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The Crystal Structure of Copper Mercury Oxynitrate Trihydrate, $Cu(NO_3)_2 . HgO . 3H_2O$

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The crystal structure of copper(II) mercury(II) oxynitrate trihydrate has been determined by single-crystal three-dimensional X-ray analysis. There are two formula units in the monoclinic unit cell of dimensions $a=7{\cdot}33$, $b=8{\cdot}87$, $c=6{\cdot}75$ Å, $\beta=112°32'$ and space group $P2_1/c$. The copper ion is coordinated by two oxygen atoms from two nitrate ions at 2·14 Å, two oxygen atoms from two hydroxide ions at 2·15 Å and two oxygen atoms from two water molecules at 2·02 Å in an octahedron. Both hydroxide ions and both water molecules belong simultaneously to the mercury ion, at 2·30 and 2·54 Å respectively, whose octahedral coordination is completed with nitrate-oxygen atoms at 2·78 Å. The octahedra about copper and mercury are linked alternately by sharing two opposite edges along the *c* axis as well as two opposite corners along the *b* axis. The solution of the structure shows that the best definition of the chemical formula of this compound is $HgCu(OH)_2(NO_3)_2 . 2H_2O$.

Introduction

Among various basic salts there is a large group of those with the general formula $mMX_2 . nHgO . xH_2O$ where M = Ca, Sr, Ba, Mn, Co, Ni, Cu, Zn, Cd, Hg, and X = Cl^-, Br^-, NO_3^-, SO_4^{2-}, SeO_4^{2-}, ClO_3^-, BrO_3^-. (André, 1887; Maihle, 1902; Finzi, 1913; Denk & Dewald, 1951; Denk, Leschhorn & Rosmer, 1962; Denk & Leschhorn, 1966). With the exception of mercury oxyhalides, basic mercuric sulphates, chlorate and bromate where M = Hg, the structures of other salts are still unknown (Grdenić, 1965).

We have undertaken the crystal-structure investigation of the basic nitrate $Cu(NO_3)_2 . HgO . 3H_2O$ in order to establish to which structural type it belongs (Basset, 1947). It was particularly interesting to find out the coordination about mercury in the presence of another metal. At the same time, in spite of many solved structures, the stereochemistry of copper still attracts attention. Not of less interest have been also the ligand properties of the nitrate ion, particularly since Wallwork & Addison (1965) proposed its bidentate character in the structure of anhydrous α-copper(II) nitrate.

Experimental

$(NO_3)_2Hg . CuO . 5H_2O$ is reported to have been obtained by dissolving mercuric oxide in an aqueous solution of cupric nitrate (Maihle, 1902). By the same method $Cu(NO_3)_2 . HgO . 3H_2O$ was prepared in the form of pale blue needle-shaped crystals ((Finzi, 1913). All our attempts to prepare both compounds have always resulted in the trihydrate.

The crystal data are as follows:

$a=7{\cdot}33\pm0{\cdot}02$ Å	Formula weight 458·2
$b=8{\cdot}87\pm0{\cdot}02$	$V=405{\cdot}3$ Å^3
$c=6{\cdot}75\pm0{\cdot}02$	$\varrho_m=3{\cdot}74$ g.cm^{-3}
$\beta=112°32'\pm15'$	$\varrho_x=3{\cdot}75$ g.cm^{-3}
Space group $P2_1/c$	$Z=2$

The cell parameters were measured from oscillation and Weissenberg photographs. Density was determined pycnometrically. The systematic absence of reflexions *h*0*l* for *l* odd and 0*k*0 for *k* odd uniquely determined the space group as $P2_1/c$. Except for some weak reflexions, all *hkl* reflexions fulfil the condition $k+l=2n$ required by the special positions of the heavy atoms. Three-dimensional intensity data (*h*0*l* ... *h*6*l*, *hk*0 ... *hk*6) were recorded on integrated equi-inclination Weissenberg photographs with multiple films with Cu $K\alpha$ radiation and determined photometrically. Within the limiting sphere 526 independent reflexions were strong enough to be observed. After correction for Lorentz and polarization factors, the intensities were placed on the same

relative scale. The crystal was spherically ground to 0·1 mm in diameter and the intensities were corrected for absorption ($\mu r = 2{\cdot}06$). Calculations were carried out on the Ferranti MERCURY computer at the University of Sheffield and on the Science Research Council ATLAS computer at Didcot.

