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# Structure of Phuralumite


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**Abstract.** $Al_2[(OH)_2(PO_4)_2(UO_2)_3].(OH)_4.10H_2O$ (a mineral from Kobokobo, Kivu, Zaïre), monoclinic, $P2_1/a$, $a = 13{\cdot}836$ (6), $b = 20{\cdot}918$ (6), $c = 9{\cdot}428$ (3) Å, $\beta = 112{\cdot}44$ (3)°, $Z = 4$, $V = 2522$ Å$^3$, $D_m = 3{\cdot}5$, $D_c = 3{\cdot}52$ Mg m$^{-3}$. Structure type: phosphuranylite. The $[(OH)_2(PO_4)_2(UO_2)_3]_n^{2n-}$ layers are connected principally by $Al_4O_{14}$ groups, composed of two octahedra and two trigonal bipyramids sharing edges.


**Introduction.** Phuralumite is a mineral recently described by Deliens & Piret (1979). The results are here completed with the structure determination. The space group was determined from Weissenberg and precession photographs (systematic absences, *hkl*: none; *h*0*l*: $h = 2n + 1$; 0*k*0: $k = 2n + 1$). Final cell dimensions and intensities were measured on a Syntex $P2_1$ four-circle diffractometer with the experimental conditions given in Table 1. Intensities were corrected for absorption by an experimental method (Syntex, 1976). Scattering factors were those given by Cromer & Mann (1968) for neutral atoms; that for U was corrected for anomalous scattering (Cromer, 1965). The structure was solved by the use of the Patterson function. Refinement by Fourier methods and least squares (block-diagonal) gave a final residual $R$ of 0·070 for all observed reflexions.* Calculations were performed with the XRAY system (1972). The final coordinates and temperature factors are given in Table 2.

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34417 (19 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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**Discussion.** The structure consists of $[(OH)_2(PO_4)_2(UO_2)_3]_n^{2n-}$ layers similar to those in phosphuranylite (Shashkin & Sidorenko, 1974), dumontite (Piret-Meunier, Léonard & Van Meerssche,

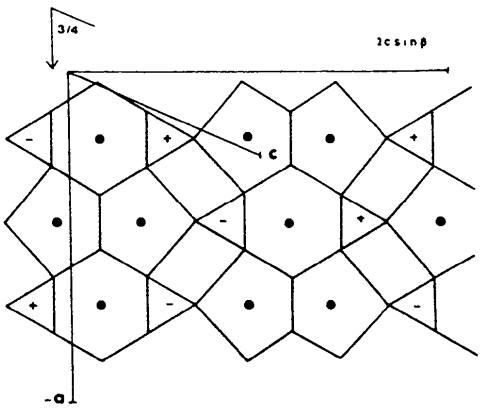


Fig. 1. Idealized $[(OH)_2(PO_4)_2(UO_2)_3]_n^{2n-}$ layer, with symmetry elements of the real layer. Full circles are $UO_2$, plus signs P—O, and minus signs O—P.

Table 1. *Experimental conditions*

| |
|---|
| Radiation: Mo $K\alpha$, $\lambda = 0{\cdot}71069$ Å |
| Graphite monochromator |
| $\omega$ scan: −0·7° to +0·7° (65 s) (background 2 × 16 s) |
| $2\theta_{max} = 47°$ |
| Total number of independent reflexions: 3730 |
| Total observed $[I \geq 2{\cdot}5\,\sigma(I)]$: 2971 |
| Crystal dimensions along **a**, **b**, **c**: 0·08 and 0·25, 0·18, 0·07 mm (rectangular trapezohedron) |
| $\mu$(Mo $K\alpha$) = 18·68 mm$^{-1}$ |

