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The Crystal Structure of Di-μ-hydroxobis(dimethylaminecopper (II)) Sulfate Monohydrate

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The crystal structure of di-μ-hydroxobis(dimethylaminecopper(II)) sulfate monohydrate, $Cu_2(NH_2CH_3)_4(OH)_2SO_4 . H_2O$, has been determined by X-ray analysis. The crystals are triclinic with space group $P\bar{1}$ and the cell dimensions are, $a = 9{\cdot}28_1$, $b = 11{\cdot}31_1$, $c = 7{\cdot}42_5$ Å, $\alpha = 98{\cdot}6_8$, $\beta = 92{\cdot}9_4$, $\gamma = 113{\cdot}1_9°$, with two formula units in the cell. The final parameters were evaluated by a full-matrix least-squares treatment of three-dimensional data.

The structure contains two crystallographically independent copper(II) atoms having a tetragonal pyramidal coordination. Each copper atom is coordinated by two hydroxyl anions and two nitrogen atoms of methylamine to form a binuclear complex ion. The two hydroxyl ions are shared by the two copper atoms. The complex ion is puckered at the hydroxyl ions and this results in a rather close approach, 2·78 Å, between the copper atoms. Two such complex ions are bound together to form a dimer, in which the hydroxyl ion in one of the complex ions is coordinated as a fifth ligand to the copper atom in the other. A water molecule is coordinated to another copper atom of the complex ion as a fifth ligand. The dimers are piled up along the *c* axis, and sulfate ions are attached to them through hydrogen bonds. These columnar units of the structure are packed together parallel to the *c* axis to complete the structure.

Experimental

In the course of a study of the hydrogenation catalysis by cupric salts dissolved in organic bases, a new compound with the composition $Cu_2(NH_2CH_3)_4(OH)_2SO_4 . H_2O$ was found to deposit in reaction flasks. In view of the significance of the structural correlation of this complex with the substrate, a structural analysis was undertaken on it by X-ray diffraction.

The complex was prepared by dissolving $CuSO_4 . 5H_2O$ in a 40% aqueous solution of methylamine in a water bath with a molar ratio of copper to methylamine 1:4. After filtration of the dark blue solution obtained, a small amount of alcohol was added to it. The solution was then suddenly cooled to liquid nitrogen temperature in order to stimulate crystallization. Many small crystals were obtained as a precipitate when the solution was kept in a refrigerator for a while. The crystal suitable for the X-ray work was grown from the solution at room temperature by using a crystal from the precipitate as a seed crystal.

The crystals collected were dark blue, elongated along the *c* axis, and often twinned with the twinning axis *c*. The crystals were unstable and easily decomposed on exposure to the air. During the exposure to X-rays, the specimen was kept in a thin-walled Pyrex glass capillary filled with methylamine and ethyl alcohol vapours. Although the results of chemical analysis showed poor reproducibility because of such instability of the specimen, the molar proportions of copper, methylamine, sulfate and water were found to be approximately 2:4:1:3, where the water content was determined by Karl Fischer's method. In the course of the structure determination, it became clear that two of the three 'water molecules' determined by Karl Fischer's method

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were actually hydroxyl ions, and the chemical formula of the complex was thus established as $Cu_2(NH_2CH_3)_4(OH)_2SO_4 \cdot H_2O$.

The cell dimensions were determined from 30° precession photographs of 0*kl* and *h*0*l* taken with Cu $K\alpha$ radiation ($\lambda = 1{\cdot}5418$ Å). They were calibrated against quartz. The crystals belong to the triclinic system with:

$$a = 9{\cdot}28_1,\quad b = 11{\cdot}31_1,\quad c = 7{\cdot}42_5\ \text{Å},$$
$$\alpha = 98{\cdot}6_8,\quad \beta = 92{\cdot}9_4,\quad \gamma = 113{\cdot}1_9^\circ\ .$$

The density measured by the flotation method is 1·83 g.cm^{-3}, while the calculated density assuming two formula units in the cell is 1·89 g.cm^{-3}. The presence of the symmetry center was deduced by Wilson's statistical method (Howells, Phillips & Rogers, 1950), and the space group was determined as $P\bar{1}$. The crystals used for the intensity measurement were long needles with the cross sections about $0{\cdot}05 \times 0{\cdot}02$ mm, and were mounted along the *c* axis. The whole of the intensity data were collected only from the *c*-axis equi-inclination Weissenberg photographs, because attempts to cut the crystals normal to the needle axis were not successful. The layers from *hk*0 to *hk*4 were taken with Cu $K\alpha$ radiation by the multiple film technique. Intensities were estimated visually with a calibrated intensity scale. A total of 1733 reflexions were observed, of which 403 were with relative intensities less than 1 in a full intensity scale of 2000. Lorentz and polarization corrections were applied but no correction was made for absorption.

Determination of the structure

Since in a two-dimensional Patterson synthesis calculated from the *hk*0 data the overlapping of peaks was found to take place severely, a three-dimensional sharpened Patterson synthesis was calculated and the positions of the two copper atoms and a sulfur atom could be located in the map. A three-dimensional Fourier synthesis was then computed with the use of the signs based on the contributions of these atoms. The electron density map showed all the light atoms as well resolved peaks. A new set of coordinates was obtained from the second Fourier and difference Fourier syntheses and the approximate structure was well established. At this stage, the *R* value was 0·20 for all reflexions excluding unobserved ones.

The first stage of the refinement was carried out by the least-squares method using diagonal approximations. After five cycles of refinement with full three-dimensional data the *R* index dropped to 0·16. Next, a full-matrix least-squares refinement was carried out on a CDC G-20 computer, with the program ORFLS of Busing, Martin & Levy (1962). In three cycles of refinement, all 77 parameters were allowed to vary. These comprised all positional and isotropic thermal parameters for each atom and five scale factors for each layer line. The *R* value was then reduced to 0·132. The final parameters are listed in Table 1. Their standard deviations derived directly from the inverse least-squares matrix are given in Table 2. The observed and calculated structure factors are listed in Table 3. The following atomic scattering factors were used for the refinement: for carbon atoms, the calculation SX-6, for nitrogen, SX-7, for oxygen, SX-8, for sulfur, SXC-69, for copper, SX-68, all listed in *International Tables for X-ray Crystallography* (1962, pp.202 and 204).

Table 1. *Final atomic parameters*

	x/a	*y/b*	*z/c*	*B*
Cu(1)	0·1610	0·0181	0·0988	2·15 Å^2
Cu(2)	0·2134	0·2813	0·1731	2·22
S	0·4448	0·2256	0·6715	1·48
O(1)(OH)	0·1229	0·1330	0·2944	1·27
O(2)(OH)	0·1098	0·1374	−0·1411	1·38
O(3)(H_2O)	0·4724	0·2897	0·1834	2·69
O(4)(SO_4)	0·2717	0·1457	0·6370	3·37
O(5)(SO_4)	0·4728	0·3666	0·7209	2·75
O(6)(SO_4)	0·5086	0·1872	0·8268	2·73
O(7)(SO_4)	0·5183	0·2061	0·5061	2·89
N(1)	0·2882	0·4160	0·4085	2·00
N(2)	0·2646	−0·0531	0·2722	1·65
N(3)	0·2054	−0·0680	−0·1379	1·82
N(4)	0·2851	0·4210	0·0190	2·25
C(1)	0·1575	0·4492	0·4814	4·01
C(2)	0·1458	−0·1592	0·3552	3·24
C(3)	0·2149	−0·1986	−0·1522	3·60
C(4)	0·1727	0·4847	−0·0182	4·33

Table 2. *Standard deviations of the atomic parameters*

	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$	$\sigma(B)$
Cu(1)	0·0029 Å	0·0028 Å	0·0037 Å	0·06 Å^2
Cu(2)	0·0029	0·0028	0·0037	0·06
S	0·0052	0·0049	0·0070	0·08
O(1)	0·0127	0·0123	0·0160	0·21
O(2)	0·0129	0·0124	0·0164	0·22
O(3)	0·0164	0·0157	0·0191	0·30
O(4)	0·0177	0·0175	0·0201	0·34
O(5)	0·0162	0·0158	0·0188	0·30
O(6)	0·0164	0·0159	0·0193	0·30
O(7)	0·0166	0·0164	0·0196	0·31
N(1)	0·0178	0·0172	0·0217	0·30
N(2)	0·0171	0·0165	0·0212	0·29
N(3)	0·0172	0·0166	0·0212	0·29
N(4)	0·0185	0·0179	0·0226	0·33
C(1)	0·0320	0·0311	0·0338	0·62
C(2)	0·0272	0·0264	0·0307	0·50
C(3)	0·0302	0·0291	0·0324	0·58
C(4)	0·0273	0·0268	0·0303	0·52

Description and discussion of the structure

The structure of the complex ion

The structure of the complex ion found in the present structure analysis is unusual in the respect that it consists of two tetragonal pyramidal coordination polyhedra of copper(II) atoms joined together with one of the edges of each polyhedron in common to form a binuclear complex ion, and that two of these binuclear ions are again bound together by sharing one of the longer edges to form a dimer ion. Details of the structure will be discussed below.

The crystal contains two kinds of crystallographically independent copper atom [Cu(1) and Cu(2)] in a cell.

One of the each kind is surrounded, as the nearest neighbours, by the two hydroxyl ions and the two nitrogen atoms of methylamine to form a rectangular coordination. The two rectangles formed by Cu(1) and Cu(2) are bound together by sharing two hydroxyl ions between the two copper atoms and form a binuclear complex ion. The planes of these two rectangular groups are inclined to each other at an angle of 50·8° and this results in a rather close approach of the copper atoms (Cu · · · Cu, $2{\cdot}78_2$ Å). These binuclear complex ions are again bound together in pairs coordinating the hydroxyl ion as a fifth ligand of the copper atom in the opposite complex ion. In this way, a dimer ion of the composition $[Cu_2(NH_2CH_3)_4(OH)_2 . H_2O]_2^{4+}$ is formed. The structure of the dimer ion is illustrated in Fig. 1.

