The Crystal Structure of $Cu(H_2PO_3)_2$

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$Cu(H_2PO_3)_2$ crystallizes in space group $P2_1/c$ with $a = 7.490$, $b = 9.938$, $c = 7.465$ Å, $\beta = 99.6°$, $Z = 4$. The structure was refined by means of three-dimensional least-squares method. The final R value for 1013 observed structure factors is 0.115. The characteristic feature of the structure are pairs of distorted octahedra with one common edge. These pairs are bonded together by $H_2PO_3^-$ groups so that the entire structure may be considered as representing a coordination polymer. Cu—O bonds in octahedra are 1.98, 1.97, 1.92, 1.96, 2.33, and 3.15 Å respectively.

The crystal structure of $Cu(H_2PO_3)_2$ was determined as a further part of general study of the structure and properties of phosphites. Crystals were prepared by *Nassler* [1]. The aim of the structure analysis of $Cu(H_2PO_3)_2$ was to determine the coordination of copper and to elucidate the role of the phosphite group $H_2PO_3^-$ in this incongruently soluble copper(II) complex.

Experimental

The substance forms clear blue prismatic crystals elongated in the direction of the growth axis a. From the precession photographs and from the rotation and Weissenberg photographs around the axis a the following parameters of the unit cell were determined:

$$a = 7.490(7),\ b = 9.938(6),\ c = 7.465(3)\ \text{Å},\ \beta = 99.6(1)°.$$

Density determined by the suspension method (bromoform—benzene) has the value 2.68(1) g cm^{-3}. The theoretical value of density based on four formula units per cell is 2.71 g cm^{-3}.

Determination of intensities was performed on the basis of Weissenberg photographs of the layers $0kl - 6kl$ with CuK_α-filtered radiation and the multiple-film technique. The intensities of strong reflexions were determined photometrically from the integrated photographs. Weak intensities were estimated visually from the nonintegrated photographs. For the nondetectable reflexions 1/3 of the lowest observed intensity in the respective layer-line was taken [2]. Corrections of the intensities on the individual layer-lines were made for the Lorentz, polarization and absorption factor. The values of $(F^2)_{corr}$ obtained in this way were then transformed to the common scale by comparison of $h0l$ spectra. Thus, 1013 independent values were found.

Systematic extinction of diffractions of the type

$$h0l \text{ for } l = 2n$$

$$0k0 \text{ for } k = 2n$$

means that only the space group No. 14 C_{2h}^5 in the setting $P2_1/c$ is possible. In this group there is only one fourfold position and hence if $Z = 4$, all the atoms are in general positions.

Determination and refinement of the crystal structure

The structure model was suggested on the basis of interpretation of the three-dimensional Patterson function $P(uvw)$, from which the positions of the atoms Cu, P(1), P(2) were determined. The positions of all oxygen atoms were then found by means of the electron-density projections $\varrho(yz)$ and $\varrho(xz)$. The entire structure was preliminary refined by successive Fourier $F_o - F_c$ syntheses.

The basic model was further refined using all the three-dimensional data by the least-squares method with the GIER computer [3]; the individual isotropic temperature factors were taken first. After six cycles the R factor was 17.8%. Then the anisotropic temperature factors were introduced and after subsequent ten cycles the R index dropped to 11.7%. The block-diagonal approximation was used in the programme. The Hughes [4] weighting scheme was used for the refinement. In this stage of refinement no significant parameter changes were observed and thus a control with three-dimensional difference synthesis [5] was performed. In this map, except for random deviations, which were smaller than 0.8 e Å^{-3} (for maxima at 10—50 e Å^{-3}) two larger peaks appeared (1.2 e Å^{-3}) which could be interpreted as peaks arising from hydrogen atoms bonded to the phosphorus atoms. From this, the positions of two hydrogen atoms were determined and used in the three last refinement cycles. Their positions in structure were not refined. Since these hydrogen atoms are chemically bonded atoms with low atomic number, where there is uncertainty of exact value of atomic scattering factor [6] and since for the calculations the respective values from *International Tables* [7] for an isolated atom were taken, refinement of the temperature factor of hydrogen atoms would be meaningless. Thus, the mean value of the individual isotropic temperature factor coefficients of the phosphorus atoms, as determined in the least-squares isotropic cycle, was conventionally assigned to them. The resulting R factor dropped to the value of 11.5% and the value of error-square-sum $\Sigma w(|F_o| - |F_c|)^2$ decreased by 0.62 to reach the final value 14.69.

