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Crystal Chemistry of *cyclo*-Hexaphosphates. IV. Structures of Tris(ethylenediammonium) *cyclo*-Hexaphosphate Dihydrate and Copper Bis(ethylenediammonium) *cyclo*-Hexaphosphate Hexahydrate

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Abstract. Tris(ethylenediammonium) *cyclo*-hexaphosphate dihydrate, $[C_2H_{10}N_2]_3P_6O_{18}.2H_2O$, $M_r = 696{\cdot}204$, monoclinic, $P2_1/n$, $a = 11{\cdot}064\,(5)$, $b = 12{\cdot}317\,(5)$, $c = 9{\cdot}342\,(5)$ Å, $\beta = 90{\cdot}53\,(5)°$, $V = 1273\,(2)$ Å^3, $Z = 2$, $D_x = 1{\cdot}816$ Mg m^{-3}, λ(Mo $K\overline{\alpha}$) $= 0{\cdot}7107$ Å, $\mu = 0{\cdot}528$ mm^{-1}, $F(000) = 724$, $T = 295$ K, final $R = 0{\cdot}030$ for 2530 unique reflections. Copper bis(ethylenediammonium) *cyclo*-hexaphosphate hexahydrate, $Cu[C_2H_{10}N_2]_2P_6O_{18}.6H_2O$, $M_r = 769{\cdot}694$, monoclinic, $P2_1/a$, $a = 13{\cdot}378\,(8)$, $b = 11{\cdot}574\,(6)$, $c = 8{\cdot}687\,(3)$ Å, $\beta = 103{\cdot}15\,(3)°$, $V = 1310\,(2)$ Å^3, $Z = 2$, $D_x = 1{\cdot}951$ Mg m^{-3}, λ(Mo $K\overline{\alpha}$) $= 0{\cdot}7107$ Å, $\mu = 1{\cdot}344$ mm^{-1}, $F(000) = 790$, $T = 295$ K, final $R = 0{\cdot}032$ for 3646 unique reflections. In the first compound two kinds of ethylenediammonium groups coexist, one with no internal symmetry, the second one centrosymmetric. Layers containing P_6O_{18}, water molecules and the centrosymmetric organic groups alternate along the b axis. Layers of the first kind of ethylenediammonium groups alternate with those of the second type. The second compound can also be described as a layer organization: layers containing the P_6O_{18} ring anions and $[Cu(H_2O)_6]$ octahedra alternate with layers containing the organic groups, along the a axis. For both compounds, H-atom positions have been refined and the networks of hydrogen bonds are described.

Introduction. A series of ethylenediammonium–divalent cation–*cyclo*-tetraphosphate compounds has been previously reported by the authors. These compounds have very different stoichiometries: $Ca[eda]P_4O_{12}.15/2H_2O$ (Averbuch-Pouchot, Durif & Guitel, 1988);* $M[eda]P_4O_{12}.5H_2O$ for M = Pb or Sr (Bagieu-Beucher, Durif & Guitel, 1988); $M[eda]_3[P_4O_{12}]_2.14H_2O$ for M = Cu, Ni, Co, Mn, Mg, Zn and Cd (Averbuch-Pouchot & Durif, 1989).

The present work reports the first results we obtained in a similar systematic study, but this time with a larger-ring phosphoric anion: P_6O_{18}.

Experimental.

(I) *Tris(ethylenediammonium) cyclo-hexaphosphate dihydrate*, $3[NH_3(CH_2)_2NH_3]^{2+}.(P_6O_{18})^{6-}.2H_2O$

Single crystals were prepared by using a process deriving from the Boullé metathesis reaction (Boullé, 1938) but involving in the present case the use of $Ag_6P_6O_{18}.H_2O$, recently described (Averbuch-Pouchot, 1989).