In copper complexes, binuclear structures have been reported in several acetate complexes, such as copper acetate dihydrate, $Cu_2(CH_3COO)_4 . 2H_2O$ (van Niekerk & Schoening, 1953), and the orthorhombic (Hanic, Štempelová & Hanicová, 1964) and monoclinic forms of monopyridine copper acetate, $Cu_2(CH_3COO)_4$

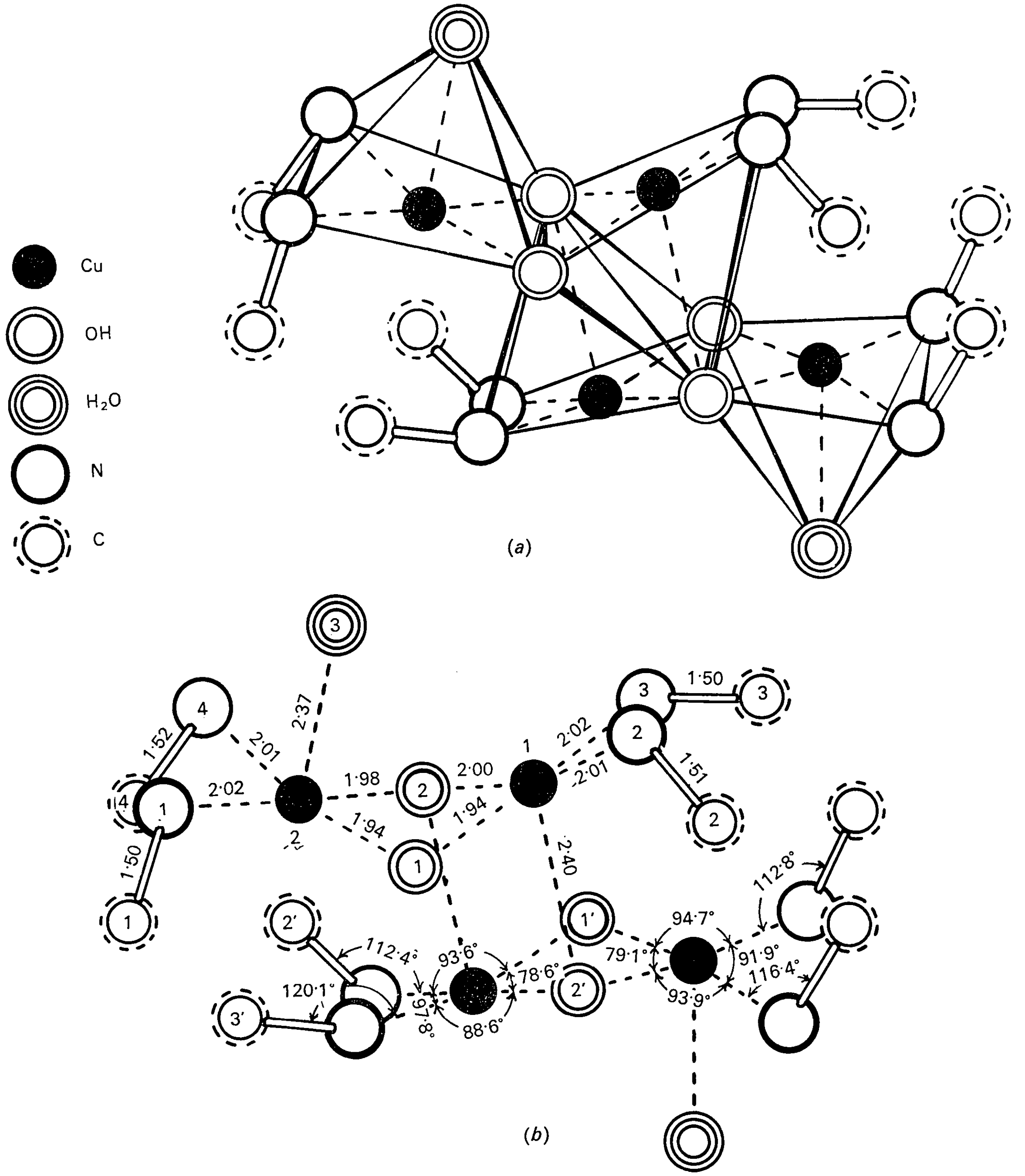

Fig. 1. Structure of the dimer complex ion. (*a*) The union of the tetragonal pyramidal coordination polyhedra of copper atoms. (*b*) Interatomic distances (Å) and bond angles.

