Table 3. *Hydrogen-bond geometry* (Å *and* °)

O—H···O	O···O	O···H	O—H···O
O(7)—H(7)···O(3^{i})	2·776 (5)	1·99 (9)	136 (7)
O(7)—H(71)···O(3^{ii})	2·839 (5)	1·87 (7)	175 (6)
O(8)—H(8)···O(3^{iii})	2·768 (6)	1·82 (6)	164 (5)
O(8)—H(81)···O(9)	2·836 (6)	2·20 (5)	122 (5)
O(9)—H(9)···O(6^{iv})	2·796 (6)	1·99 (7)	139 (8)
O(9)—H(91)···O(3^{ii})	2·780 (6)	1·81 (5)	174 (5)

Symmetry code: (i) $x + 0·5, 1·5 - y, z - 1$; (ii) $x, y, z - 1$; (iii) $1 + x, y, z - 1$; (iv) $1 - x, 1 - y, 1 - z$.

molecules and is therefore formally pentacoordinated. A similar type of hydrogen bonding was earlier observed, *e.g.* in trisodium D-2-phosphoglycerate hexahydrate (Lis, 1985).

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Crystal Chemistry of *cyclo*-Hexaphosphates. IX. Structure of Tetraammonium Dimanganese *cyclo*-Hexaphosphate Oxalate Hexahydrate

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Abstract. $Mn_2(NH_4)_4(P_6O_{18})(C_2O_4).6H_2O$, $M_r = 851·966$, triclinic, $P\bar{1}$, $a = 9·747 (3)$, $b = 9·751 (3)$, $c = 7·689 (3)$ Å, $\alpha = 99·92 (5)$, $\beta = 105·88 (5)$, $\gamma = 100·08 (5)$°, $V = 673·1$ Å^3, $Z = 1$, $D_x = 2·101$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 1·465$ mm^{-1}, $F(000) = 432$, $T = 294$ K, final $R = 0·030$ for 2577 reflections. The atomic arrangement is built up by infinite ribbons of P_6O_{18} ring anions and MnO_6 octahedra spreading parallel to the b axis. These ribbons are themselves interconnected by the oxalic groups located between two MnO_6 octahedra belonging to two different ribbons. The hydrogen-bond scheme is described.

Introduction. Phosphates with two different phosphoric anions of different degrees of condensation are becoming more and more familiar. A review of this type of compound has recently been reported by one of us (Averbuch-Pouchot, 1985). But up to now the coexistence in an atomic arrangement of a condensed phosphoric anion with a non-phosphoric one has not been reported. In this work we describe what we believe is the first example of such a compound: manganese ammonium *cyclo*-hexaphosphate oxalate hexahydrate, $Mn_2(NH_4)_4(P_6O_{18})(C_2O_4).6H_2O$. In fact, in a good number of compounds (Boudjada, 1985), a condensed phosphoric anion coexists with a $Te(OH)_6$ group but due to the neutrality of the telluric acid they cannot be considered as mixed-anion salts but as adducts.

Experimental. Crystals of the title compound have been prepared by slow diffusion of an aqueous solution of manganese oxalate into an aqueous solution

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of ammonium *cyclo*-hexaphosphate. After some days at room temperature, crystals of the title compound appeared with various morphologies; short, stout multifaceted prisms, sometimes elongated, calcite-like or thick diamond-like plates. They are very slightly water soluble and stable for months at room temperature.

Crystal size: 0·16 × 0·16 × 0·11 mm. Density not measured. Philips PW1100 diffractometer, graphite monochromator. 20 reflections ($11{\cdot}0 < \theta < 13{\cdot}5°$) for refining unit-cell dimensions. ω scan; scan width 1·20°; scan speed 0·02° s^{-1}. Total background measuring time 10 s. 3187 reflections collected ($3 < \theta < 30°$); $\pm h$, $\pm k$, l; $h_{max} = 13$, $k_{max} = 13$, $l_{max} = 10$. Two orientation and intensity control reflections (023 and $0\overline{23}$) measured every four hours without any significant variation. 2951 reflections obtained after averaging Friedel pairs ($R_{int} = 0{\cdot}013$). Lorentz and polarization corrections, no absorption correction. Structure solved by direct methods with *MULTAN*77 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1977). H atoms located by difference Fourier syntheses. Anisotropic full-matrix least-squares refinement (on F), isotropic for H atoms. Unit weights. Final refinements with 2577 reflections corresponding to $I > 4\sigma_I$. Final $R = 0{\cdot}030$ ($wR = 0{\cdot}034$), $S = 0{\cdot}896$, max. $\Delta/\sigma = 0{\cdot}06$, max. peak height in the final difference Fourier synthesis = 0·429 e $Å^{-3}$. Secondary extinction refined according to Stout & Jensen (1968) to $g = 6{\cdot}3 \times 10^{-7}$. 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. For the complete set of 2951 reflections, the R value is 0·035.