Table 1. *Observed and calculated structure factors*

The values listed are $50F_o$ and $50F_c$.

h	k	l	F_o	F_c	h	k	l	F_o	F_c	h	k	l	F_o	F_c
0	0	2	8061	8868	1	1	−7	1743	1705	1	6	−2	5689	5478
		4	4612	4935			−5	2134	2109			−1	1461	1315
		6	2736	3099			−4	1105	42			0	4911	5038
0	1	1	4493	3964			−3	4584	4670			1	1345	928
		2	4488	−3572			−2	3688	−3175			2	5569	4660
		3	4287	3891			−1	4571	4270			4	3717	3469
		5	2835	2398			0	2004	−1773			6	1055	1863
		7	1348	1203			1	4330	4203	1	7	−5	1690	1692
0	2	0	8134	8080			2	1678	−638			−3	2885	2515
		2	7444	6892			3	3278	3006			−1	3484	2990
		3	1177	602			4	1353	1141			1	1547	2417
		4	6461	5826			5	3099	2850			3	3554	1958
		5	927	−722			7	973	993			5	1182	1490
		6	3749	3473	1	2	−8	1913	1904	1	8	−6	1161	1833
0	3	1	5384	5007			−6	3566	3450			−4	3140	3144
		2	1391	−995			−5	636	781			−2	3917	3556
		3	3975	3348			−4	5820	5426			0	3176	3066
		4	1179	778			−2	6951	6636			2	3345	2918
		5	2483	2285			0	8717	9932			4	2134	2469
		7	1262	1434			1	1220	310	1	9	−5	836	1120
0	4	0	6306	5784			2	8988	8392			−3	1312	1647
		1	1433	−679			3	2080	945			−1	1605	1554
		2	8375	7550			4	6018	4951			1	1426	1597
		4	5733	4980			6	3132	2680			3	1407	1371
		6	2967	2740	1	3	−7	1426	1414	1	10	−4	1482	1888
0	5	1	3019	2537			−5	2725	2597			−2	2599	2348
		2	1374	596			−3	3868	3458			0	2415	2697
		3	2626	2653			−2	1189	−793			2	2138	2165
		5	2010	2077			−1	5466	4666	1	11	−1	947	1287
		7	1153	1316			0	2765	2271			1	870	1422
0	6	0	5155	4974			1	4368	3854	2	0	−8	1827	2111
		1	1494	392			3	3658	2992			−6	2963	3792
		2	5683	5169			4	1330	567			−4	4955	6074
		4	3916	3511			5	2075	1770			−2	5797	6496
		6	2064	2310			7	1282	1280			0	6753	7927
0	7	1	2584	3117	1	4	−6	3354	3162			2	9646	10078
		2	985	579			−4	5007	4217			4	5532	4322
		3	2670	2067			−3	1253	588			6	2201	2289
		5	1234	1328			−2	8115	7694	2	1	−7	1987	2197
0	8	0	4421	4398			−1	1629	−281			−5	2066	2215
		2	3918	3475			0	8122	8492			−3	3836	3920
		4	2328	2315			1	798	−611			−2	1395	−972
0	9	1	1340	1740			2	7268	6517			−1	4323	4267
		3	1565	1408			4	4911	4142			0	2186	2186
		5	511	1040			6	2297	2202			1	4550	4318
0	10	0	2193	2640	1	5	−7	1025	1320			3	3089	2605
		2	2313	2246			−5	2197	2276			4	1348	−809
0	11	1	1040	1264			−3	2224	1758			5	2369	2105
1	0	−8	1306	1648			−2	1177	598			7	788	944
		−6	3544	3632			−1	2952	2881	2	2	−8	1743	1843
		−4	7423	8612			1	3355	3278			−6	3432	3398
		−2	6704	9083			2	1397	−562			−4	5959	6122
		0	7055	9324			3	3121	2927			−3	1122	1297
		2	6953	6325			5	1517	1207			−2	8062	8397
		4	6169	4858	1	6	−6	2248	2414			−1	883	591
		6	3965	3742			−4	3936	3526			0	8084	8884