An agreement between the observed and calculated structure factors is shown in Table 1. The final coordinates, and for the refined atoms also their standard deviations are listed in Table 2. In Table 3 the coefficients of anisotropic temperature factors and their standard deviations are presented. Coefficients of isotropic temperature factors of $B = 1.91$ Å^2, were assigned to the hydrogen atoms.

Description of the structure

From the calculations of interatomic distances, bond angles and their standard deviations [8] it follows that the coordination polyhedron around the copper atom has the shape of an elongated distorted octahedron (Fig. 1, Table 4*a*). Four shorter and one longer distances correspond to the Cu—O bonds, whereas each oxygen atom belongs to different $H_2PO_3^-$ group. This configuration is completed by an oxygen atom O(3) from a hydroxyl group which is linked by the weakest bond to the next $H_2PO_3^-$ group. Thus the oxygen atoms from six different $H_2PO_3^-$ groups participate in the coordination around the Cu atom.

The $H_2PO_3^-$ group forms a distorted tetrahedron (Table 4*b*) with P atom in its centre. Accurate determinations of bond lengths show that the distances P(1)—O(3), or P(2)—

Table 1. Observed and calculated structure factors
In the columns from left to right the values l, $100|F_o|$ and $100\,F_c$ are listed. Undetectable diffractions are marked by n