Table 3. *Observed and calculated structure factors*

H	K	L	|Fobs|	Fcal
0	1	0	59.25	65.10
0	2	0	32.19	-31.61
0	3	0	7.64	8.58
0	4	0	57.45	56.13
0	5	0	29.13	25.35
0	6	0	11.52	9.14
0	7	0	46.26	45.19
0	8	0	17.74	11.51
0	9	0	0.00	-5.77
0	10	0	14.59	9.13
0	11	0	0.00	-0.42
0	12	0	5.96	-12.70
1	0	0	13.51	-8.95
1	1	0	46.44	-44.56
1	2	0	103.37	103.11
1	3	0	16.21	23.20
1	4	0	9.20	-9.07
1	5	0	47.64	-46.48
1	6	0	59.92	53.57
1	7	0	43.51	37.78
1	8	0	30.37	-27.57
1	9	0	19.20	-22.50
1	10	0	11.51	-14.75
1	11	0	9.98	-11.86
1	12	0	10.60	-10.05
-1	1	0	83.55	129.14
-1	2	0	41.13	43.03
-1	3	0	12.46	12.31
-1	4	0	0.00	7.01
-1	5	0	6.83	3.75
-1	6	0	23.79	-18.98
-1	7	0	49.57	42.75
-1	8	0	68.24	63.06
-1	9	0	14.01	13.89
-1	10	0	14.27	9.14
-1	11	0	29.37	27.29
-1	12	0	16.17	18.10
2	0	0	74.82	-67.79
2	1	0	23.81	-25.54
2	2	0	73.61	-59.75
2	3	0	45.66	-49.27
2	4	0	50.90	-46.93
2	5	0	15.53	12.16
2	6	0	23.07	20.35
2	7	0	61.74	-56.77
2	8	0	27.17	-23.35
2	9	0	0.00	1.27
2	10	0	0.00	-6.47
2	11	0	15.94	-21.89
-2	1	0	10.11	-6.42
-2	2	0	45.47	-37.95
-2	3	0	15.85	-22.65
-2	4	0	5.39	8.75
-2	5	0	39.12	43.14
-2	6	0	17.52	-10.91
-2	7	0	36.70	-34.25
-2	8	0	44.95	38.77
-2	9	0	55.96	54.02
-2	10	0	8.53	5.75
-2	11	0	10.28	10.20
-2	12	0	14.97	15.69
-2	13	0	18.85	13.39
3	0	0	141.58	-152.75
3	1	0	53.25	-45.51
3	2	0	21.74	-20.87
3	3	0	38.28	-38.45
3	4	0	44.21	-43.07
3	5	0	17.08	-8.98
3	6	0	45.27	-46.03
3	7	0	16.06	-17.19
3	8	0	11.93	8.78
3	9	0	10.95	-11.53
3	10	0	14.44	-21.01
-3	1	0	56.77	-55.56
-3	2	0	63.57	61.28
-3	3	0	9.82	-5.30
-3	4	0	70.54	-66.53
-3	5	0	17.61	-20.22
-3	6	0	7.78	6.39
-3	7	0	15.56	-21.74
-3	8	0	52.70	-49.50
-3	9	0	16.54	16.22
-3	10	0	12.10	7.59
-3	11	0	16.91	-15.77
-3	12	0	5.45	-3.58
-3	13	0	9.00	-5.57
-3	14	0	5.04	-4.14
4	0	0	35.41	33.82
4	1	0	6.11	6.84
4	2	0	62.60	-66.07
4	3	0	34.71	-30.79
4	4	0	31.95	33.34
4	5	0	20.27	20.85
4	6	0	17.18	-18.83
4	7	0	8.52	-5.09
4	8	0	0.00	-7.46
4	9	0	0.00	-1.29
4	10	0	0.00	7.46
-4	1	0	73.21	-72.12
-4	2	0	49.35	-42.57
-4	3	0	51.92	48.50
-4	4	0	40.55	-38.02
-4	5	0	54.38	-58.19
-4	6	0	33.31	-33.21
-4	7	0	25.14	-23.28
-4	8	0	52.52	-48.72
-4	9	0	51.52	-50.60
-4	10	0	0.00	4.24
-4	11	0	15.83	-18.06
-4	12	0	19.87	-20.00
-4	13	0	5.57	-5.54
-4	14	0	0.00	-6.93
5	0	0	4.73	6.25
5	1	0	28.22	-21.92
5	2	0	14.06	12.79
5	3	0	54.75	59.10
5	4	0	46.11	43.94
5	5	0	12.12	-10.43
5	6	0	11.91	5.57
5	7	0	19.14	21.84
5	8	0	6.59	8.42
5	9	0	0.00	2.64
-5	1	0	35.46	33.21
-5	2	0	29.81	-31.47
-5	3	0	4.45	1.25
-5	4	0	49.97	47.46
-5	5	0	41.71	-37.42
-5	6	0	30.49	-30.97
-5	7	0	31.00	-25.28
-5	8	0	13.90	-8.11
-5	9	0	37.55	-31.67
-5	10	0	6.09	-5.46
-5	11	0	0.00	6.98
-5	12	0	22.04	-18.56
-5	13	0	15.64	-14.08
-5	14	0	3.28	4.09
6	0	0	22.88	23.10
6	1	0	23.85	21.55
6	2	0	40.15	38.64
6	3	0	35.17	38.35
6	4	0	0.00	-4.02
6	5	0	8.34	10.50
6	6	0	25.45	29.21
6	7	0	0.00	2.35
6	8	0	0.00	-5.75
-6	1	0	13.31	11.68
-6	2	0	16.87	17.49
-6	3	0	13.82	-13.44
-6	4	0	55.25	53.41
-6	5	0	40.50	39.87
-6	6	0	13.85	9.27
-6	7	0	17.42	16.35
-6	8	0	29.98	24.54
-6	9	0	6.07	-3.00
-6	10	0	22.71	-20.75
-6	11	0	26.08	22.45
-6	12	0	23.15	21.21
-6	13	0	0.00	-2.68
-6	14	0	13.10	-11.74
7	0	0	11.82	7.87
7	1	0	12.04	9.72
7	2	0	32.15	30.23
7	3	0	0.00	-1.26
7	4	0	0.00	-8.50
7	5	0	7.25	5.84
7	6	0	0.00	-6.87
7	7	0	0.00	-4.55
-7	1	0	26.57	23.52
-7	2	0	28.06	27.50
-7	3	0	12.58	-9.49
-7	4	0	12.59	10.53
-7	5	0	55.13	55.15
-7	6	0	33.77	34.00
-7	7	0	15.18	12.30
-7	8	0	23.40	20.80
-7	9	0	47.56	42.54
-7	10	0	5.97	-2.18
-7	11	0	12.46	-13.36
-7	12	0	23.54	19.53
-7	13	0	21.42	17.73
-7	14	0	7.07	8.58
8	0	0	8.61	-7.53
8	1	0	15.80	19.42
8	2	0	0.00	-3.32
8	3	0	22.53	-26.66
8	4	0	0.00	-6.57
8	5	0	0.00	-7.07
-8	1	0	16.09	-13.50
-8	2	0	15.49	13.78
-8	3	0	20.00	18.82
-8	4	0	40.11	-42.70
-8	5	0	0.00	0.35
-8	6	0	43.02	42.72
-8	7	0	30.00	27.10
-8	8	0	12.87	-6.31
-8	9	0	0.00	-2.50
-8	10	0	23.42	19.41
-8	11	0	5.25	3.09
-8	12	0	0.00	4.32
-8	13	0	19.47	15.79
9	0	0	7.92	3.42
9	1	0	7.42	-3.41
9	2	0	27.52	-31.69
9	3	0	7.94	-13.44
-9	1	0	14.21	-13.25
-9	2	0	30.21	-37.41
-9	3	0	0.00	-2.03
-9	4	0	0.00	4.07
-9	5	0	29.47	-30.79
-9	6	0	16.42	-15.76
-9	7	0	5.93	-3.29
-9	8	0	8.19	-1.57
-9	9	0	5.55	2.17
-9	10	0	0.00	2.97
-9	11	0	6.55	-2.48
-9	12	0	15.80	-14.65
-9	13	0	5.78	6.03
10	0	0	0.00	-3.57
10	1	0	14.21	-17.08
10	2	0	5.51	-10.68
-10	1	0	0.00	-1.11
-10	2	0	0.00	-5.37
-10	3	0	18.45	-19.14
-10	4	0	10.84	-10.76
-10	5	0	19.71	-18.55
-10	6	0	17.18	-19.88
-10	7	0	9.23	0.52
-10	8	0	13.03	-11.71
-10	9	0	21.90	-22.60
-10	10	0	5.12	-4.56
-10	11	0	3.67	7.04
-10	12	0	5.37	-7.85
-11	1	0	4.33	6.78
-11	2	0	0.00	-3.17
-11	3	0	5.71	-2.82
-11	4	0	6.03	6.11
-11	5	0	0.00	-0.40
-11	6	0	28.68	-27.60
-11	7	0	19.31	-19.93
-11	8	0	14.30	15.21
-11	9	0	3.57	3.68
-11	10	0	15.40	-17.88
0	-1	1	54.83	58.69
0	-2	1	10.85	9.79
0	-3	1	44.78	44.32
0	-4	1	94.28	101.00
0	-5	1	27.83	27.45
0	-6	1	27.53	-24.41
0	-7	1	43.71	40.32
0	-8	1	48.00	54.62
0	-9	1	13.91	-13.10
0	-10	1	0.00	2.52
0	-11	1	25.88	28.69
0	-12	1	14.06	19.54
0	1	1	20.96	18.77
0	2	1	60.28	56.00
0	3	1	64.09	68.39
0	4	1	16.64	-15.05
0	5	1	47.45	-40.50
0	6	1	65.82	59.51
0	7	1	32.57	28.21
0	8	1	40.64	-31.08
0	9	1	8.14	-6.95
0	10	1	20.58	17.75
-1	0	1	101.75	126.86
-1	-1	1	68.74	76.57
-1	-2	1	32.17	25.81
-1	-3	1	56.60	61.46
-1	-4	1	29.44	25.60
-1	-5	1	8.21	-3.97
-1	-6	1	35.12	34.67
-1	-7	1	26.71	28.89
-1	-8	1	15.59	-14.11
-1	-9	1	8.14	-8.74
-1	-10	1	11.02	15.73
-1	-11	1	5.93	-0.57
-1	-12	1	10.75	-18.78
-1	1	1	7.28	12.35
-1	2	1	19.95	-17.93
-1	3	1	49.40	58.79
-1	4	1	101.17	102.03
-1	5	1	15.51	14.58
-1	6	1	27.95	-22.47
-1	7	1	61.91	56.02
-1	8	1	57.25	50.32
-1	9	1	0.00	-4.19
-1	10	1	8.05	5.57
-2	0	1	12.93	13.13
-2	-1	1	62.64	-71.91
-2	-2	1	9.84	-2.60
-2	-1	1	66.97	-71.91
-2	-4	1	25.61	-25.97
-2	-5	1	23.51	-27.82
-2	-6	1	0.00	0.90
-2	-7	1	13.38	12.96
-2	-8	1	11.39	-9.85
-2	-9	1	11.25	-10.54
-2	-10	1	12.64	-12.24
-2	-11	1	19.03	-19.55
-2	1	1	92.75	113.78
-2	2	1	0.00	-1.03
-2	3	1	44.04	-42.14
-2	4	1	13.43	-6.14
-2	5	1	34.29	31.89
-2	6	1	40.32	32.74
-2	7	1	33.21	27.42
-2	8	1	53.04	44.37
-2	9	1	27.58	20.91
-2	10	1	8.12	1.59
-2	11	1	18.79	20.07
-2	12	1	14.87	12.56
-3	0	1	74.20	-83.01
-3	-1	1	35.91	-30.55
-3	-2	1	33.22	-27.43
-3	-3	1	73.00	-71.07
-3	-4	1	74.86	-84.57
-3	-5	1	7.11	-3.00
-3	-6	1	18.78	15.96
-3	-7	1	30.12	-32.77
-3	-8	1	31.12	-33.82
-3	-9	1	7.53	1.05
-3	-10	1	6.41	-7.42
-3	-11	1	7.98	-11.39
-3	1	1	5.98	-6.82
-3	2	1	33.50	30.43
-3	3	1	59.64	-54.28
-3	4	1	24.33	-24.58
-3	5	1	16.67	13.86
-3	6	1	20.46	-18.88
-3	7	1	11.91	-10.91
-3	8	1	24.66	21.28
-3	9	1	26.28	25.80
-3	10	1	11.42	-10.17
-3	11	1	0.00	2.59
-3	12	1	16.98	15.06
-4	0	1	37.71	-36.40
-4	-1	1	23.17	-23.00
-4	-2	1	35.39	-43.42
-4	-3	1	51.60	-57.53
-4	-4	1	0.00	4.49
-4	-5	1	13.35	13.67
-4	-6	1	44.21	-47.70
-4	-7	1	27.87	-29.07
-4	-8	1	13.11	10.50
-4	-9	1	0.00	-0.92
-4	-10	1	11.09	-16.38
-4	1	1	56.92	-56.96
-4	2	1	16.05	9.78
-4	3	1	7.35	2.89
-4	4	1	64.00	-67.49
-4	5	1	25.75	-23.59
-4	6	1	0.00	-0.73
-4	7	1	61.92	-55.24
-4	8	1	66.75	-60.35
-4	9	1	15.85	13.15
-4	10	1	0.00	7.83
-4	11	1	30.31	-26.65
-4	12	1	17.23	-14.19
-4	13	1	0.00	2.41
-5	0	1	0.00	2.61
-5	-1	1	19.67	20.35
-5	-2	1	0.00	3.19
-5	-3	1	12.87	12.42
-5	-4	1	20.71	26.12
-5	-5	1	5.10	-11.00
-5	-6	1	0.00	3.54
-5	-7	1	15.01	18.85
-5	-8	1	0.00	1.52
-5	-9	1	5.06	-9.37
-5	1	1	57.03	-56.47
-5	2	1	34.24	-36.21
-5	3	1	30.83	28.39
-5	4	1	8.64	-2.27