Table 2. *Atomic coordinates* ($\times 10^4$) *and thermal parameters* [$U = B/(8\pi^2)$]

| | $x$ | $y$ | $z$ | $U \times 10^2$ (Å$^2$) |
|---|---|---|---|---|
| U(1) | 1755·1 (6) | 2602·7 (4) | 8482·9 (9) | 1·07 (2) |
| U(2) | 4701·2 (6) | 2187·9 (5) | 0629·2 (9) | 1·01 (2) |
| U(3) | 3572·8 (6) | 2278·2 (4) | 6277·1 (9) | 1·01 (2) |
| Al(4) | 5648 (6) | 6111 (4) | 6168 (9) | 1·55 (16) |
| Al(5) | 5500 (6) | 5088 (4) | 3869 (9) | 1·68 (16) |
| P(6) | 7272 (5) | 7189 (3) | 7856 (7) | 0·87 (12) |
| P(7) | 4366 (5) | 7416 (3) | 5216 (7) | 1·01 (12) |
| O(8) | 8769 (12) | 8164 (8) | 1544 (19) | 1·4 (4) |
| O(9) | 7815 (12) | 6597 (8) | 1539 (18) | 1·3 (3) |
| O(10) | 0110 (14) | 8030 (9) | 9500 (20) | 2·0 (4) |
| O(11) | 0437 (13) | 6352 (9) | 9124 (19) | 1·8 (4) |
| O(12) | 1680 (12) | 6444 (8) | 4181 (18) | 1·3 (3) |
| O(13) | 1150 (13) | 8121 (9) | 3343 (20) | 1·8 (4) |
| O(14) | 1759 (14) | 7199 (9) | 1532 (21) | 2·1 (4) |
| O(15) | 6845 (14) | 7552 (9) | 8946 (21) | 2·1 (4) |
| O(16) | 8431 (13) | 7124 (8) | 8886 (20) | 1·6 (4) |
| O(17) | 4889 (12) | 8038 (8) | 1575 (18) | 1·2 (3) |
| O(18) | 4869 (12) | 7753 (7) | 4220 (18) | 1·0 (3) |
| O(19) | 3207 (13) | 7447 (9) | 4179 (20) | 1·9 (4) |
| O(20) | 9581 (15) | 7230 (9) | 6675 (22) | 2·4 (4) |
| O(21) | 4719 (14) | 6725 (10) | 5479 (22) | 2·6 (4) |
| O(22) | 6756 (14) | 6512 (9) | 7451 (22) | 2·6 (4) |
| O(23) | 7068 (13) | 7564 (8) | 6349 (19) | 1·4 (4) |
| O(24) | 6666 (15) | 4745 (10) | 3632 (22) | 3·0 (5) |
| O(25) | 6327 (13) | 5718 (9) | 5139 (20) | 1·9 (4) |
| O(26) | 5350 (14) | 5544 (9) | 7320 (21) | 2·4 (4) |
| O(27) | 5134 (14) | 5647 (10) | 2083 (22) | 2·6 (4) |
| O(28) | 5513 (14) | 4523 (9) | 5448 (20) | 2·1 (4) |
| O(29) | 3632 (17) | 4427 (12) | 9545 (26) | 4·2 (6) |
| O(30) | 6723 (19) | 3680 (12) | 2243 (27) | 4·5 (6) |
| O(31) | 2581 (18) | 5740 (12) | 2320 (27) | 4·6 (6) |
| O(32) | 0437 (24) | 4356 (16) | 8393 (36) | 7·2 (8) |
| O(33) | 8354 (28) | 6059 (19) | 5895 (43) | 9·4 (11) |
| O(34) | 7558 (26) | 4433 (17) | 0632 (39) | 8·2 (9) |
| O(35) | 1104 (36) | 4768 (24) | 1769 (53) | 12·6 (15) |
| O(36) | 8434 (31) | 5275 (21) | 3621 (46) | 10·3 (12) |
| O(37) | 0621 (40) | 5889 (28) | 6073 (61) | 14·5 (18) |

1962) and phurcalite (Piret & Declercq, 1978). The disposition of the layer in the unit cell of phuralumite is shown in Fig. 1, which allows the comparison with similar figures for the three other minerals (Piret & Declercq, 1978). In Fig. 2 the detailed configuration of the sheet is given. The coordination figures are: for U(1) a hexagonal bipyramid, for U(2) and U(3) pentagonal bipyramids. The mean U—O distances are for U(1)—O(uranyl) 1·77, for U(2)— and U(3)—O(uranyl) 1·795, for U(1)—O (others) 2·51, for U(2)— and U(3)—O (others) 2·36 Å. The mean P—O distance is 1·54 Å. The layers are connected by two Al atoms, four OH ions and ten $H_2O$ molecules. The centrosymmetrical Al—O coordination is shown in Fig. 3. Each octahedron shares one edge with another, and two edges with each of the two trigonal bipyramids. The mean Al—O distance in the octahedron is 1·89 Å. In the bipyramid four Al—O distances are near 1·77 Å, but the fifth is 2·19 Å. The $Al_4O_{14}$ group is connected to the layers principally by O(21) and O(22) of the $PO_4$ anions, but also by hydrogen bonds, as shown in Fig. 3. Distances less than 2·805 Å are given

