) Å
Cu —O(4)	2·02 (4)
Cu —O(6′)	2·31 (4)
Cu —N(1)	1·93 (6)
Cu —N(2)	1·91 (5)
Cu —O(2)	2·50 (4)
O(1)–N(4)	1·31 (5)
O(2)–N(4)	1·30 (7)
O(3)–N(4)	1·23 (5)
O(4)–N(3)	1·35 (8)
O(5)–N(3)	1·21 (5)
O(6)–N(3)	1·21 (5)
N(1)–C(1)	1·04 (7)
C(1)–C(2)	1·54 (8)
N(2)–C(3)	1·03 (7)
C(3)–C(4)	1·60 (9)
	Angle
O(1)–Cu —N(1)	93 (2)°
O(1)–Cu —N(2)	95 (2)
O(1)–Cu —O(6′)	86 (1)
N(1)–Cu —O(4)	83 (2)
N(1)–Cu —O(6′)	99 (2)
N(2)–Cu —O(4)	89 (2)

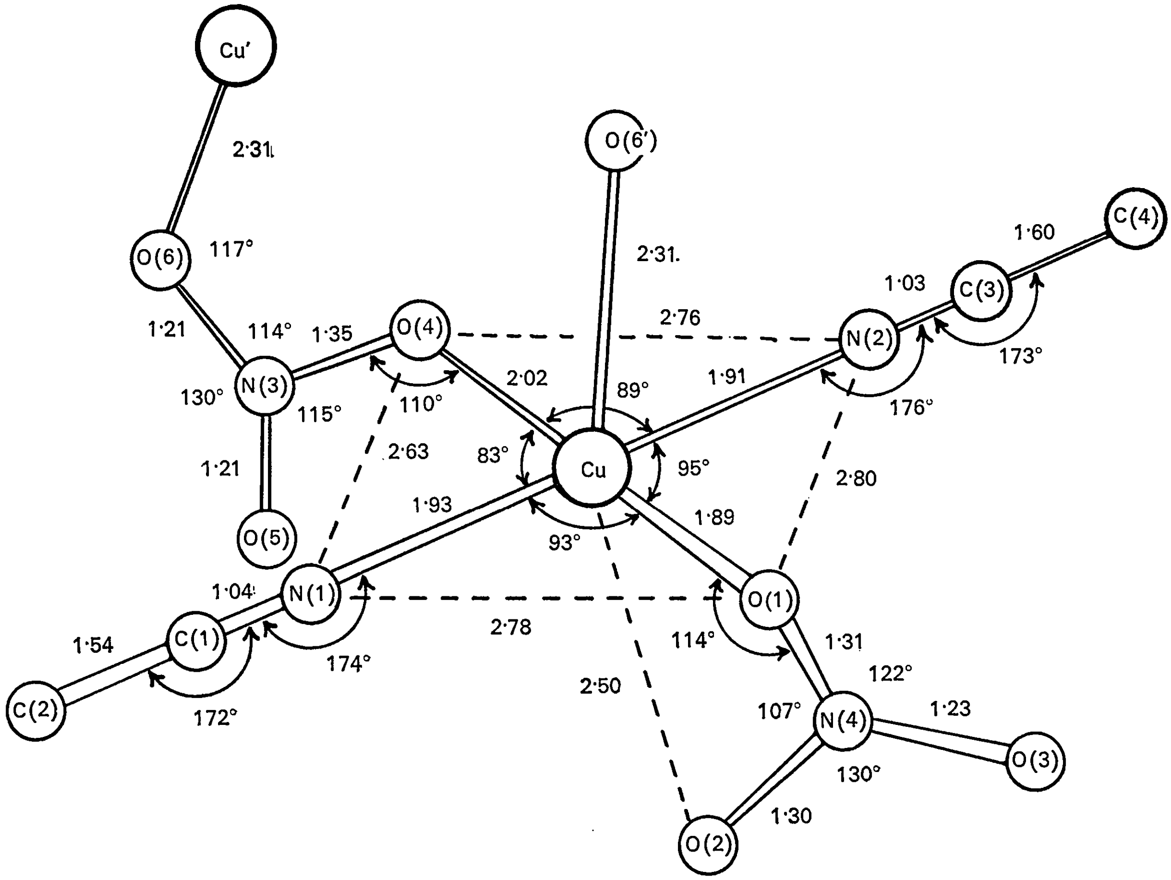

Fig. 1. Interatomic bond distances and angles.