Discussion. Table 1 reports the final atomic coordinates.*

The P_6O_{18} ring anion develops around the inversion centre located at ($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$) and so is built by only three independent PO_4 tetrahedra. As is commonly observed for P_6O_{18} anions with $\overline{1}$ internal symmetry, the ring is significantly distorted. The P—P—P angles vary between 93·14 and 116·13°. This distortion is comparatively much less important than that observed in some *cyclo*-hexaphosphates. In $Cs_6P_6O_{18}.6H_2O$ for instance, the same angles spread between 93·2 and 145·5° (Averbuch-Pouchot & Durif, 1989). In spite of this distortion the local arrangement observed for the PO_4 tetrahedra (P—O distances and P—O—P or O—P—O angles as well as P—P distances) are in accordance with values generally observed in condensed phosphoric anions. The main geometrical features of this ring are reported in Table 2.

Table 1. *Final atomic coordinates and* B_{eq} *with e.s.d.'s in parentheses*

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

	x	y	z	B_{eq} ($Å^2$)
Mn	0·84208 (5)	0·11847 (4)	0·70887 (6)	1·190 (7)
P(1)	0·17081 (7)	0·40931 (7)	0·37697 (9)	1·09 (1)
P(2)	0·63293 (8)	−0·21426 (7)	0·6301 (1)	1·19 (1)
P(3)	0·37492 (8)	−0·35663 (7)	0·3171 (1)	1·20 (1)
O(*E*11)	0·0394 (2)	0·4170 (2)	0·2285 (3)	1·68 (4)
O(*E*12)	0·1536 (2)	0·3809 (2)	0·5538 (3)	1·83 (4)
O(*L*12)	0·7575 (2)	0·7064 (2)	0·7169 (3)	1·48 (4)
O(*L*13)	0·7060 (2)	0·4459 (2)	0·5685 (3)	1·73 (4)
O(*E*21)	0·7029 (3)	−0·0871 (2)	0·5761 (3)	2·05 (5)
O(*E*22)	0·5459 (2)	−0·1985 (3)	0·7583 (3)	2·24 (5)
O(*L*23)	0·5419 (2)	−0·3315 (2)	0·4408 (3)	1·52 (4)
O(*E*31)	0·3591 (3)	−0·4438 (3)	0·1318 (3)	2·04 (5)
O(*E*32)	0·3339 (2)	−0·2169 (2)	0·3301 (4)	2·28 (5)
O(1)	0·0348 (2)	0·0210 (2)	0·7936 (3)	1·69 (4)
O(2)	0·1451 (2)	0·9156 (2)	0·0101 (3)	1·84 (4)
O(*W*1)	0·9075 (3)	0·1655 (3)	0·4750 (3)	2·09 (5)
O(*W*2)	−0·0020 (3)	0·6739 (2)	0·1387 (3)	1·92 (4)
O(*W*3)	0·5653 (4)	0·9481 (3)	0·1881 (5)	5·34 (8)
N(1)	0·3020 (3)	0·2850 (3)	0·8798 (4)	2·36 (6)
N(2)	0·7216 (3)	0·2989 (4)	0·1666 (4)	2·71 (6)
C	0·9476 (3)	0·0192 (3)	0·0564 (4)	1·27 (5)

The oxalic group, C_2O_4, is centrosymmetric and located around the inversion centre at (0, 0, 0). All its O atoms take part in the coordination of the Mn atom. The coordination polyhedron of this Mn atom is a distorted octahedron built up by two O atoms shared with the phosphoric ring, two water molecules and two O atoms belonging to the oxalic group. The main geometrical features of this coordination polyhedron are reported in Table 2.

As shown in Fig. 1, this atomic arrangement can easily be described as a succession of ribbons parallel to the **b** direction and built up by the phosphoric ring anions and the managanese octahedra. These ribbons are themselves interconnected through the oxalic groups. Due to this connection of the ribbons by the organic groups, an unusual situation occurs around the inversion centre located at the origin of the unit cell. Two manganese octahedra are related by this inversion centre and a very short O—O distance [O(1)—O(2) = 2·232 Å] is observed between the two polyhedra. This situation is depicted schematically in Fig. 2.