The reaction is:

$$3(eda)Cl_2 + Ag_6P_6O_{18}.H_2O \rightarrow 6AgCl + (eda)_3P_6O_{18}.$$

After filtration of the insoluble silver chloride the resulting solution is kept at room temperature until the formation of large stout colourless monoclinic prisms of $(eda)_3P_6O_{18}.2H_2O$.

Crystal size: 0·30 × 0·30 × 0·35 mm. Density not measured. Philips PW1100 diffractometer, graphite monochromator. Systematic absences: $h0l$ ($h + l =$

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* eda = $C_2H_{10}N_2$.

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$2n$); $0k0$ ($k = 2n$). 22 reflections ($13 < \theta < 14{\cdot}5°$) for refining the unit-cell dimensions. $\omega/2\theta$ scan. 3491 reflections collected ($3 < \theta < 30°$), $\pm h, k, l$, $h_{\max} = 15$, $k_{\max} = 17$, $l_{\max} = 13$. Scan width: 1·20°, scan speed: $0{\cdot}03°\ \mathrm{s}^{-1}$, total background measuring time 10 s. Two intensity and orientation reference reflections every two hours (145 and $1\bar{4}5$), no variation. Lorentz and polarization corrections, no absorption correction. 3314 unique reflections ($R_{\mathrm{int}} = 0{\cdot}028$).

Structure solved by direct methods (*MULTAN*77; Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1977). H atoms from difference-Fourier synthesis. Anisotropic full-matrix least-squares refinement (on F), isotropic for H atoms. Unit weights. Final refinement cycles with 2530 reflections corresponding to $I > 9\sigma_I$. Final $R = 0{\cdot}030$ ($wR = 0{\cdot}039$), $S = 0{\cdot}948$, max. $\Delta/\sigma = 0{\cdot}05$. Max. peak height in the final difference-Fourier synthesis $0{\cdot}46\ \mathrm{e\ Å^{-3}}$. No extinction correction. For the total set of 3314 unique reflections, $R = 0{\cdot}037$. Scattering factors for neutral atoms and f', f'' from *International Tables for X-ray Crystallography* (1974). Enraf–Nonius (1977) *SDP* used for all calculations. Computer used: MicroVAX II.*

(II) *Copper bis(ethylenediammonium) cyclo-hexaphosphate hexahydrate*, $\mathrm{Cu^{2+}.[NH_3(CH_2)_2NH_3]_2^{2+}.(P_6O_{18})^{6-}.6H_2O}$

Single crystals prepared by a process similar to that described for the first compound; they appear as turquoise stout monoclinic prisms or rectangular platelets.

Crystal size: 0·55 × 0·14 × 0·64 mm. Density not measured. Phillips PW 1100 diffractometer, graphite monochromator. Systematic absences: $h0l$ ($h = 2n$), $0k0$ ($k = 2n$). 19 reflections ($0 < \theta < 20°$) for refining the unit-cell dimensions. $\omega/2\theta$ scan.