-5	5	1	57.10	-55.27
-5	6	1	46.74	-38.54
-5	7	1	14.45	-9.22
-5	8	1	51.46	-47.58
-5	9	1	58.51	-52.72
-5	10	1	14.00	10.78
-5	11	1	0.00	0.76
-5	12	1	25.18	-17.85
-5	13	1	15.93	-17.60
-6	0	1	36.92	34.95
-6	-1	1	0.00	-0.56
-6	-2	1	0.00	5.59
-6	-3	1	38.78	40.21
-6	-4	1	29.57	35.46
-6	-5	1	7.95	11.01
-6	-6	1	14.67	13.90
-6	-7	1	12.71	12.43
-6	-8	1	6.85	11.42
-6	1	1	16.92	17.25
-6	2	1	32.87	-34.35
-6	3	1	6.78	8.85
-6	4	1	35.45	37.89
-6	5	1	0.00	-6.52
-6	6	1	25.32	-18.56
-6	7	1	0.00	-5.11
-6	8	1	22.39	19.94
-6	9	1	14.02	-11.94
-6	10	1	16.01	-14.40
-6	11	1	0.00	3.54
-6	12	1	6.79	-2.24
-6	13	1	0.00	-2.57
-7	0	1	7.89	-8.90
-7	-1	1	8.05	-8.55
-7	-2	1	29.20	30.75
-7	-3	1	28.92	35.07
-7	-4	1	0.00	-5.99
-7	-5	1	0.00	-3.50
-7	-6	1	16.90	18.54
-7	-7	1	4.38	9.49
-7	1	1	39.82	43.84
-7	2	1	31.00	35.63
-7	3	1	0.00	-6.14
-7	4	1	36.53	36.58
-7	5	1	48.46	44.55
-7	6	1	20.50	18.44
-7	7	1	27.58	23.57
-7	8	1	27.99	23.74
-7	9	1	8.10	8.22
-7	10	1	0.00	0.23
-7	11	1	23.02	18.78
-7	12	1	18.05	12.49
-7	13	1	7.10	-10.78
-8	0	1	0.00	0.64
-8	-1	1	15.95	15.87
-8	-2	1	7.76	12.40
-8	-3	1	12.51	-17.53
-8	-4	1	6.47	-10.73
-8	-5	1	9.21	13.52
-8	-6	1	3.23	-8.48
-8	1	1	0.00	2.75
-8	2	1	22.80	25.54
-8	3	1	13.92	15.62
-8	4	1	0.00	5.21
-8	5	1	39.01	42.83
-8	6	1	29.62	27.89
-8	7	1	0.00	0.11
-8	8	1	24.10	20.17
-8	9	1	32.10	29.56
-8	10	1	7.46	-6.77
-8	11	1	11.67	-11.20
-8	12	1	25.74	21.03
-8	13	1	24.17	23.90
-9	0	1	0.00	-1.51
-9	-1	1	0.00	7.46
-9	-2	1	0.00	-7.97
-9	-3	1	9.66	-11.48
-9	-4	1	0.00	-2.87
-9	1	1	0.00	-7.24
-9	2	1	0.00	-2.46
-9	3	1	0.00	-6.60
-9	4	1	21.17	-24.42
-9	5	1	0.00	-6.51
-9	6	1	25.13	27.29
-9	7	1	0.00	7.11
-9	8	1	26.35	-25.09
-9	9	1	0.00	-3.01
-9	10	1	14.95	21.17
-9	11	1	5.91	1.03
-9	12	1	0.00	-8.27
-10	0	1	8.53	4.52
-10	-1	1	0.00	1.62
-10	-2	1	12.35	-16.12
-10	1	1	19.69	-24.30
-10	2	1	21.89	-26.28
-10	3	1	7.17	-4.23
-10	4	1	10.24	-11.40
-10	5	1	29.77	-37.48
-10	6	1	20.32	-19.79
-10	7	1	9.88	8.19
-10	8	1	0.00	5.78
-10	9	1	13.91	-11.33
-10	10	1	11.06	-12.11
-10	11	1	0.00	0.15
-11	1	1	4.33	8.74
-11	2	1	10.03	-11.75
-11	3	1	17.23	-20.78
-11	4	1	0.00	-1.53
-11	5	1	0.00	-5.43
-11	6	1	18.14	-17.71
-11	7	1	5.55	-5.18
-11	8	1	5.18	-4.78
-11	9	1	7.89	-5.42
-11	10	1	3.42	-0.54
1	0	1	18.00	-16.83
1	-1	1	71.63	88.03
1	-2	1	9.46	12.10
1	-3	1	53.18	-64.96
1	-4	1	0.00	4.58
1	-5	1	62.96	65.74
1	-6	1	30.35	29.40
1	-7	1	38.27	-36.31
1	-8	1	32.52	33.03
1	-9	1	47.86	52.54
1	-10	1	0.00	9.34
1	-11	1	7.83	5.72
1	-12	1	15.35	17.62
1	-13	1	9.23	13.20
1	1	1	43.36	-47.13
1	2	1	14.59	-7.00
1	3	1	32.55	-27.14
1	4	1	17.55	-30.58
1	5	1	8.90	6.14
1	6	1	18.44	-12.16
1	7	1	48.39	-48.47
1	8	1	11.35	-12.78
1	9	1	11.31	2.83
2	0	1	100.14	-115.05
2	-1	1	74.30	-82.30
2	-2	1	49.14	57.37
2	-3	1	0.00	-1.50
2	-4	1	50.03	-56.34
2	-5	1	42.04	-41.75
2	-6	1	12.92	-10.12
2	-7	1	6.51	-3.60
2	-8	1	10.12	-10.12
2	-9	1	13.43	15.32
2	-10	1	0.00	5.87
2	-11	1	7.98	-3.56
2	-12	1	7.25	5.09
2	-13	1	8.35	8.19
2	-14	1	6.21	-7.37
2	1	1	0.00	-0.71
2	2	1	21.47	-16.79
2	3	1	65.76	-50.07
2	4	1	64.95	-52.60
2	5	1	9.52	-3.07
2	6	1	10.55	-6.00
2	7	1	31.22	-27.00
3	0	1	22.59	-16.55
3	-1	1	76.55	-81.25
3	-2	1	35.78	-42.78
3	-3	1	19.15	13.97
3	-4	1	67.39	-63.37
3	-5	1	53.82	-58.07
3	-6	1	18.74	-20.37
3	-7	1	29.30	-34.46
3	-8	1	47.34	-49.44
3	-9	1	7.75	-3.78
3	-10	1	0.00	-2.22
3	-11	1	22.55	-24.96
3	-12	1	20.96	-24.46
3	-13	1	0.00	6.45
3	-14	1	0.00	4.13
3	1	1	34.79	-30.38
4	0	1	5.59	6.91
4	-1	1	23.10	-19.37
4	-2	1	55.01	-52.31
4	-3	1	0.00	0.16
4	-4	1	9.41	10.99
4	-5	1	41.11	-46.26
4	-6	1	25.52	-29.21
4	-7	1	30.28	28.58
4	-8	1	29.88	-32.80
4	-9	1	58.36	-65.82
4	-10	1	8.10	-8.64
4	-11	1	8.03	11.50
4	-12	1	16.67	-18.82
4	-13	1	26.34	-25.19
4	-14	1	0.00	-3.75
5	0	1	51.10	50.17
5	-1	1	57.03	50.14
5	-2	1	6.07	-6.16
5	-3	1	19.98	-16.44
5	-4	1	47.54	44.14
5	-5	1	43.60	46.56
5	-6	1	5.72	-8.42
5	-7	1	10.03	-7.22
5	-8	1	30.87	36.43
5	-9	1	7.94	-2.79
5	-10	1	29.66	-34.01
5	-11	1	0.00	-3.80
5	-12	1	12.80	10.65
5	-13	1	8.95	-8.27
5	-14	1	4.73	-6.92
6	-1	1	47.55	47.83
6	-2	1	56.98	58.40
6	-3	1	0.00	1.75
6	-4	1	22.85	18.81
6	-5	1	57.75	53.93
6	-6	1	32.53	31.29
6	-7	1	0.00	-0.08
6	-8	1	7.86	10.17
6	-9	1	33.17	26.50
6	-10	1	18.07	17.50
6	-11	1	0.00	1.65
6	-12	1	10.12	11.65
6	-13	1	0.00	0.15
6	-14	1	4.46	-1.78
7	-1	1	24.78	-23.88
7	-2	1	21.78	20.43
7	-3	1	34.16	32.62
7	-4	1	13.16	-10.27
7	-5	1	0.00	7.59
7	-6	1	25.81	25.87
7	-7	1	0.00	0.31
7	-8	1	16.08	14.81
7	-9	1	36.32	30.03
7	-10	1	11.21	15.65
7	-11	1	0.00	2.38
7	-12	1	17.92	18.50
7	-13	1	25.35	26.38
7	-14	1	3.78	2.33
8	-2	1	28.03	-26.96
8	-3	1	0.00	-3.50
8	-4	1	0.00	-6.99
8	-5	1	19.75	-22.13
8	-6	1	11.41	12.07
8	-7	1	14.03	15.70
8	-8	1	21.31	-19.70
8	-9	1	7.94	0.37
8	-10	1	31.22	29.78
8	-11	1	7.03	9.54
8	-12	1	12.26	-13.15
8	-13	1	6.89	7.49
9	-3	1	0.00	-6.57
9	-4	1	0.00	-3.96
9	-5	1	27.56	-26.58
9	-6	1	28.57	-26.93
9	-7	1	11.04	10.15
9	-8	1	7.68	8.32
9	-9	1	27.46	-26.65
9	-10	1	27.42	-23.55
9	-11	1	6.19	7.13
9	-12	1	5.19	-2.86
9	-13	1	10.15	-13.71
10	-6	1	20.05	-22.01
10	-7	1	31.10	-26.58
10	-8	1	5.72	-9.52
10	-9	1	0.00	-3.14
10	-10	1	12.76	-16.02
10	-11	1	16.81	-17.03
10	-12	1	6.51	-9.61
0	-2	2	85.50	84.47
0	-3	2	69.71	-58.16
0	-4	2	50.20	47.80
0	-5	2	79.51	78.25
0	-6	2	23.79	22.78
0	-7	2	20.49	17.83
0	-8	2	28.45	30.19
0	-9	2	31.73	32.30
0	-10	2	0.00	5.76
0	-11	2	12.19	13.66
0	-12	2	15.85	19.50
0	1	2	75.97	-93.90
0	2	2	49.82	53.72
0	3	2	15.08	14.14
0	4	2	51.12	-45.31
0	5	2	23.02	-17.34
0	6	2	0.00	3.46
0	7	2	0.00	-8.35
0	8	2	25.01	-23.05
0	9	2	0.00	2.63
0	10	2	0.00	-0.70
0	11	2	5.02	-16.30
-1	0	2	59.88	89.00
-1	-1	2	16.50	26.60
-1	-2	2	10.51	-8.21
-1	-3	2	27.75	26.78
-1	-4	2	82.75	90.00
-1	-5	2	0.00	6.07
-1	-6	2	0.00	6.46
-1	-7	2	32.11	34.08
-1	-8	2	46.03	45.02
-1	-9	2	0.00	-0.32
-1	-10	2	0.00	-8.07
-1	-11	2	14.60	18.26
-1	-12	2	0.00	8.51
-1	1	2	15.28	15.47
-1	2	2	15.05	-9.51
-1	3	2	94.16	99.67
-1	4	2	32.75	34.51
-1	5	2	14.57	17.77
-1	6	2	39.60	32.64
-1	7	2	23.21	25.61
-1	8	2	0.00	2.38
-1	9	2	10.72	6.05
-1	10	2	24.25	23.74
-1	11	2	0.00	1.45
-2	0	2	9.22	2.37
-2	-1	2	0.00	-0.53
-2	-2	2	18.38	-16.86
-2	-3	2	63.30	59.20
-2	-4	2	36.76	33.05
-2	-5	2	23.35	-20.53
-2	-6	2	13.33	7.69
-2	-7	2	12.56	7.85
-2	-8	2	21.42	-19.15
-2	-9	2	25.96	-24.64
-2	-10	2	13.73	14.43
-2	-11	2	5.92	7.42
-2	-12	2	7.52	-12.29
-2	1	2	69.83	86.71
-2	2	2	54.69	54.71
-2	3	2	67.72	58.59
-2	4	2	67.93	69.32
-2	5	2	7.64	2.52
-2	6	2	13.60	10.02
-2	7	2	63.96	59.35
-2	8	2	29.14	24.02
-2	9	2	0.00	-4.16
-2	10	2	10.53	5.09
-2	11	2	0.00	28.56
-2	12	2	0.00	7.40
-3	0	2	11.85	11.00
-3	-1	2	47.67	-46.75
-3	-2	2	13.04	-11.60
-3	-3	2	34.81	28.71
-3	-4	2	42.96	-43.02
-3	-5	2	6.68	-10.05
-3	-6	2	0.00	-8.54
-3	-7	2	30.19	-31.29
-3	-8	2	30.20	-34.78
-3	-9	2	0.00	-1.73
-3	-10	2	8.55	4.79
-3	-11	2	16.07	-19.46
-3	1	2	21.16	20.78
-3	2	2	39.97	-34.28
-3	3	2	15.02	-18.50
-3	4	2	44.29	46.24
-3	5	2	58.67	54.59
-3	6	2	40.41	-36.79
-3	7	2	20.10	-16.04
-3	8	2	37.52	32.21
-3	9	2	23.12	19.00
-3	10	2	0.00	-1.54
-3	11	2	13.94	10.79
-3	12	2	25.85	19.74
-3	13	2	8.45	8.40
-4	0	2	88.28	-96.96
-4	-1	2	26.00	-25.13
-4	-2	2	15.26	21.50
-4	-3	2	45.65	-46.52
-4	-4	2	49.50	-45.71
-4	-5	2	14.46	-12.10
-4	-6	2	18.50	-19.60
-4	-7	2	15.51	-21.56
-4	-8	2	12.35	-13.91
-4	-9	2	0.00	3.26
-4	-10	2	8.27	-12.82
-4	1	2	13.87	-14.74
-4	2	2	0.00	4.00
-4	3	2	66.19	-67.96
-4	4	2	77.02	-74.85
-4	5	2	11.54	7.85