Within a distance of 3·5 Å the two ammonium groups N(1) and N(2) are surrounded by nine and seven O atoms respectively. The N—O distances in these two polyhedra are reported in Table 2.

The three-dimensional network of hydrogen bonds interconnecting the components of this atomic arrangement is described in Table 2. As is usual in compounds involving a condensed phosphoric anion,

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* Lists of structure factors, anisotropic thermal parameters, 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 52641 (25 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Main interatomic distances* (Å) *and bond angles* (°) *in the atomic arrangement of* $Mn_2(NH_4)_4(P_6O_{18})(C_2O_4).6H_2O$ *with e.s.d.'s in parentheses*

The P_6O_{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)	1·487 (2)	2·557 (3)	2·469 (3)	2·526 (3)
O(*E*12)	118·9 (1)	1·481 (2)	2·538 (3)	2·460 (3)
O(*L*12)	106·3 (1)	111·0 (1)	1·598 (2)	2·499 (3)
O(*L*13)	110·2 (1)	106·3 (1)	103·1 (1)	1·593 (2)

$P(2)O_4$ tetrahedron

P(2)	O(*L*12)	O(*E*21)	O(*E*22)	O(*L*23)
O(*L*12)	1·607 (2)	2·514 (3)	2·478 (4)	2·465 (3)
O(*E*21)	108·7 (1)	1·487 (2)	2·569 (4)	2·484 (3)
O(*E*22)	107·1 (1)	120·5 (1)	1·472 (3)	2·546 (3)
O(*L*23)	100·2 (1)	106·8 (1)	111·6 (1)	1·606 (2)

$P(3)O_4$ tetrahedron

P(3)	O(*L*13)	O(*L*23)	O(*E*31)	O(*E*32)
O(*L*13)	1·600 (3)	2·454 (3)	2·555 (4)	2·492 (3)
O(*L*23)	100·4 (1)	1·596 (2)	2·474 (3)	2·502 (3)
O(*E*31)	112·0 (1)	107·0 (1)	1·481 (2)	2·552 (3)
O(*E*32)	107·9 (1)	108·8 (1)	119·0 (1)	1·480 (2)

P(2)—P(1)—P(3)	93·14 (3)	P(1)—P(2)	2·928 (1)
P(1)—P(2)—P(3)	103·61 (3)	P(1)—P(3)	2·942 (1)
P(1)—P(3)—P(2)	116·13 (3)	P(2)—P(3)	2·891 (1)

P(1)—O(*L*12)—P(2)	132·0 (1)
P(2)—O(*L*23)—P(3)	129·2 (1)
P(1)—O(*L*13)—P(3)	134·3 (1)

The MnO_6 octahedron

Mn	O(*E*21)	O(*E*32)	O(1)	O(2)	O(*W*1)	O(*W*2)
O(*E*21)	2·118 (2)	3·035 (3)	3·101 (3)	3·136 (3)	3·230 (3)	4·346 (3)
O(*E*32)	92·47 (9)	2·085 (2)	4·316 (3)	3·249 (3)	3·181 (4)	3·102 (3)
O(1)	90·62 (8)	171·91 (9)	2·242 (2)	2·692 (3)	3·108 (3)	3·019 (3)
O(2)	92·69 (9)	98·1 (1)	74·29 (9)	2·216 (2)	4·314 (3)	2·997 (3)
O(*W*1)	98·12 (9)	97·1 (1)	89·86 (9)	160·94 (8)	2·158 (3)	2·918 (3)
O(*W*2)	175·28 (9)	91·81 (8)	84·88 (8)	84·74 (8)	83·31 (8)	2·231 (2)

The NH_4O_n polyhedra

N(1)—O(*E*12)	2·923 (4)	N(2)—O(*E*11)	2·983 (4)
N(1)—O(*L*12)	3·297 (4)	N(2)—O(*E*12)	3·283 (4)
N(1)—O(*E*22)	3·104 (4)	N(2)—O(*L*13)	3·230 (4)
N(1)—O(*L*23)	3·285 (4)	N(2)—O(*E*22)	2·866 (4)
N(1)—O(*E*31)	2·861 (4)	N(2)—O(*E*31)	2·898 (4)
N(1)—O(*E*31)	3·426 (4)	N(2)—O(2)	2·974 (4)
N(1)—O(1)	3·158 (3)	N(2)—O(*W*1)	3·184 (4)
N(1)—O(*W*2)	2·989 (4)		
N(1)—O(*W*3)	2·846 ()		