h	k	l	F_o	F_c	h	k	l	F_o	F_c	h	k	l	F_o	F_c
2	2	1	1402	792	3	0	−2	8666	9927	3	8	−4	2983	2809
		2	7591	6789			0	5548	5918			−2	3879	3965
		4	4746	3827			2	4957	5228			0	3231	3502
		6	2408	2447			4	2782	2994			2	2239	2307
2	3	−7	1580	1431			6	1365	1851			4	1184	1609
		−5	2653	2600	3	1	−7	1931	1973	3	9	−5	1381	1154
		−4	1337	589			−5	2264	2582			−3	1381	1556
		−3	3748	3550			−4	1095	842			−1	1723	1973
		−1	4039	3781			−3	2943	3086			1	1534	1536
		0	2686	2301			−2	1046	−529			3	764	1153
		1	2908	3147			−1	4408	4702	3	10	−2	1723	2204
		2	1324	−502			0	1892	−1726			0	1714	1868
		3	2866	2513			1	3614	3739			2	523	1825
		5	1816	1844			3	2590	2682	4	0	−8	2080	2065
2	4	−6	3332	3296			5	1379	1533			−6	3309	3680
		−4	5647	5212	3	2	−8	2070	1978			−4	4469	4721
		−2	7019	6832			−6	3337	3625			−2	5632	5754
		0	6322	6542			−4	5565	5795			0	4286	4394
		2	4702	3980			−3	1855	1648			2	4574	4246
		4	4489	4152			−2	7117	7398			4	2953	3614
		6	1851	2331			−1	1485	1141	4	1	−7	1472	1649
2	5	−7	981	954			0	6600	6797			−5	2644	3088
		−5	2231	2198			2	6734	6088			−4	1085	−380
		−3	2581	2586			4	4251	3851			−3	2978	3108
		−2	1217	−613			6	1657	2207			−2	1037	−16
		−1	3351	3604	3	3	−7	1704	1719			−1	3604	3463
		1	2949	2963			−5	2476	2342			1	2623	2692
		3	2510	2424			−3	3506	3393			2	1406	1220
		5	1251	1428			−2	1048	−750			3	1738	2321
2	6	−6	2519	2631			−1	2923	2729			5	1008	1171
		−4	4103	3753			1	2615	2687	4	2	−8	2159	1996
		−2	5352	5151			3	2498	2291			−6	3181	3283
		−1	1144	1565			5	1398	1497			−4	4760	4771
		0	5428	5393	3	4	−8	1916	1811			−2	6799	6805
		2	4536	3854			−6	3232	3198			0	6062	6326
		4	3005	2888			−4	4963	4617			1	1212	638
2	7	−5	1773	1888			−2	4884	4431			2	5830	4974
		−3	1871	2050			0	6448	6587			4	3231	2885
		−1	2790	2179			2	5576	5042	4	3	−7	1693	1742
		1	2138	2009			4	3279	3032			−5	2109	1995
		3	2184	1937			6	928	1463			−3	2768	2558
		5	731	995	3	5	−7	1099	1211			−1	2797	2724
2	8	−6	1599	2023			−5	2086	2191			1	2749	2588
		−4	2777	2472			−3	3298	3075			3	1604	1551
		−2	3198	3169			−1	3197	2826			5	940	1169
		0	3428	3692			0	1338	1064	4	4	−8	1829	1702
		2	3553	3665			1	2690	2788			−6	2870	2841
		4	1969	2134			3	2286	2292			−4	4916	4761
2	9	−5	1014	1037			5	1126	1462			−2	5729	5486
		−3	1344	1429	3	6	−6	2890	2729			0	4953	4869
		−1	2169	1692			−4	3801	3950			2	3830	3380
		1	1525	1933			−2	4720	4452			4	1983	1893
		3	1096	1466			0	4717	4848	4	5	−7	1240	1495
2	10	−2	2305	2525			2	3362	3261			−5	1745	1584
		0	2070	2143			4	2402	2654			−3	2704	2646
		2	1541	1831	3	7	−5	1532	1538			−1	2823	2777
2	11	−1	699	1175			−3	1379	1649			1	2618	2605
3	0	−8	2072	2018			−1	2601	2037			3	1488	1421
		−6	2805	3263			1	1665	1706	4	6	−6	2326	2548
		−4	4916	5736			3	1047	1375			−4	3660	3691