Table 3 (*cont.*)

-4	5	2	25.25	20.28
-4	7	2	27.32	-32.08
-4	8	2	21.81	-14.68
-4	9	2	0.00	3.12
-4	10	2	0.00	-0.03
-4	11	2	9.94	-6.67
-4	12	2	20.17	16.48
-4	13	2	4.56	5.67
-5	0	2	0.00	-4.35
-5	-1	2	34.22	35.29
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-10	9	3	17.67	14.54
-10	10	3	12.48	11.98
-11	1	3	14.46	-19.95
-11	2	3	5.18	-8.74
-11	3	3	0.00	5.78
-11	4	3	8.25	-7.10
-11	5	3	12.54	-11.31
-11	6	3	6.51	-8.56
-11	7	3	0.00	-5.08
-11	8	3	11.47	-11.11
1	0	3	21.21	-20.13
1	-1	3	22.05	-23.95
1	-2	3	10.41	-9.14
1	-3	3	32.73	-28.54
1	-4	3	73.51	-79.58
1	-5	3	45.50	-54.73
1	-6	3	37.23	38.39
1	-7	3	0.00	1.53
1	-8	3	37.45	-39.52
1	-9	3	15.86	-23.10
1	-10	3	15.50	16.08
1	-11	3	0.00	-5.72
1	-12	3	11.32	-17.32
1	-13	3	0.00	3.52
1	1	3	23.53	24.73
1	2	3	58.35	-52.12
1	3	3	55.92	-75.07
1	4	3	22.57	-16.70
1	5	3	40.25	-33.73
1	6	3	19.49	-22.00
1	7	3	11.02	-9.35
1	8	3	0.00	2.89
2	0	3	13.75	12.35
2	-1	3	55.29	-56.54
2	-2	3	55.21	-52.59
2	-3	3	0.00	-0.73
2	-4	3	9.17	-11.89
2	-5	3	84.45	-96.92
2	-6	3	51.35	-51.33
2	-7	3	17.19	-17.94
2	-8	3	15.93	-13.55
2	-9	3	13.20	-12.12
2	-10	3	19.18	-19.03
2	-11	3	0.00	-9.59
2	-12	3	21.67	-22.12
2	-13	3	0.00	-3.30
2	-14	3	0.00	5.25
2	1	3	6.91	-5.57
2	2	3	52.42	-58.62
2	3	3	6.21	-9.14
2	4	3	5.37	1.37
2	5	3	0.00	1.60
2	6	3	19.05	-13.59
3	0	3	37.60	33.50
3	-1	3	37.17	35.25
3	-2	3	23.19	-19.71
3	-3	3	37.74	-36.96
3	-4	3	12.50	12.71
3	-5	3	0.00	-2.92
3	-6	3	45.58	-43.79
3	-7	3	0.00	3.41
3	-8	3	21.42	-19.85
3	-9	3	20.12	-22.33
3	-10	3	0.00	3.59
3	-11	3	7.57	10.51
3	-12	3	15.67	-19.68
3	-13	3	30.47	-34.33
3	-14	3	0.00	-7.07
4	0	3	5.75	-7.07
4	-1	3	44.17	44.14
4	-2	3	42.69	45.10
4	-3	3	47.44	40.95
4	-4	3	25.77	23.07
4	-5	3	31.29	31.87
4	-6	3	31.10	-26.59
4	-7	3	18.14	-14.68
4	-8	3	55.21	59.61
4	-9	3	21.71	23.86
4	-10	3	24.75	-29.2[illegible]
4	-11	3	0.00	-10.05
4	-12	3	15.70	16.03
4	-13	3	0.00	-2.36
4	-14	3	18.71	-21.26
5	-1	3	43.07	37.71
5	-2	3	55.32	53.56
5	-3	3	17.11	14.56
5	-4	3	0.00	5.07
5	-5	3	38.57	39.65
5	-6	3	61.41	60.06
5	-7	3	7.25	-5.67
5	-8	3	13.06	-15.25
5	-9	3	37.45	37.52
5	-10	3	32.00	36.10
5	-11	3	7.48	2.57
5	-12	3	0.00	2.50
5	-13	3	14.32	10.80
5	-14	3	0.00	2.14
6	-1	3	54.92	-50.31
6	-2	3	15.39	12.51
6	-3	3	49.59	47.91
6	-4	3	17.57	11.08
6	-5	3	14.53	-9.49
6	-6	3	19.61	18.39
6	-7	3	30.39	25.50
6	-8	3	0.00	2.14
6	-9	3	0.00	2.55
6	-10	3	17.25	15.07
6	-11	3	17.94	15.70
6	-12	3	17.52	19.35
6	-13	3	19.93	17.96
6	-14	3	10.93	10.39
7	-2	3	53.42	-52.78
7	-3	3	23.17	-21.17
7	-4	3	7.75	7.75
7	-5	3	0.00	3.45
7	-6	3	0.00	0.92
7	-7	3	0.00	3.95
7	-8	3	25.95	-23.31
7	-9	3	21.84	-22.28
7	-10	3	19.59	17.34
7	-11	3	12.02	8.25
7	-12	3	6.17	-3.64
7	-13	3	0.00	3.39
8	-3	3	21.90	-21.03
8	-4	3	7.82	-5.47
8	-5	3	17.39	-18.56
8	-6	3	34.67	-28.59
8	-7	3	10.85	-9.09
8	-8	3	13.10	12.08
8	-9	3	29.98	-30.89
8	-10	3	33.48	-35.44
8	-11	3	0.00	1.91
8	-12	3	0.00	1.65
8	-13	3	11.07	-9.74
9	-4	3	12.35	-8.53
9	-5	3	0.00	6.24
9	-6	3	0.00	-7.15
9	-7	3	30.02	-24.53
9	-8	3	11.88	-9.42
9	-9	3	13.00	12.24
9	-10	3	20.80	-19.18
9	-11	3	24.57	-22.05
9	-12	3	5.76	-4.82
10	-7	3	0.00	10.12
10	-8	3	0.00	-2.80
10	-9	3	0.00	1.68
10	-10	3	0.00	[illegible]
10	-11	3	5.54	-7.[illegible]
0	0	4	34.67	-36.03
0	-2	4	22.21	19.94
0	-3	4	16.25	11.96
0	-4	4	52.42	-46.50
0	-5	4	30.39	-12.45
0	-6	4	16.64	15.28
0	-7	4	0.00	-1.01
0	-8	4	8.18	-10.58
0	-9	4	0.00	8.22
0	-10	4	3.13	5.35
0	-11	4	0.00	-4.86
0	-12	4	0.00	4.93
0	-13	4	8.16	13.44
0	1	4	20.15	17.75
0	2	4	21.07	-20.15
0	3	4	57.35	-57.97
0	4	4	24.73	-17.59
0	5	4	0.00	3.57
0	6	4	29.73	-25.71
0	7	4	30.50	-28.59
0	8	4	0.00	-3.34
0	9	4	7.25	-7.05
-1	0	4	27.04	-34.02
-1	-1	4	39.35	41.65
-1	-2	4	39.41	37.03
-1	-3	4	36.42	-31.93
-1	-4	4	11.14	9.49
-1	-5	4	44.10	43.42
-1	-6	4	41.78	3.02
-1	-7	4	11.10	-11.91
-1	-8	4	14.33	13.95
-1	-9	4	10.28	-7.79
-1	-10	4	13.43	13.76
-1	-11	4	0.00	2.83
-1	-12	4	8.51	5.88
-1	1	4	0.00	0.89
-1	2	4	35.92	40.10
-1	3	4	8.01	-8.14
-1	4	4	37.92	-40.07
-1	5	4	10.28	-7.79
-1	6	4	15.30	-9.32
-1	7	4	18.53	-15.46
-1	8	4	8.28	-8.91
-1	9	4	0.00	-1.42
-1	10	4	28.47	-23.34
-2	0	4	49.35	53.39
-2	-1	4	49.25	50.72
-2	-2	4	11.82	-3.53
-2	-3	4	0.00	5.90
-2	-4	4	40.19	40.24
-2	-5	4	44.39	45.57
-2	-6	4	7.75	6.24
-2	-7	4	14.17	15.27
-2	-8	4	34.10	41.75
-2	-9	4	0.00	5.50
-2	-10	4	0.00	-3.43
-2	-11	4	0.00	9.25
-2	1	4	24.38	32.56
-2	2	4	15.52	23.03
-2	3	4	25.24	28.74
-2	4	4	20.23	-15.13
-2	5	4	20.21	14.20
-2	6	4	31.90	27.38
-2	7	4	0.00	-4.62
-2	8	4	23.51	-16.53
-2	9	4	17.70	14.95
-2	10	4	24.24	15.77
-2	11	4	9.45	-7.45
-3	0	4	28.23	30.20
-3	-1	4	40.42	43.01
-3	-2	4	11.74	-10.25
-3	-3	4	15.86	12.59
-3	-4	4	27.51	29.59
-3	-5	4	7.73	7.53
-3	-6	4	0.00	2.55
-3	-7	4	22.02	22.38
-3	-8	4	0.00	-10.60
-3	-9	4	13.08	-22.53
-3	-10	4	0.00	2.38
-3	-11	4	7.55	11.85
-3	1	4	11.53	10.53
-3	2	4	34.78	31.00
-3	3	4	74.25	75.33
-3	4	4	29.32	31.94
-3	5	4	25.35	-22.85
-3	6	4	17.77	13.47
-3	7	4	52.14	51.75
-3	8	4	22.00	15.03
-3	9	4	0.00	-2.10
-3	10	4	25.07	16.77
-3	11	4	21.21	16.68
-4	0	4	27.41	25.54
-4	-1	4	37.40	-40.25
-4	-2	4	19.42	-17.45
-4	-3	4	35.00	34.55
-4	-4	4	0.00	-2.60
-4	-5	4	23.17	-23.19
-4	-6	4	0.00	-9.21
-4	-7	4	0.00	-6.09
-4	-8	4	15.25	-18.51
-4	-9	4	0.00	-5.57
-4	-10	4	0.00	-5.54
-4	1	4	24.39	22.55
-4	2	4	39.57	-35.12
-4	3	4	0.00	-3.54