The C_2O_4 group

C—C	1·564 (4)	O(1)—C—O(2)	126·4 (3)
C—O(1)	1·259 (4)	C—C—O(1)	116·0 (3)
C—O(2)	1·242 (4)	C—C—O(2)	117·7 (3)

The hydrogen bonds

O(N)—H···O	O(N)—H	H···O	O(N)—O	O(N)—N···O
N(1)—H(1N1)···O(*W*3)	0·89 (5)	1·99 (5)	2·846 (5)	160 (4)
N(1)—H(2N1)···O(*E*12)	0·80 (6)	2·22 (5)	2·923 (4)	146 (5)
N(1)—H(3N1)···O(1)	0·90 (6)	2·36 (5)	3·158 (3)	148 (6)
N(1)—H(4N1)···O(*E*31)	0·94 (4)	1·98 (4)	2·861 (4)	154 (4)
N(2)—H(1N2)···O(2)	0·80 (6)	2·20 (6)	2·974 (4)	163 (6)
N(2)—H(2N2)···O(*E*31)	0·81 (6)	2·11 (6)	2·898 (4)	163 (5)
N(2)—H(3N2)···O(*E*22)	0·89 (5)	1·99 (5)	2·867 (4)	169 (4)
N(2)—H(4N2)···O(*E*11)	0·96 (4)	2·35 (6)	2·983 (4)	123 (4)
O(*W*1)—H(1*W*1)···O(*E*12)	0·89 (4)	1·86 (4)	2·745 (3)	172 (4)
O(*W*1)—H(2*W*1)···O(1)	0·84 (5)	1·92 (5)	2·754 (3)	174 (5)
O(*W*2)—H(1*W*2)···O(*E*11)	0·63 (5)	2·09 (5)	2·712 (3)	168 (6)
O(*W*2)—H(2*W*2)···O(*E*11)	0·78 (5)	2·01 (5)	2·778 (3)	168 (4)
O(*W*3)—H(1*W*3)···O(*E*22)	0·93 (6)	1·92 (6)	2·852 (4)	178 (5)
O(*W*3)—H(2*W*3)···O(*E*21)	0·96 (5)	2·10 (6)	3·023 (4)	161 (5)

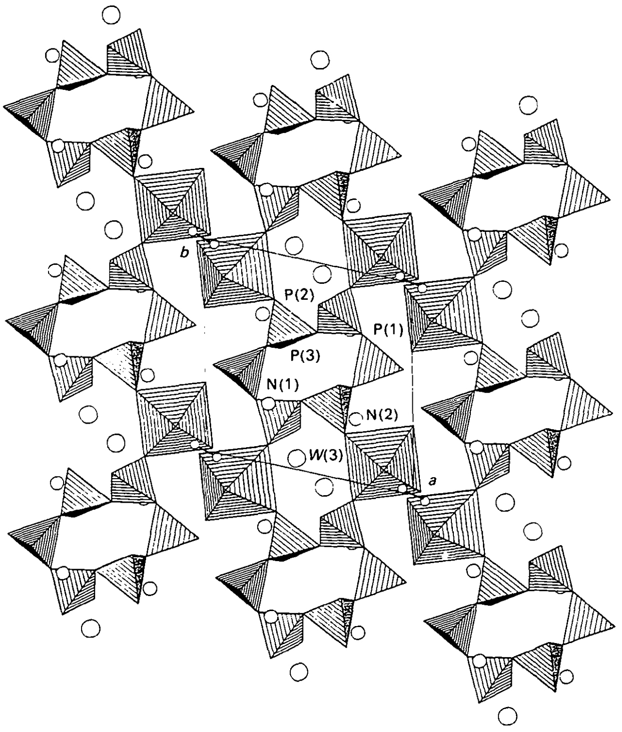

Fig. 1. Projection of the atomic arrangement of $(NH_4)_4Mn_2(P_6O_{18})(C_2O_4).6H_2O$ along the *c* axis.

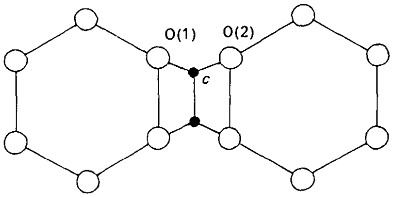

Fig. 2. Schematic representation of the situation around the inversion centre at (0, 0, 0). The two related MnO_6 octahedra are represented by hexagons.

the bonding O atoms [O(*L*)] do not take part in such a network. The drawings were made with *STRUPLO* (Fischer, 1985).

