

$\text{K}_{0.78}\text{W}_3\text{O}_9$ $hP28$ (182) $P6_322$ – ihge $\text{K}_{0.26}\text{WO}_3$ [1], HTB (hexagonal tungsten bronze)Structural features: WO_6 octahedra share vertices to form a 3D-framework; K in channels of hexagonal cross-section parallel to [001].

Pye M.F., Dickens P.G. (1979) [1]

 $\text{K}_{0.78}\text{O}_9\text{W}_3$ $a = 0.7385$, $c = 0.753$ nm, $c/a = 1.020$, $V = 0.3557$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	$12i$	1	0.426	0.217	0.028		non-colinear W_2
O2	$6h$	$\bar{2}$	0.516	0.032	$\frac{1}{4}$		non-colinear W_2
W3	$6g$	$\bar{2}$	0.47926	0	0		octahedron O_6
K4	$4e$	$3\bar{2}$	0	0	0.22	0.39	

Transformation from published data: $-x, -y, -z$; origin shift $0\ 0\ \frac{1}{2}$ Experimental: powder, diffractometer, neutrons, $R_B = 0.073$

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

References: [1] Pye M.F., Dickens P.G. (1979), Mater. Res. Bull. 14, 1397-1402.