Table 3 (*cont.*)

	Angle
N(2)–Cu —O(6′)	86 (2)
O(4)–Cu —O(6′)	88 (2)
O(1)–N(4)–O(2)	107 (4)
O(1)–N(4)–O(3)	122 (5)
O(2)–N(4)–O(3)	130 (5)
O(4)–N(3)–O(5)	115 (6)
O(4)–N(3)–O(6)	114 (5)
O(5)–N(3)–O(6)	130 (7)
N(1)–C(1)–C(2)	172 (7)
N(2)–C(3)–C(4)	173 (6)
Cu —O(1)–N(4)	114 (4)
Cu —O(4)–N(3)	110 (4)
Cu —N(1)–C(1)	174 (6)
Cu —N(2)–C(3)	176 (4)
Cu′—O(6)–N(3)	117 (3)

Each copper atom in the structure has four nearest neighbours arranged around it in square planar positions with a next nearest neighbour lying above the copper atom perpendicular to the square plane. The copper atom thus has a slightly distorted (4+1) tetragonal pyramidal coordination. In the square plane, two nitrogen atoms from methyl cyanide molecules occupy *trans* positions and form bonds of length 1·91 and 1·93 Å to the copper atom. The other two *trans* positions in the copper square plane are occupied by oxygen atoms, one from each of the two nitrate groups in the asymmetric unit, and these atoms form bonds of length 1·89 and 2·02 Å to copper. The weaker fifth bond, Cu–O(6′), of length 2·31 Å, directed towards the apex of the tetragonal pyramid, is to an oxygen atom of a nitrate group in an adjacent copper square plane and links copper atoms related by the twofold screw axes in the structure to form infinite chains parallel to the *b* axis. Forces between adjacent chains are due to weak van der Waals interactions.

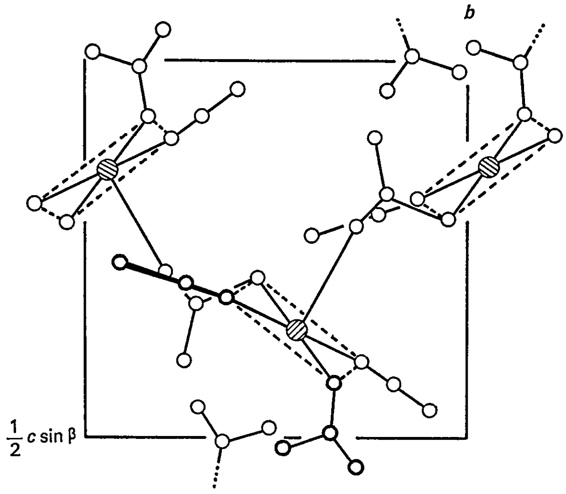

Fig. 2. Projection of the structure along [100].

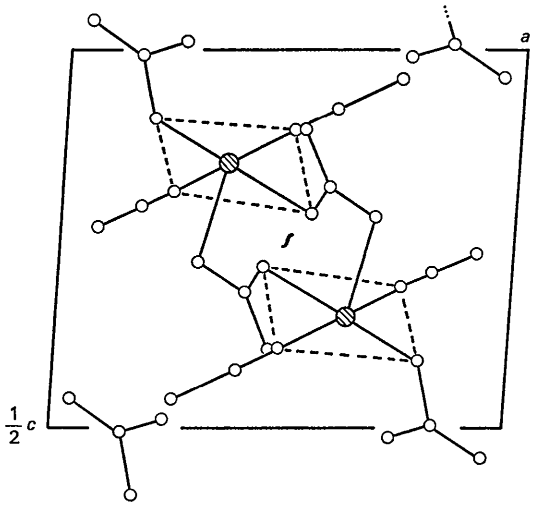

Fig. 3. Projection of the structure along [010].

One of the two nitrate groups in the asymmetric unit thus acts as a bridging ligand and forms bonds of length 2·02 and 2·31 Å to copper atoms related by the twofold screw axes. While the second nitrate group forms only one strong bond, Cu–O(1), of length 1·89 Å, a Cu–O(2) distance of 2·50 Å and a O(1)–N(4)–O(2) bond angle of 107° suggest a tendency for this nitrate group to act as a bidentate ligand and complete an octahedral copper coordination sphere. However, the angles O(1)–Cu–O(2) of 55° and Cu–O(2)–N(4) of 84° indicate that if such a bond were formed it would involve considerable strain.

The nitrate groups are planar within experimental error with bond lengths and angles, except for O(1)–N(4)–O(2), not significantly different from literature values. The methyl cyanide molecules are linear within experimental error and the apparent shortening of the N≡C-bonds on coordination from the value of 1·156 Å in the free molecule (Sutton, 1958) has been observed to a smaller extent in the structure of the methyl cyanide–boron trifluoride complex (Hoard, Owen, Buzzell & Salmon, 1950).