Table 1. *Final atomic coordinates for* $(eda)_3\mathrm{P_6O_{18}.2H_2O}$

$B_{\mathrm{eq}} = (4/3)\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	B_{eq}(Å^2)
P(1)	0·09060 (5)	0·16826 (5)	0·12389 (6)	1·300 (8)
P(2)	0·24871 (5)	0·97280 (5)	0·14304 (6)	1·273 (8)
P(3)	0·33951 (5)	0·39202 (5)	0·63381 (6)	1·454 (9)
O(*E*11)	0·1139 (2)	0·2248 (2)	0·2603 (2)	2·32 (3)
O(*E*12)	0·4288 (2)	0·7341 (1)	0·5082 (2)	1·96 (3)
O(*L*13)	0·4817 (1)	0·4175 (1)	0·6413 (2)	1·75 (3)
O(*L*12)	0·6985 (2)	0·4125 (1)	0·5878 (2)	1·90 (3)
O(*L*23)	0·1828 (2)	0·8901 (1)	0·0365 (2)	1·90 (3)
O(*E*21)	0·6202 (2)	0·0230 (2)	0·8848 (2)	2·21 (3)
O(*E*22)	0·2015 (2)	0·9478 (2)	0·2877 (2)	1·92 (3)
O(*E*31)	0·7765 (2)	0·0153 (2)	0·2007 (2)	2·03 (3)
O(*E*32)	0·8161 (2)	0·2193 (2)	0·1866 (2)	2·33 (3)
N(11)	0·9186 (2)	0·3409 (2)	0·4128 (2)	1·80 (3)
N(21)	0·0178 (2)	0·1635 (2)	0·7163 (2)	2·24 (4)
C(11)	0·0176 (3)	0·7325 (2)	0·3507 (3)	2·24 (4)
C(21)	0·0803 (2)	0·7551 (2)	0·4929 (3)	1·84 (4)
N(2)	0·6534 (2)	0·0545 (2)	0·4540 (2)	1·65 (3)
C(2)	0·0416 (2)	0·5109 (2)	0·9379 (2)	1·84 (4)
O(*W*)	0·2966 (2)	0·6355 (2)	−0·0086 (2)	2·78 (4)

5385 reflections collected ($3 < \theta < 35°$), $\pm h, k, l$; $h_{\max} = 21$, $k_{\max} = 18$, $l_{\max} = 13$. Scan width = 1·20°, scan speed: $0{\cdot}03°\ \mathrm{s}^{-1}$, total background measuring time 6 s. Two intensity and orientation reference reflections every two hours: ($4\bar{4}4$, $\bar{4}4\bar{4}$) no variation. Lorentz and polarization corrections, no absorption correction. 5120 unique reflections ($R_{\mathrm{int}} = 0{\cdot}02$). Structure solved with the same stategy as for compound (I). Final refinement cycles with 3646 reflections corresponding to $I > 9\sigma_I$. Final $R = 0{\cdot}032$ ($wR = 0{\cdot}038$), $S = 0{\cdot}983$, max. $\Delta/\sigma = 0{\cdot}03$. Max. peak height in the final difference-Fourier synthesis $0{\cdot}770\ \mathrm{e\ Å^{-3}}$. No extinction correction. For the total set of 5120 unique reflections $R = 0{\cdot}040$.

Discussion.

(I) $(eda)_3\mathrm{P_6O_{18}.2H_2O}$

Table 1 reports the final atomic coordinates for the non-H atoms.

The $\mathrm{P_6O_{18}}$ *ring anion*. The two $\mathrm{P_6O_{18}}$ ring anions are located around the inversion centres at (000) and ($\frac{1}{2}\frac{1}{2}\frac{1}{2}$). As previously observed in centrosymmetric $\mathrm{P_6O_{18}}$ groups, the three P—P—P angles are very significantly different: here $91{\cdot}76 < \mathrm{P—P—P} < 111{\cdot}90°$. This result is to be compared with what was observed in $\mathrm{Cu_3P_6O_{18}.14H_2O}$ (Averbuch-Pouchot & Durif, 1989) in which P—P—P varies from 96·3 to 139·9°. On the other hand, the local arrangement around one $\mathrm{PO_4}$ tetrahedron and the P—O—P bond angles are quite similar to what is normally observed in all other condensed phosphoric anions. Table 2 reports the main interatomic distances and bond angles in this $\mathrm{P_6O_{18}}$ ring anion.

The ethylenediammonium groups. Two types of ethylenediammonium groups coexist in this atomic arrangement. The first one, built up of C(11), C(21), N(11) and N(21), has no internal symmetry, while the second one is centrosymmetric, located around the inversion centres ($0\frac{1}{2}0$) and ($\frac{1}{2}0\frac{1}{2}$). The conformations of these two groups are reported in Table 2.

The atomic arrangement may be considered as a succession of two types of layers perpendicular to the b axis. The first type of layer ($y \sim 0$ and 0·5) contains the phosphoric groups, the centrosymmetric ethylenediammonium groups and the water molecules. These layers alternate with layers ($y \sim 0{\cdot}25$, 0·75) containing the second kind of organic group (Fig. 1).