Table 3 (*cont.*)

-4	4	4	61.16	60.07
-4	5	4	30.42	31.14
-4	6	4	17.54	-13.33
-4	7	4	8.27	-5.91
-4	8	4	30.48	24.33
-4	9	4	13.92	9.41
-4	10	4	17.89	14.49
-4	11	4	24.27	20.27
-5	0	4	64.17	-69.57
-5	-1	4	27.08	-33.38
-5	-2	4	23.00	21.77
-5	-3	4	11.34	-9.45
-5	-4	4	35.11	-39.45
-5	-5	4	16.60	-19.71
-5	-6	4	0.00	0.32
-5	-7	4	0.00	-11.99
-5	-8	4	10.45	-17.50
-5	-9	4	0.00	-2.77
-5	1	4	19.85	-18.11
-5	2	4	14.03	7.35
-5	3	4	37.20	-38.75
-5	4	4	19.53	-14.53
-5	5	4	0.00	1.50
-5	6	4	0.00	0.04
-5	7	4	0.00	-8.52
-5	8	4	0.00	0.96
-5	9	4	0.00	-6.41
-5	10	4	19.05	-13.10
-5	11	4	8.49	9.95
-5	12	4	18.77	23.55
-6	0	4	15.80	-16.00
-6	-1	4	8.13	-7.78
-6	-2	4	16.48	-15.98
-6	-3	4	26.30	-32.38
-6	-4	4	0.00	-9.67
-6	-5	4	0.00	8.58
-6	-6	4	7.47	-13.03
-6	-7	4	19.03	-21.96
-6	-8	4	4.13	6.14
-6	1	4	31.97	-38.84
-6	2	4	21.97	-20.79
-6	3	4	28.57	-30.58
-6	4	4	26.39	-23.74
-6	5	4	0.00	7.78
-6	6	4	8.32	-6.51
-6	7	4	40.34	-37.97
-6	8	4	29.43	-20.25
-6	9	4	0.00	6.14
-6	10	4	0.00	-7.57
-6	11	4	23.63	-20.40
-7	0	4	0.00	-9.28
-7	-1	4	8.72	12.14
-7	-2	4	0.00	5.87
-7	-3	4	0.00	-2.97
-7	-4	4	7.51	12.05
-7	-5	4	0.00	-3.69
-7	-6	4	7.75	-9.33
-7	-7	4	0.00	8.85
-7	1	4	14.35	-15.29
-7	2	4	11.65	10.44
-7	3	4	15.48	13.57
-7	4	4	32.10	-29.28
-7	5	4	28.85	-26.48
-7	6	4	14.40	10.57
-7	7	4	0.00	5.15
-7	8	4	40.35	-34.25
-7	9	4	24.32	-18.84
-7	10	4	0.00	-3.53
-7	11	4	10.23	-10.20
-8	0	4	31.26	41.50
-8	-1	4	15.54	24.37
-8	-2	4	0.00	-0.79
-8	-3	4	13.65	15.67
-8	-4	4	13.30	15.58
-8	-5	4	0.00	4.78
-8	1	4	0.00	4.80
-8	2	4	21.80	-21.96
-8	3	4	15.48	17.97
-8	4	4	23.31	23.34
-8	5	4	0.00	-5.46
-8	6	4	17.95	-15.70
-8	7	4	13.45	12.44
-8	8	4	7.35	9.11
-8	9	4	13.28	-10.99
-8	10	4	0.00	-6.03
-8	11	4	0.00	-2.44
-9	0	4	0.00	7.03
-9	-1	4	0.00	-5.51
-9	-2	4	10.10	12.88
-9	-3	4	15.55	19.99
-9	1	4	32.39	35.54
-9	2	4	0.00	10.40
-9	3	4	0.00	-3.70
-9	4	4	0.00	4.48
-9	5	4	14.98	13.37
-9	6	4	7.32	10.58
-9	7	4	16.98	16.92
-9	8	4	27.10	19.33
-9	9	4	0.00	5.52
-9	10	4	0.00	0.89
-10	0	4	0.00	-2.61
-10	-1	4	0.00	2.20
-10	1	4	5.70	3.40
-10	2	4	12.09	10.79
-10	3	4	0.00	1.79
-10	4	4	0.00	4.72
-10	5	4	10.78	11.57
-10	6	4	0.00	5.21
-10	7	4	0.00	5.80
-10	8	4	25.14	25.18
-10	9	4	14.96	16.77
-11	3	4	0.00	-2.52
-11	4	4	0.00	-9.14
-11	5	4	9.00	1.95
-11	6	4	6.22	10.19
1	0	4	7.21	2.70
1	-1	4	49.89	-47.72
1	-2	4	61.57	-59.51
1	-3	4	18.33	-20.25
1	-4	4	19.07	-15.75
1	-5	4	47.32	-52.48
1	-6	4	20.71	-24.05
1	-7	4	0.00	-1.73
1	-8	4	29.03	-31.61
1	-9	4	15.55	-15.23
1	-10	4	0.00	6.81
1	-11	4	0.00	-5.03
1	-12	4	18.51	-22.17
1	-13	4	0.00	-4.66
1	1	4	33.45	-42.22
1	2	4	51.53	-51.58
1	3	4	27.11	-26.23
1	4	4	16.45	13.01
1	5	4	32.63	-28.92
1	6	4	34.01	-27.34
1	7	4	16.42	14.32
2	0	4	10.54	9.03
2	-1	4	23.49	17.08
2	-2	4	0.00	-9.50
2	-3	4	0.00	-4.33
2	-4	4	25.74	-20.34
2	-5	4	35.71	-35.00
2	-6	4	34.05	-38.60
2	-7	4	14.48	12.01
2	-8	4	0.00	0.34
2	-9	4	33.78	-43.47
2	-10	4	23.47	-25.92
2	-11	4	11.12	4.35
2	1	4	34.39	-32.74
2	2	4	29.50	-24.57
2	3	4	16.29	13.48
2	4	4	0.00	1.55
2	5	4	14.31	-12.89
3	0	4	23.14	21.07
3	-1	4	71.43	70.73
3	-2	4	0.00	3.17
3	-3	4	0.00	-6.55
3	-4	4	40.36	42.00
3	-5	4	30.53	33.37
3	-6	4	33.07	-34.57
3	-7	4	27.05	-31.85
3	-8	4	13.67	14.26
3	-9	4	16.46	16.91
3	-10	4	20.36	-23.22
3	-11	4	11.21	-12.87
3	-12	4	0.00	-0.57
3	-13	4	0.00	-9.08
4	0	4	22.96	-16.89
4	-1	4	21.82	18.25
4	-2	4	70.68	70.25
4	-3	4	17.37	15.30
4	-4	4	23.09	-21.65
4	-5	4	35.75	41.57
4	-6	4	39.35	43.03
4	-7	4	0.00	0.64
4	-8	4	0.00	-1.12
4	-9	4	16.55	17.79
4	-10	4	15.54	16.25
4	-11	4	0.00	3.34
4	-12	4	18.81	17.75
4	-13	4	0.00	7.58
5	-1	4	31.78	-29.36
5	-2	4	15.07	-13.81
5	-3	4	33.21	34.57
5	-4	4	26.77	21.95
5	-5	4	0.00	1.78
5	-6	4	31.78	35.81
5	-7	4	22.54	20.44
5	-8	4	16.42	15.39
5	-9	4	24.13	24.99
5	-10	4	24.56	25.70
5	-11	4	0.00	2.00
5	-12	4	5.96	9.70
5	-13	4	27.12	26.21
5	-14	4	9.24	12.39
6	-2	4	0.00	-2.23
6	-3	4	0.00	-4.50
6	-4	4	0.00	-2.42
6	-5	4	16.17	-13.92
6	-6	4	20.05	18.96
6	-7	4	29.81	25.14
6	-8	4	8.36	-5.55
6	-9	4	18.45	-15.35
6	-10	4	19.59	19.57
6	-11	4	23.53	20.66
6	-12	4	0.00	-9.55
6	-13	4	0.00	-3.41
7	-2	4	25.18	-33.52
7	-3	4	11.75	-10.56
7	-4	4	15.51	15.53
7	-5	4	18.61	-18.27
7	-6	4	43.14	-45.22
7	-7	4	15.56	-12.21
7	-8	4	0.00	3.88
7	-9	4	17.31	-15.26
7	-10	4	30.24	-27.57
7	-11	4	0.00	1.87
7	-12	4	0.00	1.50
7	-13	4	11.45	-11.47
8	-4	4	25.77	-25.27
8	-5	4	13.89	11.65
8	-6	4	19.57	-17.12
8	-7	4	40.96	-32.55
8	-8	4	18.70	-18.38
8	-9	4	0.00	-3.70
8	-10	4	19.23	-12.00
8	-11	4	15.53	-13.78
8	-12	4	0.00	-2.97
9	-5	4	0.00	-8.14
9	-6	4	0.00	4.68
9	-7	4	0.00	-1.93
9	-8	4	0.00	0.72
9	-9	4	0.00	4.91
9	-10	4	5.51	-6.55
9	-11	4	12.90	-10.71
10	-9	4	7.37	9.15