Table 1 (*cont.*)

h	k	l	F_o	F_c	h	k	l	F_o	F_c	h	k	l	F_o	F_c
4	6	−2	4004	3691	5	6	−6	2154	2298	7	0	0	3150	3092
		0	4257	4301			−4	3710	3389	7	1	−7	1216	1400
		2	3090	3301			−2	3844	3760			−5	1522	1705
		4	1429	1994			0	3446	3368			−3	1971	1900
4	7	−5	1478	1464			2	2236	2548			−1	1607	1478
		−3	2001	1919	5	7	−5	1180	1222			1	979	1363
		−1	1914	1620			−3	1866	1472	7	2	−6	2877	2178
		1	1460	1389			−1	1044	1292			−4	2909	2704
		3	1031	1309			1	1655	1590			−2	2903	2593
4	8	−4	2715	2855	5	8	−2	2383	2786			0	2805	2518
		−2	2730	2891			0	2515	2880			2	1455	2000
		0	2675	2869			2	1001	1845	7	3	−7	991	1077
		2	1813	2186	5	9	−3	1179	1093			−5	1455	1507
4	9	−3	1264	1259	6	0	−8	1516	1648			−3	1885	1903
		−1	1369	1450			−6	2430	2787			−1	2105	2046
		1	1181	1259			−2	4140	3848			1	1090	1355
4	10	0	1754	1990			0	4128	4164	7	4	−6	2102	2183
5	0	−8	2056	1939			2	2262	2698			−4	3031	2797
		−6	2937	3084			4	865	1560			−2	3309	2974
		−4	3696	3891	6	1	−7	1333	1369			0	2445	2332
		−2	5034	5167			−5	1900	1968			2	1190	1370
		0	5554	5708			−3	2650	2679	7	5	−5	1312	1386
		1	2919	2470			−1	2510	2241			−3	1136	1187
		3	1283	1658			1	1972	1526			−1	1274	1107
5	1	−7	1401	1487			3	787	1186	7	6	−4	2117	2135
		−5	2307	2552	6	2	−8	1804	1669			−2	2301	2543
		−4	769	133			−6	2878	2684			0	1777	2169
		−3	2603	2513			−5	1084	960	7	7	−3	984	1221
		−2	1445	1091			−4	3933	3465			−1	855	1283
		−1	2572	2625			−2	3987	3589	8	0	−6	1907	1793
		1	2919	2470			0	3351	3118			−4	2490	2445
		3	1283	1658			2	2118	2248			−2	2431	2389
		5	635	693	6	3	−7	1312	1362			0	1713	1753
5	2	−8	2287	1834			−5	1851	2043	8	1	−5	1219	1244
		−6	3027	3031			−3	1758	1838			−3	1323	1414
		−4	4442	4332			−1	2125	2077			−1	1368	1493
		−2	6112	5472			1	1780	2077	8	2	−6	2150	1714
		−1	1646	1010			3	1149	1383			−4	2091	2092
		0	4628	4592	6	4	−6	2527	2293			−3	930	829
		2	3034	2943			−4	2881	2962			−2	2260	2084
		4	1711	1927			−2	4305	4106			−1	1171	687
5	3	−7	1554	1538			0	3761	3673			0	1966	1893
		−5	2006	2151			2	2286	2613	8	3	−5	1217	1395
		−3	2632	2504	6	5	−7	1278	1227			−3	1506	1606
		−1	2855	2576			−5	1717	1638			−1	1113	1113
		0	1245	−1026			−3	1929	1523	8	4	−4	2290	1962
		1	2168	1943			−2	1262	871			−2	2204	1991
		3	1663	1665			−1	1642	1470			0	1742	1963
5	4	−6	2985	2841			1	1000	1138	8	5	−3	962	985
		−4	4054	3823	6	6	−6	1760	2228			−1	826	922
		−2	4315	3925			−4	2855	2900	9	0	−4	1639	1503
		0	3306	3191			−2	2931	3041			−2	1296	1533
		2	3549	3579			0	2265	2258	9	1	−5	1075	1166
		4	1546	2342	6	7	−3	1666	1405			−3	1282	1181
5	5	−7	1122	1407			−1	1383	1592			−1	682	1007
		−5	1603	1570	6	8	−2	2678	2398	9	2	−4	1918	1618
		−3	2599	2412			0	1749	1947			−2	1647	1636
		−1	2274	2398	7	0	−6	2398	2144	9	3	−3	1066	936
		1	1467	1614			−4	3170	2929					
		3	952	1062			−2	3416	3298					