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* Lists of structure factors, anisotropic thermal parameters for non-H atoms, H-atom coordinates, and bonds and angles involving H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52136 (58 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Main interatomic distances* (Å) *and bond angles* (°) *in* $(eda)_3P_6O_{18}.2H_2O$

The P_6O_{18} ring

$P(1)O_4$ tetrahedron

P(1)	O(*E*11)	O(*E*12)	O(*L*13)	O(*L*12)
O(*E*11)	1·472 (2)	2·550 (2)	2·532 (2)	2·522 (2)
O(*E*12)	118·8 (1)	1·490 (2)	2·539 (2)	2·454 (2)
O(*L*13)	110·3 (1)	109·8 (1)	1·611 (2)	2·455 (2)
O(*L*12)	110·7 (1)	105·5 (1)	110·07 (9)	1·592 (2)

$P(2)O_4$ tetrahedron

P(2)	O(*L*12)	O(*L*23)	O(*E*21)	O(*E*22)
O(*L*12)	1·602 (2)	2·484 (2)	2·436 (2)	2·540 (2)
O(*L*23)	101·95 (9)	1·596 (2)	2·531 (2)	2·459 (2)
O(*E*21)	104·5 (1)	110·8 (1)	1·477 (2)	2·584 (2)
O(*E*22)	110·6 (1)	105·8 (1)	121·4 (1)	1·486 (2)

$P(3)O_4$ tetrahedron

P(3)	O(*L*13)	O(*L*23)	O(*E*31)	O(*E*32)
O(*L*13)	1·605 (2)	2·476 (2)	2·484 (2)	2·527 (2)
O(*L*23)	100·82 (9)	1·608 (2)	2·547 (2)	2·482 (2)
O(*E*31)	107·3 (1)	111·1 (1)	1·479 (2)	2·554 (3)
O(*E*32)	109·9 (1)	106·9 (1)	119·3 (1)	1·481 (2)

P(1)—O(*L*13)—P(3)	126·9 (1)	P(1)—P(2)	2·9803 (8)
P(1)—O(*L*12)—P(2)	137·8 (1)	P(1)—P(3)	2·8779 (8)
P(2)—O(*L*23)—P(3)	132·3 (1)	P(2)—P(3)	2·9300 (8)

P(2)—P(1)—P(3)	110·85 (2)
P(1)—P(2)—P(3)	91·76 (2)
P(1)—P(3)—P(2)	111·90 (2)

The ethylenediammonium groups

The first group

N(11)—C(21)	1·475 (3)	N(11)—C(21)—C(11)	112·1 (2)
C(21)—C(11)	1·518 (3)	N(21)—C(11)—C(21)	109·2 (2)
C(11)—N(21)	1·477 (3)		

The second group

N(2)—C(2)	1·482 (3)	N(2)—C(2)—C(2)	109·8 (2)
C(2)—C(2)	1·512 (3)		

The hydrogen-bond network

N(O)—H···O	N(O)—H	H···O	N(O)···O	N(O)—H···O
N(11)—H(1N11)···O(*E*21)	0·86 (3)	2·04 (3)	2·803 (3)	147 (3)
N(11)—H(2N11)···O(*E*21)	0·90 (3)	2·17 (3)	2·968 (3)	149 (3)
N(11)—H(3N11)···O(*E*32)	0·90 (4)	1·94 (4)	2·819 (3)	164 (4)
N(21)—H(1N21)···O(*W*)	0·87 (3)	2·10 (3)	2·859 (3)	145 (3)
N(21)—H(2N21)···O(*E*12)	0·88 (3)	1·92 (3)	2·776 (3)	165 (3)
N(21)—H(3N21)···O(*E*22)	0·99 (3)	1·81 (3)	2·786 (3)	168 (3)
N(2)—H(1N2)···O(*E*12)	0·83 (3)	1·95 (3)	2·781 (3)	175 (3)
N(2)—H(2N2)···O(*E*22)	0·90 (3)	2·04 (3)	2·886 (3)	156 (3)
N(2)—H(3N2)···O(*E*31)	0·95 (3)	1·84 (3)	2·783 (3)	173 (3)
O(*W*)—H(1*W*)···O(*E*11)	0·96 (4)	1·78 (4)	2·745 (3)	176 (3)
O(*W*)—H(2*W*)···O(*E*32)	0·82 (4)	1·96 (4)	2·735 (3)	157 (3)