Table 4. *Interatomic distances and angles found in the complex ion, and their standard deviations*

Atoms O(1), N(1) *etc.* are those located at the coordinates given in Table 1 and atoms O(1′), N(1′) etc. are those related to this set by the symmetry center at (0, 0, 0).

Cu(1)-O(1)	1·941 ± 0·015 Å	O(1)—Cu(1)-O(2)	78·6 ± 0·8°
-O(2)	2·000	O(1)—Cu(1)-N(2)	93·6
-N(2)	2·007 ± 0·019	N(2)—Cu(1)-N(3)	97·8
-N(3)	2·020	N(3)—Cu(1)-O(2)	88·6
-O(2′)	2·403 ± 0·015	O(2′) -Cu(1)-O(1)	94·1
		O(2′) -Cu(1)-O(2)	90·7
O(1)—N(2)	2·878 ± 0·025	O(2′) -Cu(1)-N(2)	104·5
N(2)—N(3)	3·034	O(2′) -Cu(1)-N(3)	90·0
N(3)—O(2)	2·807		
O(1)—O(2)	2·497		
Cu(2)-O(1)	1·938 ± 0·015	O(1)—Cu(2)-O(2)	79·1
-O(2)	1·983	O(1)—Cu(2)-N(1)	94·7
-N(1)	2·024 ± 0·019	O(2)—Cu(2)-N(4)	93·9
-N(4)	2·011	N(1)—Cu(2)-N(4)	91·9
-O(3)	2·365 ± 0·015	O(3)—Cu(2)-O(1)	97·4
		O(3)—Cu(2)-O(2)	99·4
O(1)—N(1)	2·915 ± 0·025	O(3)—Cu(2)-N(1)	87·4
O(2)—N(4)	2·919	O(3)—Cu(2)-N(4)	86·7
N(1)—N(4)	2·900		
N(1)—C(1)	1·503 ± 0·038	C(1)—N(1)—Cu(2)	112·8 ± 0·9
N(2)—C(2)	1·512	C(2)—N(2)—Cu(1)	112·4
N(3)—C(3)	1·504	C(3)—N(3)—Cu(1)	120·1
N(4)—C(4)	1·517	C(4)—N(4)—Cu(2)	116·4
Cu(1)-Cu(2)	2·782 ± 0·005	N(1) -O(1)—N(2)	126·1 ± 1·0
Cu(1)-Cu(1′)	3·107	N(3) -O(2)—N(4)	131·4
		Cu(1)-O(2)—Cu(1′)	89·3 ± 0·7
		Cu(2)-O(2)—Cu(1′)	127·9

$2C_5H_5N$ (Barclay & Kennard, 1961*b*). In these structures, however, five nearest atoms are coordinated to the copper atom in the form of a tetragonal pyramid and a distorted octahedral coordination around the copper atom is completed by Cu–Cu short contacts of the lengths 2·630 – 2·645 Å. Dimer structures have also been reported in several copper complexes such as in bis (dimethylglyoximato)copper(II) (Frasson, Bardi & Bezzi, 1959), anhydrous copper(II) formate (Barclay & Kennard, 1961*a*) and the β form of anhydrous copper 8-hydroxyquinolinate (Palenik, 1964). In these cases, each of the fifth bonds lying in the direction of the axis of the 5-coordination pyramid joins a pair of molecules together.

Bond lengths and angles found in the present structure determination are listed in Table 4 with their standard deviations. Some of these values are also given in Fig. 1(*b*). Within the rectangular coordination groups all the copper–nitrogen bond distances are in the range $2{\cdot}00_7$ to $2{\cdot}02_4$ Å, being typical values found in other copper complexes. Freeman, Robinson & Schoone (1964) tabulated the copper–nitrogen distances in peptide complexes, and found that the distances for copper–amino nitrogen are in the range of 1·984 – 2·045 Å and those for copper–peptide nitrogen atoms are in the range of slightly smaller values, 1·867 – 1·938 Å. The copper–oxygen distances within the rectangular coordination groups found in the present study are $1{\cdot}94_1$ and $1{\cdot}93_8$ Å for those involving O(1), while significantly longer distances of $2{\cdot}00_0$ and $1{\cdot}98_3$ Å are found for Cu(1)–O(2) and Cu(2)–O(2). Although all these bond distances are within the range of reported values (Jaggi & Oswald, 1961; Barclay & Kennard, 1961*a*, *b*; Jarvis, 1961; Freeman *et al.*, 1964), the long distances would be explained by the fact that the O(2) atom is bonded to the third copper atom Cu(1′), which causes the displacement of the O(2) atom.

The four ligands in each of the rectangular coordination groups take the approximately planar configuration. The equation of the least squares plane through atoms Cu(1), O(1), O(2), N(2) and N(3) is

$$0{\cdot}7061X+0{\cdot}3696Y-0{\cdot}0985Z=1{\cdot}2010,$$

and that through atoms Cu(2), O(1), O(2), N(1) and N(4) is

$$0{\cdot}9950X-0{\cdot}4839Y-0{\cdot}0360Z=0{\cdot}3168,$$

where X, Y and Z denote the coordinates referred to the triclinic axes expressed in Å. The former corresponds to the plane of the base of the pyramidal coordination around Cu(1) and the latter that around the Cu(2) atom. The deviations of atoms from the planes are listed in Table 5. It is seen that each copper atom lies slightly out of the basal plane in the direction of the fifth ligand. This trend is similar to that found in other structures containing copper(II) atoms with tetragonal pyrimidal arrangement of ligands (Frasson, Bardi & Bezzi, 1959; Barclay & Kennard, 1961*a*; Freeman *et al.*, 1964). The oxygen atom O(2) is twisted out from the plane of the binuclear ion in such a way that a close approach to the copper atom Cu(1′) is attained.

Table 5. *Deviations of the atoms from the least-squares planes*

Through atoms Cu(1), O(1), O(2), N(2), N(3).		Through atoms Cu(2), O(1), O(2), N(1), N(4).	
Cu(1)	−0·142 Å	Cu(2)	0·068 Å
O(1)	−0·055	O(1)	0·011
O(2)	0·123	O(2)	−0·044
N(2)	0·112	N(1)	−0·042
N(3)	−0·038	N(4)	0·006

The copper atom Cu(1) forms four normal bonds in the basal plane of the coordination pyramid and a fifth longer bond ($2{\cdot}40_3$ Å) to the O(2′) atom of another complex ion related first by a center of symmetry. A water oxygen atom lies at the apex of the coordination pyramid formed by the Cu(2) atom. The lengths of these bonds, Cu(1)–O(1′), $2{\cdot}40_3$ Å and Cu(2)–O(3), $2{\cdot}36_5$ Å, are in good agreement with those found in other 5-coordination copper complexes.

Other atoms are found at rather short distances from the copper atom in the opposite direction to the apex of the pyramid. These are Cu(1) · · · O(3), $3{\cdot}22_9$ Å; Cu(2) · · · N(3′), $3{\cdot}64_9$ Å; Cu(2) · · · C(3′), $3{\cdot}69_6$ Å. Neither the distance nor the direction corresponds to a possible bond, however. The methyl group $C(3')H_3$ is situated just at the opposite position to the fifth ligand of the Cu(2) atom. The puckering of the binuclear complex ion seems to occur due to the steric effect between the copper and the bulky methyl group.

The C–N distances found in the four methylamine molecules are $1{\cdot}50_3$, $1{\cdot}51_2$, $1{\cdot}50_4$, $1{\cdot}51_7$ Å. The average value $1{\cdot}51_2$ Å is in good agreement with the sum of the single-bond radii, 0·77 Å for carbon and 0·74 Å for nitrogen atoms. In solid methylamine the value of 1·48 Å has been reported at −150 °C. (Atoji & Lipscomb, 1953).

The structure of the sulfate ion

The bond distances and angles for the sulfate ion are listed in Table 6. It will be seen that the SO_4 tetrahedron is quite regular, with a mean S–O bond length of $1{\cdot}47_8$ Å in good agreement with the value of 1·474 Å found in $FeSO_4 . 7H_2O$ (Baur, 1964*a*) and 1·473 Å in $MgSO_4 . 4H_2O$ (Baur, 1964*b*).