	F_o	F_c
0 0 L		
2	7191	-8137
4	2810	3393
6	10080	-9176
8	543	433
0 1 L		
1	9123	9870
2	5353	-5692
3	1046	-1003
4	1528	-1540
5	2989	-3141
6	2704	-2415
7	2823	-2573
8	1469	1086
9n	214	-023
0 3 L		
1	2269	2778
2	1897	-2292
3	1730	-1701
4	9375	-8899
5	687	459
6n	358	213
7	1432	-1287
8	1081	-970
9	1381	927
0 5 L		
1	4491	-5010
2	2202	-2387
3n	305	217
4	2562	-2462
5n	356	257
6n	357	174
7	4230	3529
8	770	-364
0 7 L		
0	1116	-1287
1	1112	-1065
2	5421	-6189
3	5033	-5551
4	2049	2185
5	2528	-2536
6	2146	1668
7	693	-382
8	1790	1303
0 9 L		
1	394	301
2	2634	2489
3n	414	-192
4	2378	2100
5	1243	-739
6	1380	1010
0 11 L		
1	1963	1673
2	1076	1157
3	656	457
4	2069	1814
1 0 L		
0	883	934
1n	225	-277
2	1855	1561
3	923	1221
1 2 L		
0	9745	-9242
1	6621	-6900
2	6813	6578
3	973	-1301
4	7489	-6975
5n	465	-712
6	950	857
7	1763	2077
8	979	-1464
-1	2480	-3042
-2	11737	12392
-3	1050	-771
-4	3225	-3458
-5	3987	3755
-6	4129	3895
-7	1809	2362
-8	1582	-2330
-9n	304	364
1 3 L		
0	15088	-13415
1n	283	-040
2	2385	-2382
3	707	-587
4n	426	-260
5	1332	1658
6	2097	2101
7	1039	-1228
8	1378	1704
-1	3457	-3478
-2	1547	-1925
-3n	354	343
-4	1142	1357
-5	2211	2324
-6	5446	5121
-7n	491	-315
-8	1023	1432
-9n	273	-080
1 5 L		
0	2077	-2221
1	9507	-10188
2	3999	4405
3	1125	1020
4	3650	3555
5	1074	-1089
6	867	699
7	3294	3016
8	602	-512
-1	1740	-1462
-2	8209	-7504
-3	2326	-2286
-4	753	-367
-5	5539	5263
-6n	501	-114
-7	1047	1246
-8	855	676
1 7 L		
0	4214	-4398
1	1641	1379
2	3669	-3935
3	1410	-1757
4	2059	2092
5	7152	-6731
6n	497	-154
7n	490	073
8	1492	1972
-1	4605	5763
-2	2886	-3070
-3	4493	5084
-4	1563	-1731
-5	759	521
-6	5620	5432
-7n	499	397
-5	856	522
-6	3712	3037
-7	786	683
-8	667	-905
1 6 L		
0	409	-410
1	1027	-739
2	764	230
3	1310	-1321
4	7439	6815
5	1097	1369
6n	467	474
7	663	433
8	390	106
-1	2249	-1869
-2	8282	-7969
-3	2716	2099
-4	1194	-1529
-5n	502	-285
-6	839	-606
-7	721	425
-8	1070	1506
1 8 L		
0n	455	108
1	1292	1132
2	1167	1310
3	2328	2724
4n	501	261
5	3834	3328
6	739	-797
7	902	-1167
-1	2733	-2572
-2	3703	3549
-3	6584	-5705
-4	1229	-1213
-5n	495	448
-6	782	-582
-7	630	-726
1 9 L		
0	847	-936
1	2057	2141
2	1596	1767
3	1229	1329
4	1071	1019
5	772	-506
6n	367	260
7	551	-815
-1	2316	2769
-2	2075	-1999
-3n	502	085
-4	1386	-1651
-5	1017	-1351
-6	689	506
-7	1709	-1850
2 2 L		
0	3524	2982
1	868	582
2	2345	2950
3	482	312
4	772	-518
5	663	-245
6n	280	170
-1n	501	243
-2n	498	221
-3	1071	-1145
-4	798	-397
-5n	407	247
-6	2691	-2520
		2956
1	5139	4388
2	1915	-2456
3n	427	-414
4	711	755
5	710	843
-1n	477	-267
-2	1020	-1127
-3	963	972
-4	1560	2016
-5	2155	-2239
1 11 L		
0	913	1190
1	706	-585
2	940	1046
3	588	-522
4	502	779
-1	1971	1325
-2n	397	-197
-3	997	1215
-4	510	-540
1 12 L		
0	692	-726
1	1367	1356
2	459	424
-1	861	-1145
-2	1870	2099
-3n	470	607
2 1 L		
0	1426	990
1	9848	-10395
2	2696	2462
3	5458	-5853
4	2808	2665
5	991	-802
6n	605	-297
7	1976	1961
8	776	788
-1	1770	1349
-2	6088	-6581
-3	4314	4463
-4	2008	-2214
-5	4976	5070
-6n	589	305
-7n	602	204
2 3 L		
0	764	-699
1	2104	2133
2	1825	1361
3	2607	-2557
4	5163	4741
5	4505	4020
6	2665	2556
7	1879	-1979
8	925	-801
-1	4806	-5006
-2	9857	-10339
-3	3228	2405
-4	2515	-2178
-5n	559	259
-6	2086	-1781
-7n	591	-547
2 4 L		
0	1025	-361
1	2098	-1399
2	885	1124
3	2257	2369
4	2189	2276
5	3502	3787
6	1028	-656
7n	512	208
8	619	-668
-1	4239	-4443
-2	1480	1126
-3	6052	-6288
-4	1377	1223
-5n	580	337
-6	2350	-2341
-7	1115	750
2 5 L		
0	783	349
1	2077	1664
2	2549	-1991
3	5964	6277
4	2933	2574
5	1049	-713
6	1313	1510
7n	471	371
8	488	426
-1	883	702
-2	7022	-7035
-3	898	-464
-4	2486	2338
-5	4550	-3896
-6	1565	-1525
-7n	546	-261
2 6 L		
0	2935	3031
1	2765	2587
2	4249	4660
3	2855	-2760
4	1171	1101
5	1550	1569
6n	534	459
7n	412	-269
-1	2985	-2325
-2n	531	331
-3	3603	3365
-4	3440	-2740
-5	2678	-2308
-6	2573	-2568
-7	866	753
2 7 L		
0	1460	1389
1	5464	5631
2	2974	-2863
-1	14023	-13017
-2	1929	2436
-3	3883	-3753
-4	2083	1454
-5	2106	-1989
-6	3006	3215
-7	3208	3314

Table 1 (Continued)