Structure determination

Three Patterson projections, obtained by means of the Von Eller photosommateur, proved that the mercury and copper atoms occupy the 2(*a*) and 2(*c*) special positions respectively. A three-dimensional difference synthesis computed on the basis of mercury and copper atom positions enabled the preliminary locations of all light atoms to be found. The structure was then refined by four cycles of the least-squares method assuming isotropic thermal motion and with the data uncorrected for absorption. At this stage of refinement the reliability index was $R = 0{\cdot}129$. After absorption corrections the refinement process was continued with the anisotropic thermal parameters. Unit weight was used for all observations. The final reliability index for observed reflexions was $R = 0{\cdot}109$. Table 1 lists the observed structure amplitudes and calculated structure factors based on the final atomic coordinates given in Table 2. Atomic scattering factors used for mercury and copper were those of Thomas & Umeda (1957) and for oxygen and nitrogen those of Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955). The thermal parameters are given in Table 3.

Description and discussion of the structure

The crystal structure contains two water molecules per formula unit. The previously assumed third water mol-

ecule is present together with the oxide oxygen in the form of the hydroxide ions. The hydroxide ion, and water molecules are distinguished in the structure according to the possible directions of hydrogen bonds, as well as by considering the distances and angles of hydrogen-bonded oxygen atoms. Consequently, the compound is appropriately defined by the formula $HgCu(OH)_2(NO_3)_2.2H_2O$.

The structure is built up of the octahedra about copper and mercury ions. An idealized general view of the structure is given in Fig. 1. The copper ion is centrosymmetrically coordinated by two oxygen atoms from two water molecules (Cu–OH_2, 2·02 Å), two oxygen atoms from two nitrate ions (Cu–ONO_2, 2·14 Å), and two hydroxide ions at a distance of 2·15 Å. The characteristic coordination of mercury is digonal (Grdenić, 1965) with two centrosymmetrically related hydroxo oxygen atoms at 2·30 Å, which is slightly less than the sum of the ionic radii. The effective coordination about mercury is completed by two centrosymmetrically related oxygen atoms from two nitrate ions (Hg–ONO_2, 2·78 Å) as well as by two water-oxygen atoms at 2·54 Å. The octahedra about copper and mercury are linked alternately by having common edges (the hydroxide and water-oxygen atoms) along the *c*-axis direction as well as common corners (the O(1) nitrate oxygen atoms) along the *b*-axis direction. The adjacent rows of octahedra are linked together by hydrogen bonds. The water oxygen is linked by one hydrogen bond (HO–H···O(2), 2·88 Å) with the adjacent rows along the *c* axis are linked together along the *b* axis in a zigzag manner by means of nitrate-oxygen.