Table 4. *Supplementary distances* (2·805 Å < $d$ < 3·40 Å) *between atoms implicated in hydrogen bonds*

| | | | |
|---|---|---|---|
| O(27)—O(8) | 3·05 (3) | O(33)—O(37) | 3·10 (7) |
| O(29)—O(9) | 2·84 (4) | O(34)—O(11) | 3·15 (4) |
| —O(34) | 2·87 (4) | —O(36) | 3·15 (6) |
| O(30)—O(23) | 2·88 (4) | —O(37) | 3·24 (9) |
| O(31)—O(12) | 2·91 (4) | O(36)—O(9) | 3·21 (5) |
| O(32)—O(9) | 3·11 (4) | —O(37) | 3·29 (7) |
| —O(35) | 3·08 (6) | O(37)—O(11) | 3·14 (7) |
| —O(36) | 2·98 (7) | —O(12) | 2·94 (7) |
| O(33)—O(20) | 2·91 (5) | | |

Table 3. *Interatomic distances* (Å) *less than* 2·805 Å

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| U(1)—O(8) | 1·76 (2) | U(1)—O(14) | 2·23 (2) | U(2)—O(14) | 2·26 (6) | U(3)—O(14) | 2·29 (3) |
| —O(9) | 1·78 (2) | —O(15) | 2·48 (6) | —O(15) | 2·38 (2) | —O(17) | 2·40 (6) |
| U(2)—O(10) | 1·79 (2) | —O(16) | 2·65 (2) | —O(16) | 2·45 (2) | —O(18) | 2·38 (2) |
| —O(11) | 1·78 (2) | —O(17) | 2·43 (2) | —O(17) | 2·40 (2) | —O(19) | 2·36 (2) |
| U(3)—O(12) | 1·80 (2) | —O(18) | 2·69 (6) | —O(20) | 2·35 (4) | —O(23) | 2·31 (3) |
| —O(13) | 1·81 (2) | —O(19) | 2·55 (2) | | | | |
| Al(4)—O(21) | 1·76 (2) | Al(5)—O(24) | 1·86 (3) | P(6)—O(15) | 1·56 (3) | P(7)—O(18) | 1·54 (2) |
| —O(22) | 1·76 (4) | —O(25) | 1·85 (3) | —O(16) | 1·53 (4) | —O(19) | 1·53 (4) |
| —O(25) | 1·79 (3) | —O(26) | 1·84 (3) | —O(22) | 1·57 (2) | —O(20) | 1·49 (2) |
| —O(26) | 1·76 (2) | —O(27) | 1·95 (3) | —O(23) | 1·55 (2) | —O(21) | 1·52 (2) |
| —O(28) | 2·19 (4) | —O(28) | 1·90 (2) | | | | |
| | | —O(28) | 1·93 (3) | | | | |
| O(10)—O(30) | 2·79 (5) | O(17)—O(32) | 2·80 (4) | O(22)—O(26) | 2·78 (3) | O(26)—O(27) | 2·69 (3) |
| O(14)—O(15) | 2·54 (3) | O(18)—O(19) | 2·37 (3) | O(24)—O(25) | 2·63 (3) | —O(28) | 2·42 (5) |
| —O(17) | 2·65 (3) | —O(20) | 2·49 (3) | —O(26) | 2·65 (4) | —O(29) | 2·75 (5) |
| —O(19) | 2·59 (6) | —O(21) | 2·50 (3) | —O(27) | 2·80 (4) | O(27)—O(29) | 2·70 (5) |
| O(15)—O(16) | 2·39 (3) | O(19)—O(20) | 2·49 (6) | —O(28) | 2·79 (4) | O(28)—O(31) | 2·73 (7) |
| —O(22) | 2·57 (3) | —O(21) | 2·49 (4) | —O(30) | 2·60 (3) | O(30)—O(34) | 2·73 (5) |
| —O(23) | 2·58 (3) | O(20)—O(21) | 2·50 (3) | —O(36) | 2·69 (5) | O(31)—O(34) | 2·74 (5) |
| O(16)—O(17) | 2·59 (6) | O(21)—O(22) | 2·76 (6) | O(25)—O(27) | 2·72 (6) | —O(35) | 2·79 (6) |
| —O(22) | 2·54 (4) | —O(28) | 2·73 (3) | —O(28) | 2·80 (3) | O(32)—O(35) | 2·77 (6) |
| —O(23) | 2·58 (6) | O(22)—O(23) | 2·54 (3) | —O(28) | 2·44 (3) | O(33)—O(35) | 2·67 (7) |
| O(17)—O(18) | 2·57 (3) | —O(25) | 2·62 (3) | —O(33) | 2·71 (5) | —O(36) | 2·73 (6) |
| | | | | | | O(36)—O(37) | 2·73 (7) |