3n 602 -150	0 1236 -1322	7n 286 082
4n 601 -186	2 1301 -1529	-1 4465 4241
5 1467 1788	4n 336 -184	-2 816 795
6 825 -923	6 4515 3863	-3 8211 -8222
7 1733 -1938	8n 236 087	-4 867 1047
-1n 563 -592	-2 3180 -4010	-5 736 -781
-2 3348 2922	-4 2269 -2156	-6 1339 -851
-3 1785 1312	-6 1981 -1629	-7 2063 -2155
-4 1174 1175	-8 5452 4373	-8 493 227
-5 4525 -3894		
-6n 540 -208	3 1 L	3 5 L
-7 754 -859		
	0 1027 -607	0 1750 -1162
2 8 L	1 4217 -4158	1 1728 -1701
	2 4284 4252	2 5178 5243
0 1553 -1610	3 923 954	3 3135 3001
1 1564 -1621	4 1933 2092	4 653 543
2 5176 4631	5 1916 1690	5 5367 -4858
3n 601 -352	6 1895 -1685	6n 333 082
4 1312 -1349	7 3536 3030	7n 252 211
5 2666 -2493	8n 401 403	-1 10820 9813
6 682 671	-1 4323 -4606	-2 1309 1009
-1 5212 5351	-2 961 859	-3 854 -1012
-2 3391 3106	-3 3575 -4457	-4 4396 -4176
-3 1173 906	-4 4052 -4042	-5 1645 1286
-4 3461 -3379	-5 1419 -1554	-6n 373 -229
-5 1665 1576	-6n 371 177	-7 2835 -2366
-6 821 -574	-7 4272 3727	-8 566 -706
-7 1319 -1729	-8 1376 -1180	
	-9 1313 1151	3 6 L
2 9 L		
	3 2 L	0 6409 6289
0 2818 2357		1n 344 085
1 1041 688	0 2955 -3384	2 804 -880
2n 589 -084	1 7207 7926	3 837 -634
3n 562 -345	2 2279 2208	4 1627 -1403
4 1970 -2678	3 6847 6989	5n 357 -142
5 726 -622	4 1648 -1615	6 2853 -2488
6 654 -975	5n 375 -366	7 521 885
-1n 602 -014	6 3394 2771	-1 1759 -1645
-2 2891 2781	7 718 -658	-2 2457 2431
-3 1338 1224	8n 218 142	-3 2820 2656
-4 1425 1659	-1 1090 -893	-4 2199 2093
-5 1257 -1705	-2 1852 -1846	-5 1670 -1595
-6 869 -991	-3 5603 -5691	-6 2357 -1852
	-4 2917 -2922	-7 1318 1370
	-5 6041 -6232	-8 1782 -1513
	-6 1613 1551	
0 980 451	-7n 372 471	3 7 L
1n 555 107	-8 963 1063	
2 1593 -1812		0 1798 -1811
3 840 -380	3 3 L	1 2936 2565
4n 411 -366		2 1683 -1491
5 1890 -2066	0 1439 1358	3 2091 -1919
-1 2635 2604	1 3390 3673	4 933 -951
-2 1261 -753	2 8178 8906	5 835 -939
-3 1347 1292	3 3434 -3156	6 448 568
-4 1208 1329	4 564 457	-1 4771 4449
-5n 377 100	5 2271 1656	-2 1668 1678
	6 818 825	-3 959 960
2 11 L	7 994 -1124	-4n 378 -071
	8 1843 -2056	-5n 366 295
0 1103 1176	-1 1403 -1277	-6 2451 2153
1 1806 -1986	-2 347 258	-7 2888 -2511
2n 430 -421	-3 1414 1645	
3 636 -702	-4 8381 -8313	3 8 L
-1n 477 -319	-5 1615 -1399	
-2 1371 1491	-6 655 -219	0 3480 3124
-3n 412 394	-7n 366 271	1 3148 -2807
	-8 1128 -1037	2 843 -851
2 12 L		3 2297 -2197
	3 4 L	4 671 -497
0 1752 -2164		5n 283 -406
1n 322 -149	0 2497 2604	6 2064 -2073
2 539 -996	1 483 648	-1 757 853
-1 662 597	2 1829 -1416	-2 3565 3206
-2 595 667	3 8265 7557	-3 653 679
	4 736 789	-4 1292 -1229