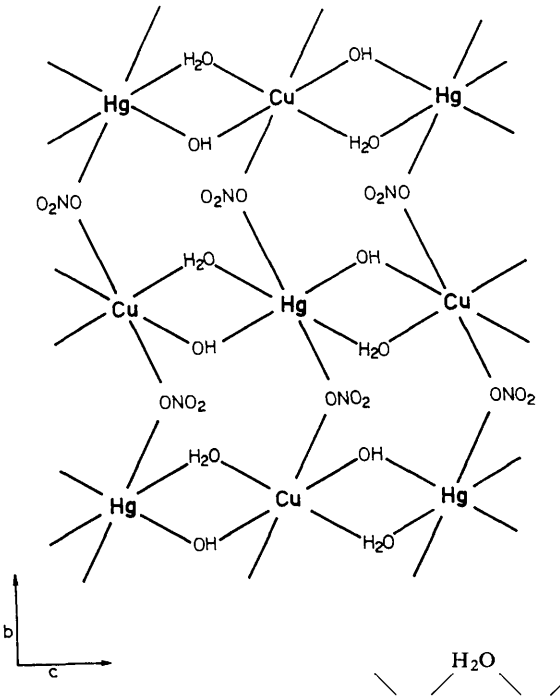


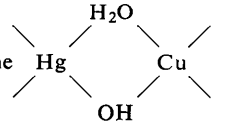
Fig. 1. General view of the structure. The 

Table 2. *Positional parameters in fractional coordinates and their estimated standard deviations*

	x/a	*y/b*	*z/c*	σ_x	σ_y	σ_z
Hg	0·000	0·000	0·000	—	—	—
Cu	0·000	0·000	0·500	—	—	—
O(1)	0·154	0·290	0·044	0·006	0·005	0·011
O(2)	0·399	0·127	0·110	0·006	0·004	0·006
O(3)	0·430	0·364	0·097	0·007	0·006	0·009
O(OH)	−0·172	0·402	0·164	0·007	0·007	0·006
$O(H_2O)$	−0·180	0·101	0·228	0·008	0·006	0·006
N	0·337	0·263	0·095	0·007	0·007	0·007

Table 3. *Thermal parameters and their estimated standard deviations*

The temperature factor is of the form

$$\exp[-(b_{11}h^2+b_{22}k^2+b_{33}l^2+b_{23}kl+b_{13}hl+b_{12}hk)].$$

	b_{11}	b_{22}	b_{33}	b_{23}	b_{13}	b_{12}
Hg	0·0157	0·0078	0·0164	0·0021	0·0119	−0·0107
	(0·0005)	(0·0003)	(0·0006)	(0·0022)	(0·0009)	(0·0020)
Cu	0·0189	0·0103	0·0193	−0·0110	0·0064	0·0265
	(0·0022)	(0·0013)	(0·0023)	(0·0054)	(0·0036)	(0·0049)
O(1)	0·0056	0·0044	0·0929	0·0151	0·0141	0·0043
	(0·0081)	(0·0050)	(0·0300)	(0·0209)	(0·0251)	(0·0110)
O(2)	0·0237	0·0033	0·0176	0·0027	−0·0248	0·0009
	(0·0110)	(0·0044)	(0·0104)	(0·0117)	(0·0172)	(0·0122)
O(3)	0·0195	0·0134	0·0525	−0·0047	0·0339	0·0108
	(0·0115)	(0·0074)	(0·0207)	(0·0221)	(0·0259)	(0·0166)
O(OH)	0·0295	0·0275	0·0076	−0·0061	0·0049	0·0311
	(0·0137)	(0·0110)	(0·0090)	(0·0172)	(0·0181)	(0·0212)
$O(OH_2)$	0·0383	0·0165	0·0123	−0·0008	0·0019	−0·0402
	(0·0158)	(0·0082)	(0·0100)	(0·0155)	(0·0208)	(0·0201)
N	0·0143	0·0234	0·0140	0·0205	−0·0325	−0·0330
	(0·0114)	(0·0111)	(0·0122)	(0·0201)	(0·0187)	(0·0198)

jacent nitrate ion and by another (HO–H···OH, 2·71 Å) with the hydroxide oxygen. The hydroxide oxygen is hydrogen-bonded (O–H···O(3), 2·80 Å) to the oxygen atom from the same adjacent nitrate ion. The arrangements of the octahedra are shown in Figs. 2 and 3 projected down the *c* and *a* axes respectively. Some interatomic distances and angles together with standard deviations (*International Tables for X-ray Crystallography*, 1959) are listed in Table 4.