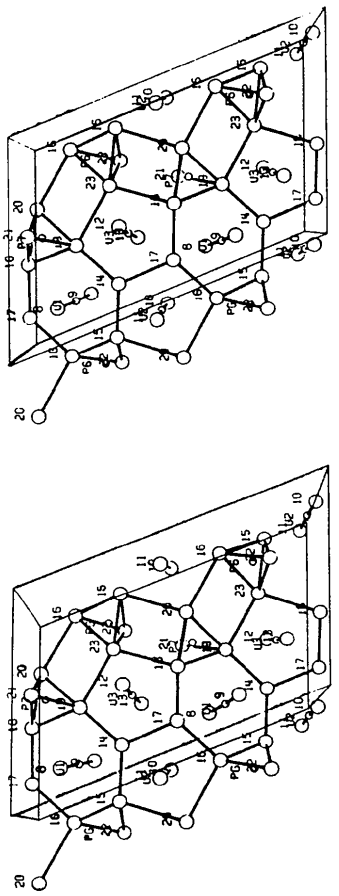

Fig. 2. Stereoscopic drawing (Johnson, 1965) of the layer (**c** across, **a** down). Limits: $x$, 0 to 1 (box) and −0·02 to 1 (atoms); $y$, 0·5 to 1 (box) and 0·633 to 0·867 (atoms); $z$, 0 to 1 (box) and −0·335 to 1 (atoms).

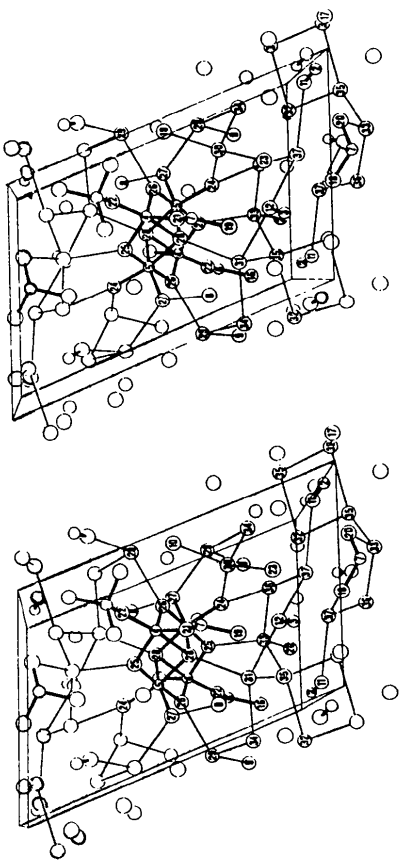

Fig. 3. Stereoscopic drawing (Johnson, 1965) of the interlayer structure (**c** across, **a** down). Limits: $x$, 0 to 1 (box) and −0·17 to 1 (atoms); $y$, 0·25 to 0·75 (box) and 0·27 to 0·76 (atoms); $z$, 0 to 1 (box) and −0·20 to 1·20 (atoms).

in Table 3. Supplementary distances implicated in hydrogen bonds are given in Table 4. It was not possible to trace the bifurcated hydrogen bond in Fig. 3. Distances and configurations indicate that atoms O(8) to O(13) belong to uranyl groups, O(15) to O(23) to $PO_4^-$, O(25), O(26), O(28) and probably O(24) to $OH^-$, O(29) to O(37) and probably O(27) to $H_2O$ molecules.

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