H(1*W*)—O(*W*)—H(2*W*)	100 (3)

Table 3. *Final atomic coordinates for* $Cu(eda)_2P_6O_{18}.6H_2O$

$B_{eq} = (4/3)\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$

	x	*y*	*z*	B_{eq}(Å^2)
Cu	0	0	0	1·861 (6)
P(1)	−0·00386 (4)	0·24000 (4)	0·48056 (7)	1·506 (8)
P(2)	0·07866 (4)	0·37628 (5)	0·75847 (7)	1·487 (8)
P(3)	0·34987 (4)	0·11241 (5)	0·26756 (6)	1·397 (8)
O(*E*11)	0·9253 (1)	0·1710 (2)	0·5521 (2)	2·36 (3)
O(*E*12)	0·5924 (1)	0·3123 (2)	0·4560 (2)	2·42 (3)
O(*L*12)	−0·0232 (1)	0·6404 (1)	0·4246 (2)	1·81 (3)
O(*L*13)	0·4346 (1)	0·2124 (1)	0·3139 (2)	2·06 (3)
O(*E*21)	0·6854 (1)	0·1667 (2)	0·7831 (2)	2·41 (3)
O(*E*22)	−0·0102 (1)	0·6675 (2)	0·1421 (2)	2·30 (3)
O(*L*23)	0·0758 (1)	0·5135 (1)	0·7692 (2)	2·03 (3)
O(*E*31)	0·1924 (1)	0·5803 (2)	0·5951 (2)	2·21 (3)
O(*E*32)	0·7817 (1)	0·3491 (2)	0·1181 (2)	2·66 (3)
N(1)	0·7052 (2)	0·8622 (2)	0·2852 (3)	2·17 (3)
C(1)	0·2514 (2)	0·0308 (2)	0·7684 (3)	2·45 (4)
C(2)	0·1923 (2)	0·4224 (2)	0·2584 (3)	2·34 (4)
N(2)	0·2798 (1)	0·8826 (2)	0·5744 (3)	2·13 (3)
O(*W*1)	0·4601 (2)	0·5015 (2)	0·7648 (2)	3·98 (5)
O(*W*2)	0·8634 (1)	0·1240 (2)	0·0052 (3)	3·18 (4)
O(*W*3)	0·5809 (1)	0·3622 (2)	0·0021 (3)	3·91 (4)

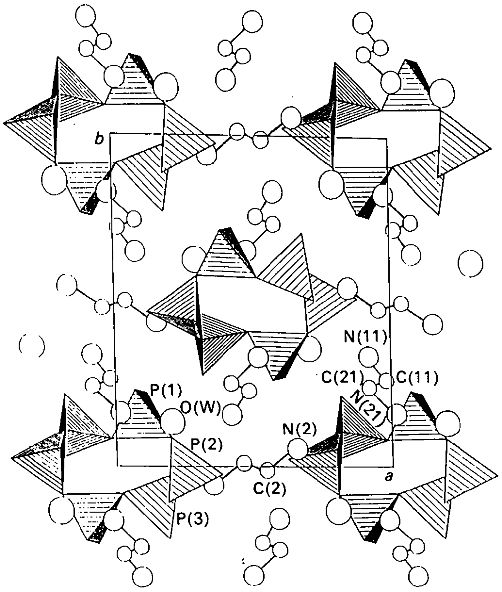

Fig. 1. Projection of the atomic arrangement of $(eda)_3P_6O_{18}.2H_2O$ along the *c* axis. H atoms are omitted.

