

$\text{K}_{0.69}\text{Li}_{0.27}\text{W}_3\text{O}_9$ $hP34$ (182) $P6_322 - \text{ih}^2\text{ge}$ $\text{K}_{0.23}\text{Li}_{0.09}\text{WO}_3$ [1], HTB (hexagonal tungsten bronze)

Structural features: WO_6 octahedra share vertices to form a 3D-framework; Li in trigonal prismatic voids, K in large channels of hexagonal cross-section parallel to [001].

Slade R.C.T. et al. (1989) [1]

 $\text{K}_{0.72}\text{Li}_{0.39}\text{O}_9\text{W}_3$ $a = 0.7392$, $c = 0.7586$ nm, $c/a = 1.026$, $V = 0.3590$ nm³, $Z = 2$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|---------------|------|---|
| O1 | 12i | 1 | 0.2135 | 0.4229 | 0.0138 | | non-coplanar triangle W_2Li |
| Li2 | 6h | ..2 | 0.2918 | 0.5836 | $\frac{1}{4}$ | 0.13 | |
| O3 | 6h | ..2 | 0.5028 | 0.0056 | $\frac{1}{4}$ | | |
| W4 | 6g | .2. | 0.485 | 0 | 0 | | octahedron O_6 |
| K5 | 4e | 3.. | 0 | 0 | 0.233 | 0.36 | |

Experimental: powder, diffractometer, neutrons, time-of-flight, $R_B = 0.153$

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Slade R.C.T., West B.C., Ramanan A., David W.I.F., Harrison W.T.A. (1989), Eur. J. Solid State Inorg. Chem. 26, 15-22.