Table 6. *Bond lengths and angles for the sulfate ion and their standard deviations*

S–O(4)	1·486 ± 0·016 Å	O(4)–S–O(5)	108·5 ± 1·1°
–O(5)	1·495	O(4)–S–O(6)	108·0
–O(6)	1·466	O(4)–S–O(7)	110·1
–O(7)	1·464	O(5)–S–O(6)	109·3
		O(5)–S–O(7)	109·2
mean	1·478	O(6)–S–O(7)	111·7

Hydrogen bonds and framework features

Two projections of the structure, along the *c* axis and the *a* axis, are shown in Figs. 2 and 3. In these figures, the hydrogen bonds are shown by chain lines and the bonds involved in the copper coordination groups by solid lines. In Fig. 2 some of the interatomic short contacts are shown by dotted lines. The distances of hydrogen bonds are listed in Table 7. It can be seen from the figures that the discrete units of dimer complex ions are situated near to the corners of the unit cell and surrounded by sulfate ions. They are connected to sulfate ions through several hydrogen bonds. There is no hydrogen bond linking the complex ions directly to one another. Important hydrogen bond systems are the following three:

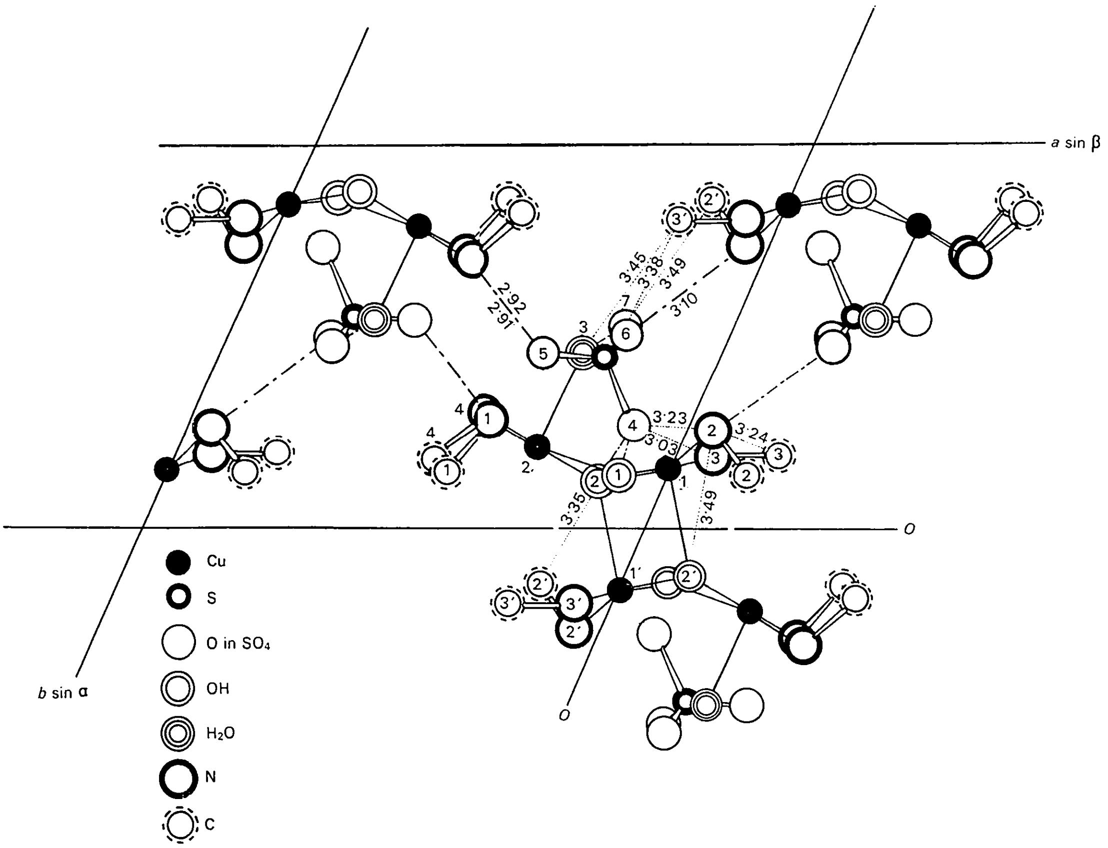


Fig. 2. Projection of the structure along the *c* axis, illustrating the structure and packing of the columnar units formed by the dimer complex ions and sulfate groups. Hydrogen bonds, copper coordination bonds and interatomic short contacts are shown by chain lines, solid lines and dotted lines, respectively.

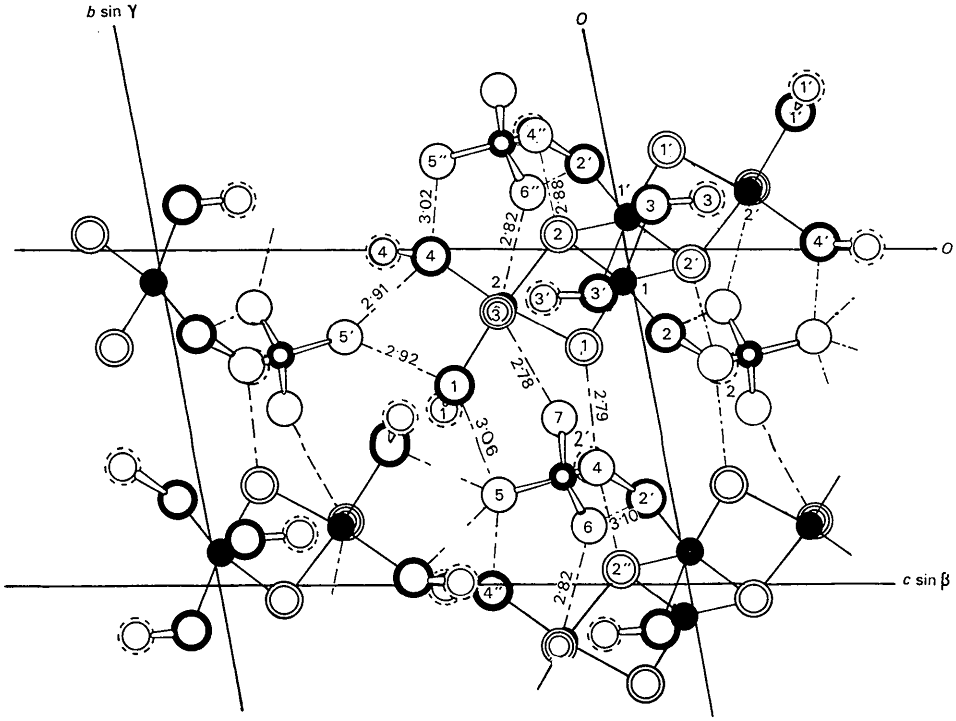
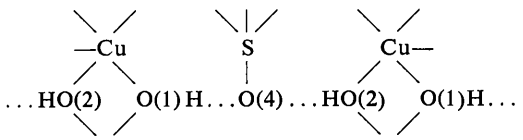
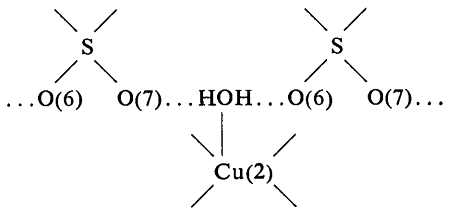
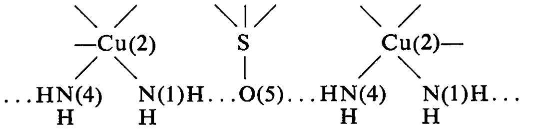


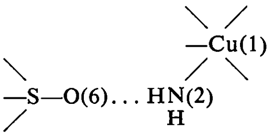
Fig. 3. Projection of the structure along the *a* axis, showing the linking of complex ions through sulfate groups. Hydrogen bonds are drawn by chain lines and copper coordination bonds by solid lines.



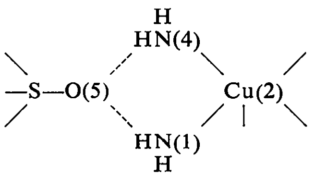




The complex ions are bound together by these hydrogen bonds to form a chain of alternating complex ions and sulfate ions. As the complex ions are linked to each other through the fifth coordination bonds of the copper atoms, two of these chains are joined together forming a column of the dimer complex ions. As seen in Fig. 2, which shows a cross section of the column, sulfate ions act as a bridge between the dimers which pile up along the *c* axis with their rectangular coordination plane faced parallel to **c**. It is also seen that the structure consists of the columns packed parallel to the *c* axis. Between the columns there are several hydrogen bonds and short contacts which hold the columns within the crystal. Among them the following two hydrogen bond systems are important.



parallel to [100]



parallel to [110]

The interatomic short distances less than 3·5 Å are shown in Fig. 2.

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Table 7. *Hydrogen bond distances and angles*

Atoms O(1), N(1) *etc.* are those located at the coordinates given in Table 1; atoms O(1′), N(1′) *etc.* are those related to this set by the symmetry center, and atoms O(1″), N(1″) *etc.* by translations.

O(1) ··· O(4)	2·787 ± 0·025 Å	Cu(1) –O(1) ··· O(4)	113·1 ± 1·0°
O(2) ··· O(4″)	2·882	Cu(2) –O(1) ··· O(4)	117·8
O(3) ··· O(6″)	2·817	Cu(1) –O(2) ··· O(4″)	106·5
O(3) ··· O(7)	2·777	Cu(2) –O(2) ··· O(4″)	117·5
N(1) ··· O(5)	3·060	Cu(1′)–O(2) ··· O(4″)	112·9
N(1) ··· O(5′)	2·920	O(7) ··· O(3) ··· O(6″)	127·2 ± 1·0
N(2′) ··· O(6)	3·100	Cu(2) –O(3) ··· O(7)	104·8 ± 1·0
N(4) ··· O(5′)	2·907	Cu(2) –O(3) ··· O(6″)	107·1
N(4) ··· O(5″)	3·023	C(1) —N(1) ··· O(5)	109·3 ± 1·2
		C(1) —N(1) ··· O(5′)	112·8
		C(2′) –N(2′) ··· O(6)	98·8
		C(4) —N(4) ··· O(5′)	100·1
		C(4) —N(4) ··· O(5″)	119·7