| $H_2Rb_{15.6}W_{27}Co_{9.2}[PO_4]_5O_{90}[OH]_3[H_2O]_{36}$ | *hP*388 | (176) $P6_3/m$ – $i^{26}h^{11}f^2a$ |
|---|---|---|

**$Rb_{15.6}Co_{0.2}[(PW_9O_{34})_3Co_9(OH)_3(H_2O)_6(HPO_4)_2]\cdot 30H_2O$** [1]

Structural features: $Co_9(OH)_3(H_2O)_6(HPO_4)_2(PW_9O_{34})_3$ units (three Keggin units consisting of twelve edge- and vertex-linked $WO_6$, $Co(O_5[OH])$ and $Co(O_4[OH][OH_2])$ octahedra sharing vertices with a central $PO_4$ tetrahedron, are interconnected via common vertices of the Co-centered octahedra and two capping $P(O_3[OH])$ tetrahedra) in a Mg-type (h.c.p.) arrangement; Rb and additional $H_2O$ between the units.

Weakley T.J.R. (1984) [1]

$Co_9H_{41}O_{131}P_5Rb_{15.62}W_{27}$

$a = 2.0243$, $c = 2.0343$ nm, $c/a = 1.005$, $V = 7.2193$ nm$^3$, $Z = 2$

| site | Wyck. | sym. | *x* | *y* | *z* | occ. | atomic environment |
|---|---|---|---|---|---|---|---|
| Rb1 | 12*i* | 1 | 0.0194 | 0.57 | 0.0393 | 0.71 | single atom ($OH_2$) |
| O2 | 12*i* | 1 | 0.0275 | 0.2493 | 0.0854 | | single atom W |
| W3 | 12*i* | 1 | 0.0297 | 0.2003 | 0.1581 | | octahedron $O_6$ |
| O4 | 12*i* | 1 | 0.031 | 0.4888 | 0.1683 | | single atom W |
| W5 | 12*i* | 1 | 0.0898 | 0.3703 | 0.0757 | | octahedron $O_6$ |
| O6 | 12*i* | 1 | 0.1047 | 0.3379 | 0.1862 | | single atom P |
| O7 | 12*i* | 1 | 0.1248 | 0.0141 | 0.1162 | | single atom W |
| O8 | 12*i* | 1 | 0.1326 | 0.2317 | 0.1515 | | non-colinear $W_2$ |
| O9 | 12*i* | 1 | 0.143 | 0.468 | 0.103 | | non-colinear WCo |
| Co10 | 12*i* | 1 | 0.155 | 0.5422 | 0.1711 | | octahedron $O_4(OH_2)(OH)$ |
| $(OH_2)$11 | 12*i* | 1 | 0.157 | 0.6175 | 0.1013 | | single atom Co |
| O12 | 12*i* | 1 | 0.1758 | 0.3599 | 0.0808 | | non-colinear $W_2$ |
| W13 | 12*i* | 1 | 0.2191 | 0.3409 | 0.1606 | | octahedron $O_6$ |
| Rb14 | 12*i* | 1 | 0.2517 | 0.1771 | 0.1132 | 0.71 | tetrahedron $(OH_2)O_3$ |
| O15 | 12*i* | 1 | 0.2643 | 0.4377 | 0.1787 | | non-colinear WCo |
| O16 | 12*i* | 1 | 0.2716 | 0.5884 | 0.1757 | | single atom P |
| O17 | 12*i* | 1 | 0.2739 | 0.0581 | 0.1727 | | non-colinear $W_2$ |
| O18 | 12*i* | 1 | 0.2846 | 0.3319 | 0.1265 | | single atom W |
| $(OH_2)$19 | 12*i* | 1 | 0.3467 | 0.1308 | 0.047 | | single atom O |
| O20 | 12*i* | 1 | 0.3703 | 0.0042 | 0.1035 | | non-colinear $W_2$ |
| O21 | 12*i* | 1 | 0.3735 | 0.2858 | 0.0067 | | single atom W |
| O22 | 12*i* | 1 | 0.4089 | 0.1185 | 0.1763 | | non-colinear $W_2$ |
| Rb23 | 12*i* | 1 | 0.4377 | 0.3451 | 0.147 | 0.71 | single atom O |
| W24 | 12*i* | 1 | 0.4489 | 0.0469 | 0.1654 | | octahedron $O_6$ |
| O25 | 12*i* | 1 | 0.5227 | 0.1024 | 0.1169 | | single atom W |
| $(OH_2)$26 | 12*i* | 1 | 0.5436 | 0.2784 | 0.1358 | | non-colinear RbO |
| O27 | 6*h* | *m*.. | 0.0116 | 0.3677 | $^1/_4$ | | single atom P |
| O28 | 6*h* | *m*.. | 0.0587 | 0.1918 | $^1/_4$ | | non-colinear $W_2$ |
| P29 | 6*h* | *m*.. | 0.0934 | 0.3784 | $^1/_4$ | | tetrahedron $O_4$ |
| O30 | 6*h* | *m*.. | 0.1473 | 0.4652 | $^1/_4$ | | single atom P |
| Rb31 | 6*h* | *m*.. | 0.1583 | 0.136 | $^1/_4$ | 0.71 | single atom O |
| (OH)32 | 6*h* | *m*.. | 0.165 | 0.6111 | $^1/_4$ | | non-coplanar triangle $Co_3$ |
| O33 | 6*h* | *m*.. | 0.2158 | 0.3117 | $^1/_4$ | | non-colinear $W_2$ |
| Co34 | 6*h* | *m*.. | 0.2778 | 0.5173 | $^1/_4$ | | octahedron $(OH)O_5$ |
| O35 | 6*h* | *m*.. | 0.3355 | 0.1971 | $^1/_4$ | | single atom W |
| W36 | 6*h* | *m*.. | 0.3435 | 0.1108 | $^1/_4$ | | octahedron $O_6$ |
| O37 | 6*h* | *m*.. | 0.5018 | 0.0869 | $^1/_4$ | | non-colinear $W_2$ |
| (OH)38 | 4*f* | 3.. | $^1/_3$ | $^2/_3$ | 0.0761 | | single atom P |
| P39 | 4*f* | 3.. | $^1/_3$ | $^2/_3$ | 0.1549 | | tetrahedron $O_3(OH)$ |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| Rb40 | 2*a* | -6.. | 0 | 0 | $^1/_4$ | 0.71 | coplanar triangle $Rb_3$ |

Experimental: single crystal, diffractometer, X-rays, R = 0.093

Remarks: Part of Co and $H_2O$ not located. We assigned an approximate value to the occupancy of the Rb sites based on the nominal composition. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In the material deposited for [1] the *x*-coordinate of former O(25) is misprinted as 0.4436 instead of 0.5436 (from ICSD).

References: [1] Weakley T.J.R. (1984), J. Chem. Soc., Chem. Commun. 1984, 1406-1407.