3 0 L	5 1561 -1063	-5 3763 3265
	6 1602 -1244	-6 566 -524
	330 -388	
		3 9 L
		0 1933 -1879
		1 734 -842
		2 1568 -1547
		3n 329 341
		4 2834 -2328
		5 1072 -1194
		-1 2523 2482
		-2 734 658
		-3 1420 -1277
		-4 3648 2938
		-5n 287 091
		-6 375 561
		3 10 L
		0 1238 1137
		1 567 -410
		2 687 -1013
		3 2063 -1939
		4 368 535
		-1 583 -739
		-2 2305 -1983
		-3 1374 1272
		-4 544 287
		-5 767 1103
		3 11 L
		0 701 982
		1 908 -945
		2 1793 -1616
		3 304 503
		-1 778 -977
		-2 615 -842
		-3 1057 -1141
		-4 1191 1170
		4 0 L
		0 2777 2734
		2 2695 3063
		4 3849 3793
		6 637 385
		-2 5007 -5745
		-4 4540 -5001
		-6 1277 -1003
		4 5 L
		0 6293 5878
		1 2310 2459
		2 1185 -857
		3 6323 6255
		4 2379 2555
		5n 390 -100
		6 2851 -3350
		7n 292 154
		-1 1381 1569
		-2 509 -326
		-3 8461 -8687
		-4n 314 -158
		-5 1480 -1649
		-6 1824 -1779
		-7 1541 -1526
		-8n 322 -383
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		4 2 L
		0 2016 -1646
		1 8438 8001
		2 4001 4263
		3 1970 -2005
		4 2434 2172
		5 1284 -1419
		6 1185 -1058
		7 2644 -2688
		-1 2729 3411
		-2 793 -948
		-3 3357 3979
		-4 3898 -4677
		-5 3093 -3335
		-6 1525 1517
		-7 1934 -1650
		-8 1313 -1214
		-9 907 -1319
		4 3 L
		0 8436 8087
		1 2343 2235
		2 2432 2747
		3 754 -924
		4 1245 -1064
		5 2078 1800
		6 2347 -2272
		7 1053 -1193
		-1 4955 -4414
		-2n 343 -153
		-3 769 298
		-4 1642 1608
		-5 831 718
		-6 4153 -3973
		-7 923 797
		-8 574 -515
		4 6 L
		0 2532 -2923
		1 1677 1381
		2 666 -567
		3 1391 -1178
		4 3569 -3436
		5 1214 1326
		6 501 526
		-1 2870 -2737
		-2 2073 2242
		-3 2708 2529
		-4 3715 3738
		-5 1867 -1706
		-6 1526 1505
		-7 1161 1026
		4 7 L
		0 1107 -656
		1 2018 1857
		2 2225 -2334
		3 4899 -4849
		4 1407 1349
		5 510 337
		-1 1972 -2164
		-2 1822 -1763
		-3 5265 5189
		-4 1546 1241
		-5n 363 098
		-6n 316 488
		-7 1158 1255
		4 8 L
		0 858 -680
		1 2919 -2931
		2 828 -806
		3 607 -035
		4 1716 -1974
		5 1015 1197
		-1 1963 -2146
		-2 1925 1894
		-3 1252 -885
		-4 856 795
		-5 1710 1665
		-6 1008 1051
		4 9 L
		0 3780 -3960
		1 691 743
		2n 336 127
		3 522 -563
		-1n 367 -032
		-2 699 -607
		-3 871 485
		-4 864 -688
		-5 515 -447
		5 0 L
		0 799 877
		1 1809 -1800
		2 807 746
		3 476 538
		-1 1524 -1519
		-2 1297 -1221
		-3 554 -599
		-4 424 270
		5 1 L
		0 757 -862
		1 419 589
		-1 466 -257
		-2 571 -918
		-3 1109 -1387
		5 0 L
		0 6559 6887
		2 3828 3730
		4 1464 -1476
		-2 392 163
		-4 1375 1536
		-6 6499 -6878
		-8n 302 284
		5 1 L
		0 3730 3958
		1 4684 4462
		2 3321 -2991