A three-dimensional network of hydrogen bonds connecting these two types of layers is described in Table 2.

(II) $Cu(eda)_2P_6O_{18}.6H_2O$

Table 3 reports the final atomic coordinates for the non-H atoms.

The P_6O_{18} *ring anion.* As in the first compound, the P_6O_{18} ring anion is centrosymmetric and here located around the $(\frac{1}{2}00)$ and $(0\frac{1}{2}0)$ inversion centres. The ring is significantly more regular than in the first compound as can be seen from the P—P—P angles: 106·51 < P—P—P < 121·09°. The main geometrical features of the phosphoric ring are reported in Table 4.

The copper coordination. The copper coordination polyhedron is a distorted octahedron built up of six water molecules and so has no common edge or corner with the phosphoric anion. This coordination

Table 4. *Main interatomic distances* (Å) *and bond angles* (°) *in* Cu(*eda*)$_2$P$_6$O$_{18}$.6H$_2$O

The P$_6$O$_{18}$ ring anion

P(1)O$_4$ tetrahedron

P(1)	O(*E*11)	O(*E*12)	O(*L*12)	O(*L*13)
O(*E*11)	1·480 (2)	2·565 (3)	2·530 (2)	2·497 (2)
O(*E*12)	120·04 (10)	1·481 (2)	2·516 (2)	2·476 (2)
O(*L*12)	109·87 (10)	108·90 (9)	1·610 (2)	2·457 (2)
O(*L*13)	108·69 (9)	107·26 (11)	100·23 (8)	1·592 (2)

P(2)O$_4$ tetrahedron

P(2)	O(*L*12)	O(*E*21)	O(*E*22)	O(*L*23)
O(*L*12)	1·606 (2)	2·505 (2)	2·519 (2)	2·441 (2)
O(*E*21)	108·40 (10)	1·481 (2)	2·570 (3)	2·537 (2)
O(*E*22)	109·17 (9)	120·23 (10)	1·483 (2)	2·461 (2)
O(*L*23)	99·54 (8)	111·23 (9)	106·28 (10)	1·592 (2)

P(3)O$_4$ tetrahedron

P(3)	O(*L*13)	O(*L*23)	O(*E*31)	O(*E*32)
O(*L*13)	1·606 (2)	2·407 (2)	2·541 (3)	2·449 (2)
O(*L*23)	97·51 (9)	1·595 (2)	2·528 (3)	2·504 (2)
O(*E*31)	110·88 (9)	110·57 (10)	1·479 (2)	2·569 (3)
O(*E*32)	105·23 (10)	109·20 (10)	120·8 (1)	1·475 (2)

P(1)—P(2)	2·8848 (7)	P(1)—O(*L*12)—P(2)	127·5 (1)
P(2)—P(3)	2·9211 (7)	P(1)—O(*L*23)—P(3)	132·8 (1)
P(1)—P(3)	2·9194 (7)	P(1)—O(*L*13)—P(3)	131·8 (1)

P(1)—P(2)—P(3)	121·09 (2)
P(2)—P(3)—P(1)	114·36 (2)
P(2)—P(1)—P(3)	106·51 (2)

Cu(H$_2$O)$_6$ octahedron

Cu—O(*W*1)	1·991 (2) × 2	O(*W*1)—Cu—O(*W*2)	90·19 (9) × 2
Cu—O(*W*2)	2·332 (2) × 2	O(*W*1)—Cu—O(*W*3)	92·06 (10) × 2
Cu—O(*W*3)	1·925 (2) × 2	O(*W*2)—Cu—O(*W*3)	93·92 (8) × 2

The organic group

C(1)—C(2)	1·508 (4)	N(1)—C(1)—C(2)	113·6 (2)
N(1)—C(1)	1·486 (3)	N(2)—C(2)—C(1)	112·7 (2)
N(2)—C(2)	1·488 (3)		