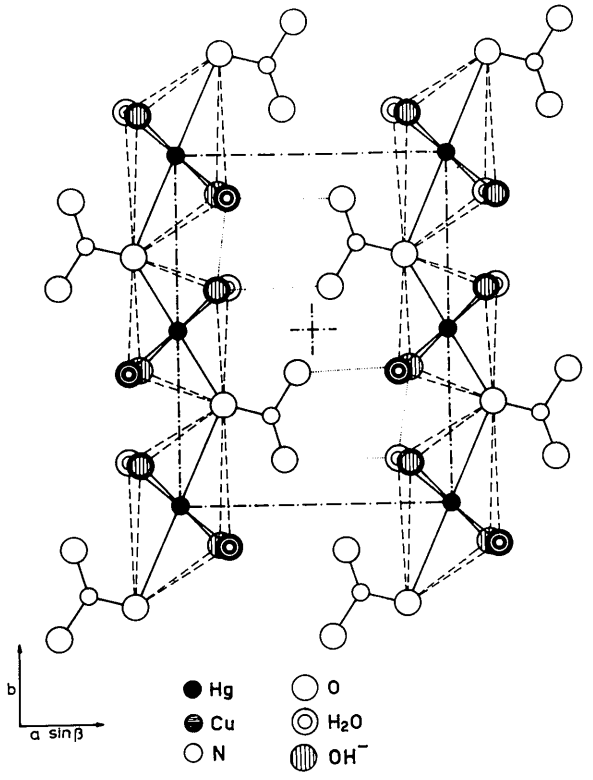


Fig. 2. The arrangements of the octahedra about mercury and copper ions projected along the *c* axis. The hydrogen bonds are shown by dotted lines.

The nitrogen–oxygen bonds within the nitrate ion are not of the same length. The N–O(1) bond with the oxygen coordinated to metal ions has a length of 1·27 Å, the N–O(2) bond with the oxygen near mercury (Hg···O(2), 2·95 Å), which is at the same time hydrogen-bonded to the water molecule, is 1·28 Å, while the N–O(3) bond with no coordinated oxygen is 1·12 Å.

The commonest stereochemical coordination of copper in cupric compounds is [4+2] with four short and two long bonds (Orgel & Dunitz, 1957; Dunitz & Orgel, 1960). The coordinations [2+4], [4+1+1], [2+2+2] occur rarely (Nowacki & Scheidegger, 1952; Zemann, 1961; Mani & Ramaseshan, 1961; Wallwork & Addison, 1965). In the present structure the coordination is [2+4] but it is interesting that six copper–oxygen distances do not differ to the usual extent. The pale bluish-green colour of the crystals is also well interpreted by the relatively regular coordination about copper (Zemann, 1961).

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Table 4. *Interatomic distances and angles*

The positions are denoted as follows:

No label	x	y	z
(i)	$-x$,	$-\frac{1}{2}+y$,	$\frac{1}{2}-z$,
(ii)	$1+x$,	y,	z,
(iii)	x,	$\frac{1}{2}-y$,	$-\frac{1}{2}+z$,
(iv)	$-x$,	$\frac{1}{2}+y$,	$\frac{1}{2}-z$,
(v)	$-x$,	$1-y$,	$-z$,
(vi)	$1-x$,	$-\frac{1}{2}+y$,	$\frac{1}{2}+z$,
(vii)	$-x$,	$-y$,	$-z$,
(viii)	$1-x$,	$1-y$,	$-z$,

(*a*) The coordination about the mercury atom.