3	791	-566	1	2995	-3027	3	1329	-1159		6 1 L			6 4 L			-2	527	-362
4	977	-617	2	2677	-2387	4	1017	1262								-3	606	-638
5	953	-534	3	1658	-1211	5	1057	1100	0	2215	2096	0	1581	-1688		-4n	277	-247
6	2014	-1956	4	1451	889	-1	1965	-1925	1	2224	-2437	1	3123	-3368		-5	2003	-1969
7	1368	-1276	5	3777	-2950	-2	1471	-979	2	4644	-4675	2	1374	1719				
-1	2493	2810	6	863	595	-3n	442	303	3	540	-561	3	1956	-1696			6 8 L	
-2	1519	1455	-1	5087	5071	-4n	426	-188	4	1356	1519	4	585	739				
-3	3654	3928	-2	2495	-2620	-5	2474	2897	5	1433	-1351	5	688	917		0n	275	169
-4	1831	1583	-3	1751	1916	-6	797	-626	6	692	-1111	-1n	282	-294		1	1488	1581
-5	3774	-3725	-4	3446	3345				-1	7043	7138	-2	2280	-2116		2	405	-431
-6n	447	241	-5	2967	2867		5 8 L		-2	4138	-4212	-3	1798	-1857		3	420	660
-7	2155	-2106	-6	1207	664				-3	1053	1017	-4	1417	-1412		-1	1107	1312
-8	586	-789	-7	1045	-1135	0	1601	-1325	-4	3817	3893	-5	4935	4724		-2	1131	-1058
			-8	644	652	1n	420	-142	-5	1726	1543	-6	494	-325		-3	536	-474
	5 2 L					2	1941	-1716	-6n	309	184	-7	398	-306		-4	405	-279
				5 5 L		3	1097	1492	-7	1956	-1824					-5	1059	-1125
0	1892	2197				4	615	734	-8	692	1193		6 5 L					
1n	325	-256	0	1354	-1241	-1n	433	-368									6 9 L	
2n	417	241	1	6546	-6313	-2n	427	107		6 2 L		0n	308	188				
3	2719	-2413	2n	442	-319	-3	2955	-2525				1	543	-677		0	390	-317
4	1472	1201	3	2501	2342	-4n	384	-056	0	1496	1573	2	2416	-2365		1	353	-174
5	3138	-2761	4	2425	-2162	-5	578	-481	1	1333	-1349	3	2163	2345		2	2474	3278
6	1503	-1245	5	698	-292	-6	1512	1671	2	1394	-1143	4	456	432		-1n	231	191
-1	1125	749	-1	1868	-1526				3	1771	-1840	5	687	753		-2	1582	1867
-2	1525	1689	-2	3441	3361		5 9 L		4	1087	-1058	-1	1551	-1202		-3	353	090
-3	4742	5015	-3	2417	-2058				5n	265	-082	-2	1452	-1632		-4	2315	-2632
-4n	396	053	-4	846	425	0n	384	-403	6	892	-1276	-3	3443	-3155				
-5n	436	174	-5	3656	3614	1	1733	-1620	-1	2202	-2226	-4	2452	1997			7 0 L	
-6	1897	-2147	-6	1147	1117	2	1294	1467	-2	4599	4518	-5	1332	-1067				
-7	1939	1837	-7	1262	909	3	474	444	-3	704	412	-6	456	704		0	2092	-1198
						-1	1413	1478	-4	1997	-1787	-7	335	694		2	3148	-3327
	5 3 L			5 6 L		-2	1475	-1335	-5	1576	1486					4	1647	-1878
						-3n	358	-180	-6	1232	1360		6 6 L			-2	1562	-1211
0	2532	-2340	0	4453	-4068	-4	1742	-1886	-7	1687	1772					-4	4839	4940
1	2033	2129	1n	445	218				-8	1603	-2036	0	1421	-1266		-6	541	552
2	2184	2147	2	3124	-2836		5 10 L					1n	312	-274				
3	1436	-1027	3n	435	-399					6 3 L		2	701	809			8 0 L	
4	6536	-6071	4	1302	1097	0	534	586				3	644	-549				
5	1913	1834	5n	457	-376	-1	596	-338	0	3020	-3011	4	1083	1132		0	4054	-3955
6n	340	-079	-1n	437	-331	-2	663	772	1	491	556	-1	1243	-1093		2n	344	172
-1	2827	-2989	-2	1449	-999	-3	2461	-2513	2	3540	-3314	-2	3768	-3132		-2	799	-838
-2	8188	8181	-3	2348	2368				3	645	-785	-3	1745	1433		-4	645	-719
-3	1615	1925	-4	1657	1300		6 0 L		4	612	-670	-4	1462	-1506		-6	1434	1443
-4	719	440	-5	1094	-1720				5n	251	102							
-5	1458	-1187	-6	2706	2378	0	1645	1840	6	253	259		6 7 L				9 0 L	
-6	1970	1740	-7	705	802	2	492	-475	-1	884	886							
-7n	397	234				4	5119	-4864	-2	450	-276	0	1564	1585		0	548	1016
-8	1603	-1654		5 7 L		6	741	-591	-3n	283	153	1	2210	2033		-2	1823	-1899
						-2	8123	8165	-4	1758	1960	2	479	-277		-4	354	-660
	5 4 L		0	776	-551	-4	933	1246	-5	544	-464	3	745	-874				
			1	3162	-3389	-6	931	-889	-6	3097	2791	4	1198	1410				
0	2122	-2078	2	434	-227	-8	1550	-1955	-7	478	-534	-1	3855	-3763				