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Crystal Chemistry of *cyclo*-Hexaphosphates. X. Structure of Dicalcium Dilithium *cyclo*-Hexaphosphate Octahydrate

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Abstract. $Ca_2Li_2P_6O_{18}.8H_2O$, $M_r = 711{\cdot}984$, triclinic, $P\bar{1}$, $a = 7{\cdot}767$ (2), $b = 10{\cdot}144$ (3), $c = 7{\cdot}225$ (2) Å, $\alpha = 105{\cdot}17$ (4), $\beta = 102{\cdot}76$ (4), $\gamma = 84{\cdot}95$ (4)°, $V = 535{\cdot}6$ Å^3, $D_x = 2{\cdot}207$ Mg m^{-3}, λ(Mo $K\bar{\alpha}$) = 0·7107 Å, $\mu = 1{\cdot}082$ mm^{-1}, $F(000) = 360$, room temperature, final $R = 0{\cdot}023$ for 2764 reflections. The atomic arrangement can be described as successive layers of planes made by LiO_6 octahedra sharing corners with the P_6O_{18} ring anions. These planes are interconnected in a three-dimensional manner by the CaO_7 polyhedra and the hydrogen bonds. The calcium–sodium salt is isotypic.

Introduction. *cyclo*-Hexaphosphates of monovalent–divalent cations belong to various structural types and have very different degrees of hydration. During a systematic investigation of this type of compound, we previously reported the existence and described the crystal structures of $Mn_2Li_2P_6O_{18}.10H_2O$ (Averbuch-Pouchot, 1989) and $Cd_2Na_2P_6O_{18}.14H_2O$ (Averbuch-Pouchot, 1990). In the present work we describe the chemical preparation and crystal structure of a new compound of this family, $Ca_2Li_2P_6O_{18}.8H_2O$. The calcium–sodium salt $Ca_2Na_2P_6O_{18}.8H_2O$ is isotypic with the following unit-cell dimensions: $a = 8{\cdot}031$ (4), $b = 10{\cdot}296$ (5), $c = 7{\cdot}279$ (3) Å, $\alpha = 105{\cdot}69$ (5), $\beta = 103{\cdot}27$ (5), $\gamma = 85{\cdot}30$ (5)°. Its preparation is similar to that described for the title compound.

Experimental. Crystals of the title compound were prepared by adding solid gypsum to an aqueous solution of lithium *cyclo*-hexaphosphate. After some days of evaporation at room temperature, crystals of $Ca_2Li_2P_6O_{18}.8H_2O$ appeared as elongated triclinic prisms, sparingly soluble in water. The compound is stable for months at room temperature.

Crystal size: 0·18 × 0·22 × 0·12 mm. Density not measured. Phillips PW1100 diffractometer, graphite monochromator. 15 reflections ($13{\cdot}0 < \theta < 17{\cdot}0°$) for refining unit-cell dimensions. $\omega/2\theta$ scan, scan width: 1·20°, scan speed: 0·02° s^{-1}. Total background measuring time: 10 s. 3827 reflections collected ($3 < \theta < 35°$); $\pm h$, $\pm k$, l; $h_{\max} = 12$, $k_{\max} = 16$, $l_{\max} = 10$. Two orientation and intensity control reflections ($\bar{1}2\bar{1}$ and $1\bar{2}1$) measured every three hours without any significant variation. 3556 reflections obtained after averaging Friedel pairs ($R_{\rm int} = 0{\cdot}01$). Lorentz and polarization corrections, no absorption correction. Structure solved by direct methods (*MULTAN77*; Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1977). H atoms located by difference Fourier syntheses. Anisotropic full-matrix least-squares refinement (on F), isotropic for H atoms. Unit weights. Final refinements with 2764 reflections corresponding to $F > 3\sigma_F$. Final $R = 0{\cdot}023$ ($wR = 0{\cdot}028$), $S = 0{\cdot}609$, max. $\Delta/\sigma = 0{\cdot}03$, max. peak height in the final difference Fourier synthesis = 0·552 e Å^{-3}. No secondary-extinction correction. 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.

Discussion. Table 1 reports the final atomic coordinates.* The P_6O_{18} ring anion has $\bar{1}$ internal symmetry and so is built by three independent P atoms. As is commonly observed for six-membered

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52642 (24 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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