		σ			σ
Hg–O(1)	2·78 Å	0·04 Å	O(1)–Hg–OH^{i}	101·3°	0·3°
Hg–OH^{i}	2·30	0·04	O(1)–Hg–OH$_2$	83·9	0·3
Hg–OH$_2$	2·54	0·04	OH^{i}–Hg–OH$_2$	75·6	0·3

(*b*) The coordination about the copper atom.

		σ			σ
Cu–O(1^{i})	2·14 Å	0·04 Å	O(1^{i})–Cu–OH^{i}	87·6°	0·4°
Cu–OH^{i}	2·15	0·04	OH^{i} –Cu–OH$_2$	91·1	0·5
Cu–OH$_2$	2·02	0·04	O(1^{i})–Cu–OH$_2$	97·6	0·3

Table 4 (*cont.*)

(*c*) Bond lengths within the nitrate ion.

		σ			σ
N–O(1)	1·27 Å	0·07 Å	O(1)–N–O(2)	120·5°	1·4°
N–O(2)	1·28	0·07	O(1)–N–O(3)	115·3	1·4
N–O(3)	1·12	0·07	O(2)–N–O(3)	123·5	1·4

(*d*) Hydrogen-bonded atoms.

		σ			σ
$O(2)\cdots OH_2^{ii}$	2·88 Å	0·08 Å	$O(2)\cdots OH_2^{ii}\cdot OH^{ii}$	87·8°	0·4°
$OH\cdots OH_2$	2·71	0·08			
$O(3)\cdots OH^{ii}$	2·80	0·07			

(*e*) Distances of approximately 3 Å.

		σ			σ
$Hg\cdots O(2)$	2·95 Å	0·05 Å	$O(2)\cdots OH_2^{vii}$	3·01 Å	0·07 Å
$O(1)\cdots OH_2^{iii}$	2·74	0·08	$O(3)\cdots O(3)^{viii}$	3·11	0·08
$O(1)\cdots OH_2^{iv}$	3·13	0·07	$O(3)\cdots OH^{v}$	2·91	0·07
$O(1)\cdots OH$	2·97	0·07	$O(4)\cdots OH_2^{iii}$	2·92	0·06
$O(1)\cdots OH^{v}$	3·10	0·08	$O(4)\cdots OH_2^{iv}$	2·98	0·08
$O(1)\cdots OH^{vi}$	3·00	0·07			

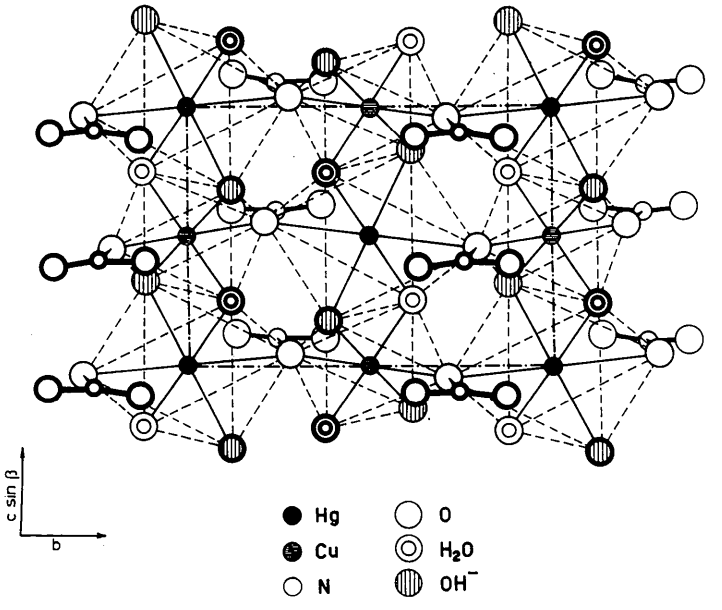

Fig. 3. The structure of $HgCu(OH)_2(NO_3)_2.2H_2O$ projected along the *a* axis.

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