Table 2

Positional parameters and for refined atoms their standard deviations

Atom	x	y	z
Cu	0.1939(2)	0.0815(2)	0.0716(2)
P(1)	0.4502(4)	0.4326(3)	0.2692(4)
P(2)	0.9634(4)	0.2978(3)	0.2291(4)
O(1)	0.4018(11)	0.0279(9)	0.2577(11)
O(2)	0.3161(11)	0.4898(9)	0.3777(12)
O(3)	0.3563(14)	0.3741(13)	0.0830(13)
C(4)	0.1022(11)	0.1880(8)	0.2512(11)
O(5)	0.9734(11)	0.3882(7)	0.3935(10)
O(6)	0.7649(15)	0.2393(11)	0.1843(16)
H(1)	0.522	0.302	0.347
H(2)	0.975	0.390	0.060

Table 3

Coefficients of anisotropic temperature factors and their standard deviations (multiplied by 10^4)

The coefficients used in: $\exp(-b_{11}h^2 - b_{22}k^2 - b_{33}l^2 - b_{12}hk - b_{13}hl - b_{23}kl)$

Atom	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
Cu	69(4)	54(2)	97(3)	12(4)	42(5)	−11(3)
P(1)	79(6)	73(3)	97(5)	−43(7)	41(8)	−5(6)
P(2)	67(6)	58(3)	89(5)	9(6)	10( )	−27(5)
O(1)	103(18)	81(9)	121(15)	85(20)	48(25)	7(19)
O(2)	67(17)	85(9)	158(16)	8(20)	160(25)	1(19)
C(3)	143(23)	190(17)	135(18)	−195(32)	77(31)	−35(28)
O(4)	92(18)	60(8)	139(16)	10(18)	41(25)	−54(18)
C(5)	92(16)	44(7)	92(13)	39(16)	−37(21)	−6(15)
O(6)	168(23)	110(12)	257(27)	53(26)	30(37)	−193(30)

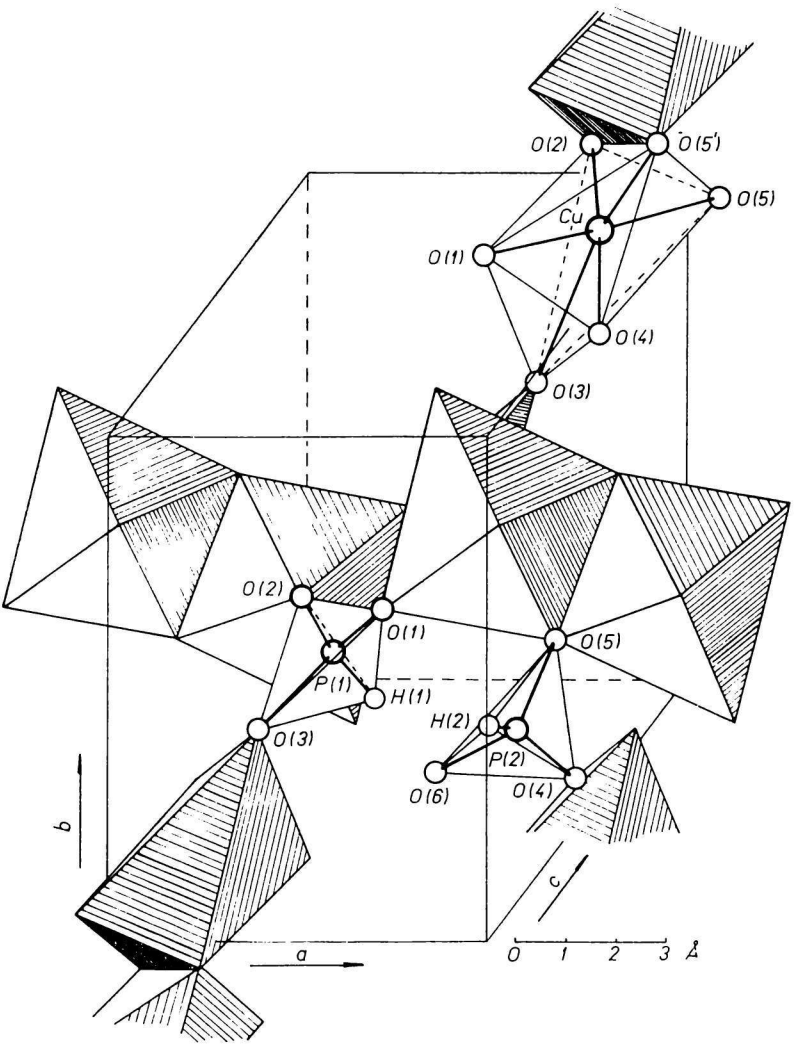

Fig. 1. The arrangement of pairs and their bonding.