The hydrogen-bond network

N(O)—H···O	N(O)—H	H···O	N(O)···O	N(O)—H···O
N(1)—H(1N1)···O(*E*31)	0·93 (4)	1·92 (4)	2·816 (3)	162 (4)
N(1)—H(2N1)···O(*E*22)	0·98 (4)	1·93 (4)	2·888 (2)	166 (4)
N(1)—H(3N1)···O(*E*21)	1·01 (5)	1·82 (4)	2·830 (3)	175 (4)
N(2)—H(1N2)···O(*E*11)	1·01 (4)	1·78 (4)	2·783 (2)	177 (4)
N(2)—H(2N2)···O(*E*12)	0·92 (4)	1·96 (4)	2·879 (3)	174 (4)
N(2)—H(3N2)···O(*E*31)	0·84 (4)	1·92 (4)	2·792 (3)	155 (4)
O(*W*1)—H(1*W*1)···O(*E*12)	0·78 (5)	2·12 (5)	2·863 (3)	159 (5)
O(*W*1)—H(2*W*1)···O(*E*11)	0·75 (5)	1·95 (5)	2·688 (3)	169 (5)
O(*W*2)—H(1*W*2)···O(*E*21)	0·75 (4)	2·03 (4)	2·747 (2)	161 (5)
O(*W*2)—H(2*W*2)···O(*E*32)	0·83 (5)	2·33 (5)	3·071 (3)	147 (4)
O(*W*3)—H(1*W*3)···O(*E*22)	0·86 (4)	1·81 (5)	2·646 (3)	165 (5)
O(*W*3)—H(2*W*3)···O(*E*32)	0·70 (4)	1·96 (4)	2·650 (3)	170 (5)

H(1*W*1)—O(*W*1)—H(2*W*1)	108 (5)
H(1*W*2)—O(*W*2)—H(2*W*2)	113 (4)
H(1*W*3)—O(*W*3)—H(2*W*3)	122 (5)

polyhedron is centrosymmetric, Cu atoms being located on inversion centres (000) and ($\frac{1}{2}\frac{1}{2}0$). The Cu—H$_2$O distances range from 1·925 to 2·332 Å (Table 4).

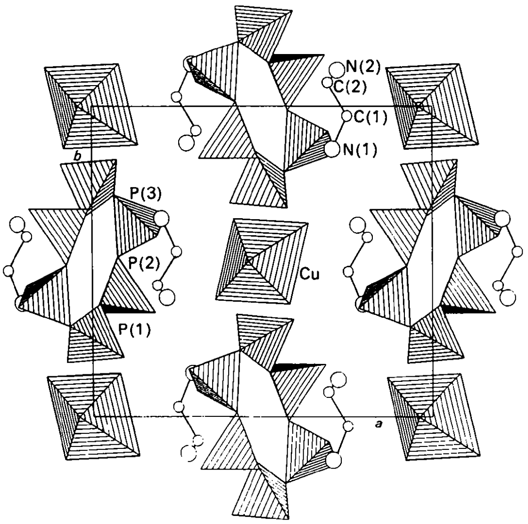

Fig. 2. Projection of the atomic arrangement of Cu(eda)$_2$P$_6$O$_{18}$.6H$_2$O along the *c* axis. H atoms are omitted.

The atomic arrangement can be clearly understood as a succession of two kinds of layers perpendicular to the *a* axis (Fig. 2). In the first type of layers are located the P$_6$O$_{18}$ groups and the Cu(H$_2$O)$_6$ octahedra. Alternating with these layers, one finds at $x \sim 0{\cdot}25$ and 0·75 the second type of layers containing the organic groups.

These two types of layers are interconnected by a three-dimensional network of hydrogen bonds, described in Table 4.

Drawings were made using the *STRUPLO* system (Fischer, 1985).

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