

$\text{W}_8\text{Sn}_5\text{O}_{22}$ $hP70$ $(176) P6_3/m - i^4h^2f^2a$ **Sn₁₀W₁₆O₄₄** [1]

Structural features: W_6O_{12} units (six edge-linked WO_5 square pyramids) share vertices with W_2O_9 units (two face-linked WO_6 octahedra) to form a 3D-framework. W_6 octahedral clusters and W_2 dumbbells.

Hibble S.J., McGrellis S.A. (1995) [1]

 $\text{O}_{22}\text{Sn}_5\text{W}_8$ $a = 0.76697$, $c = 1.86391$ nm, $c/a = 2.430$, $V = 0.9495$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
W1	12i	1	0.0564	0.2238	0.0595		5-vertex polyhedron O_5
O2	12i	1	0.1175	0.4657	0.1248		non-colinear W_2
O3	12i	1	0.2379	0.1794	0.1223		non-colinear W_2
O4	12i	1	0.4165	0.1338	0.0032		non-coplanar triangle W_2Sn
O5	6h	$m..$	0.2972	0.4694	$\frac{1}{4}$		non-colinear W_2
Sn6	6h	$m..$	0.3164	0.1924	$\frac{1}{4}$		non-colinear O_2
W7	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.1716		octahedron O_6
Sn8	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.5708		non-coplanar triangle O_3
O9	2a	-6..	0	0	$\frac{1}{4}$		coplanar triangle Sn_3

Transformation from published data: $y, x, -z$; origin shift 0 0 $\frac{1}{2}$ Experimental: powder, diffractometer, neutrons, time-of-flight, $wR_p = 0.081$

Remarks: Contrary to [2] ($\text{Sn}_{10}\text{W}_{16}\text{O}_{46}$), no significant electron density was detected in Wyckoff position 2b.

References: [1] Hibble S.J., McGrellis S.A. (1995), J. Chem. Soc., Dalton Trans. 1995, 1947-1949. [2] Goreaud M., Labbé P., Raveau B. (1980), Acta Crystallogr. B 36, 15-19.