Table 4

Interatomic distances and bond angles
The oxygen atoms O(3) and O(6) belong to the hydroxyl groups, O(5) and O(5′) are symmetrically equivalent
Data concerning the unrefined hydrogen atoms are less reliable

a) Octahedron around Cu(II)

Distances [Å]		Angles [°]	
Cu—O(1)	1.979(8)	O(1)—Cu—O(5)	172.4(4)
Cu—O(2)	1.969(10)	O(2)—Cu—O(4)	167.1(4)
Cu—O(4)	1.923(9)	O(3)—Cu—O(5′)	166.0(3)
Cu—O(5)	1.962(7)		
Cu—O(5′)	2.332(8)		
Cu—O(3)	3.148(13)		
Distances [Å]		**Angles [°]**	
O(1)—O(2)	2.807(12)	O(1)—Cu—O(2)	90.7(3)
O(2)—O(5)	2.779(12)	O(2)—Cu—O(5)	90.0(3)
O(5)—O(4)	2.788(11)	O(5)—Cu—O(4)	91.7(3)
O(4)—O(1)	2.744(12)	O(4)—Cu—O(1)	89.4(3)
O(1)—O(3)	3.675(16)	O(1)—Cu—O(3)	88.5(3)
O(2)—O(3)	3.920(16)	O(2)—Cu—O(3)	97.3(3)
O(5)—O(3)	3.957(14)	O(5)—Cu—O(3)	98.9(3)
O(4)—O(3)	3.069(15)	O(4)—Cu—O(3)	69.8(3)
O(1)—O(5′)	3.169(11)	O(1)—Cu—O(5′)	94.2(3)
O(2)—O(5′)	3.214(12)	O(2)—Cu—O(5′)	96.3(3)
O(5)—O(5′)	2.723(10)	O(5)—Cu—O(5′)	78.2(3)
O(4)—O(5′)	3.188(11)	O(4)—Cu—O(5′)	96.6(3)

b) $H_2PO_3^-$ groups

Distances [Å]	
P(1)—O(1)	1.497(9)
P(1)—O(2)	1.504(10)
P(1)—O(3)	1.561(10)
P(1)—H(1)	1.49
P(2)—O(4)	1.497(9)
P(2)—O(5)	1.512(8)
P(2)—O(6)	1.579(11)
P(2)—H(2)	1.57

Distances [Å]		Angles [°]	
O(1)—O(2)	2.519(13)	O(1)—P(1)—O(2)	114.2(5)
O(2)—O(3)	2.544(14)	O(2)—P(1)—O(3)	112.2(5)
O(3)—O(1)	2.513(14)	O(3)—P(1)—O(1)	110.5(6)
H(1)—O(1)	2.47	H(1)—P(1)—O(1)	112
H(1)—O(2)	2.46	H(1)—P(1)—O(2)	111
H(1)—O(3)	2.26	H(1)—P(1)—O(3)	96
O(4)—O(5)	2.522(11)	O(4)—P(2)—O(5)	113.9(4)
O(5)—O(6)	2.500(13)	O(5)—P(2)—O(6)	107.9(6)
O(6)—O(4)	2.543(14)	O(6)—P(2)—O(4)	111.5(5)
H(2)—O(4)	2.55	H(2)—P(2)—O(4)	112
H(2)—O(5)	2.49	H(2)—P(2)—O(5)	108
H(2)—O(6)	2.46	H(2)—P(2)—O(6)	103

—O(6) (mean value 1.570 Å) are significantly longer than the distances P(1)—O(1), or P(1)—O(2) and P(2)—O(4) or P(2)—O(5) (mean value 1.502 Å). This is in good agreement with the results of the neutron structure analysis of phosphorous acid performed by *Loopstra* [9], where the mean distances P—O of 1.496 Å and P—O(H) 1.549 Å were found; this proves also that the oxygen atoms O(3) and O(6) belong to the OH group.

Both symmetrically independent tetrahedral groups around atoms P(1) and P(2) (Fig. 1) are not crystallochemically identical. Whereas all the oxygen atoms of the first group participate in the coordination of the three $Cu[O_5OH]$ octahedra, from the second group only the atoms O(4) and O(5) belong to the octahedra. The oxygen atom O(6) from the hydroxyl group OH never participates in the coordination of copper atom; it is linked by a hydrogen bond at a distance of 2.58 Å to the oxygen atom O(2). As a consequence of this, the octahedra around Cu(II) are never isolated, they always form a pair of octahedra with one shared edge. Formation of bi-octahedra makes possible the octahedral coordination of two Cu(II) atoms by ten oxygen atoms.

Since the oxygen atoms from the octahedra $Cu[O_5OH]$ always belong to different groups $H_2PO_3^-$, the above pairs of octahedra are mutually linked in space by the tetrahedral groups $H_2PO_3^-$ and consequently the crystalline $Cu(H_2PO_3)_2$ can be considered as a coordination polymer. In the unit cell the octahedra are situated in such a way that two longer distances Cu—O(3) and Cu—O(5′), and as a consequence of this the elongated octahedron as well, are oriented approximately in the direction of the longest crystallographic axis *b*.

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