The least-squares plane through the copper atom and its four nearest neighbours is given by:

$$X'+2\cdot660Y'-3\cdot961Z'+4\cdot328=0\,,$$

where X',Y',Z' are orthogonal coordinates in Å and $X'=x+z\cos\beta$, $Y'=y$, $Z'=z\sin\beta$. The individual atom deviations, in Å, from this plane are:

$$\mathrm{O}(1)=0\cdot14,\ \mathrm{O}(4)=0\cdot06,\ \mathrm{N}(1)=-0\cdot14,\ \mathrm{N}(2)=-0\cdot06,\ \mathrm{Cu}=-0\cdot01\ \text{Å}\,.$$

Although these values may not be significant in terms of the atomic standard deviations, they are in directions expected for a distortion of the copper square plane.

All distances between non-bonded atoms in the structure have been calculated and, apart from those between adjacent atoms in the basal plane of the tetragonal pyramid, only those between C(2) at ($1-x$, $1-y$, $1-z$) and O(2), 3·11 Å, and O(5), 3·14 Å correspond to less than van der Waals contacts.

The effect on the copper coordination and nitrate bonding by introducing a weak and a strong ligand into the α-$Cu(NO_3)_2$ structure can be seen in the structures of $Cu(NO_3)_2.CH_3NO_2$ (Duffin & Wallwork, 1966) and the present work respectively. Anhydrous α-cupric nitrate contains copper atoms in a distorted octahedral (4+1+1) arrangement with all the nitrato groups acting as bridging ligands between adjacent copper atoms and each forming two strong Cu–O bonds. Half the nitrato groups, however, form two additional, weaker, bonds to copper in order to complete the copper coordination sphere. The introduction of the nitromethane molecule into the copper sphere, in the fifth octahedral position, allows all the nitrato groups to act solely as bridging groups between adjacent copper atoms while the copper coordination remains essentially a (4+1) tetragonal pyramidal arrangement. Thus the nitromethane molecules relieve some of the steric hindrance involved in the α-$Cu(NO_3)_2$ structure without affecting the strength of the main Cu–O bonds. The tetragonal pyramidal coordination of the copper atom is maintained in the $Cu(NO_3)_2.2CH_3CN$ structure although the strong methyl cyanide ligands have replaced two nitrato oxygen atoms in the copper square plane. This has resulted in a weakening of the copper–nitrate bonding so that although half the nitrato groups act as bridging ligands between adjacent copper atoms they form only one strong and one weaker Cu–O bond, the weaker bonds being directed towards the apex of the copper tetragonal pyramids. The remaining nitrato groups are essentially unidentate ligands and form only one strong bond to copper. Presumably steric hindrance prevents these groups from acting as bidentate ligands and completing an octahedral copper coordination.

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The Structures of Uranyl Chloride and its Hydrates

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X-ray powder diffraction data for UO_2Cl_2, $UO_2Cl_2.H_2O$ and $UO_2Cl_2.3H_2O$ are presented, together with the unit cells derived from these data. The structures of the three compounds are also given, with some restrictions about the positions of the oxygen ions. From the structure determination it follows that $UO_2Cl_2.H_2O$ is not a true hydrate.

As part of a study of uranyl chloride (UO_2Cl_2) and its two hydrates ($UO_2Cl_2.H_2O$ and $UO_2Cl_2.3H_2O$) the X-ray powder diffraction patterns of these compounds were indexed and an attempt was made to determine their structures. The diffraction patterns were recorded with a Guinier–de Wolff focusing camera using Cu $K\alpha$ radiation. The intensities were measured on a densitometer as peak values and integrated values were ob-

Table 1. *Space groups and unit cells* (*standard deviations in parentheses*)*

Compound	Symmetry and space group	*a*	*b*	*c*	*β*	*Z*
UO_2Cl_2	Orthorhombic; *Pnma*	5·725 (1)	8·409 (2)	8·720 (2)		4
$UO_2Cl_2.H_2O$	Monoclinic; $P2_1/m$	5·836 (3)	8·563 (3)	5·566 (2)	97·70° (3)	2
$UO_2Cl_2.3H_2O$	Orthorhombic; *Pnma*	12·738 (5)	10·495 (5)	5·547 (2)		4

* The unit cell of UO_2Cl_2 has been found previously by Baenziger & Rundle (1944). The present data are in good agreement with their result; this implies that the data in the ASTM Powder Data File, given by Dunn (1956) are in error.