

$\text{H}_{21}\text{W}_{39}\text{B}_3\text{O}_{132}[\text{H}_2\text{O}]_{69}$	<i>hP384</i>	(176) $P6_3/m - i^{27}h^{10}$
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H₂₁[B₃W₃₉O₁₃₂]·69H₂O [1]
 Structural features: B₃W₃₉O₁₃₂ units (three Keggin-related units consisting of eleven edge- and vertex-linked WO₆ octahedra sharing vertices with a central BO₄ tetrahedron, are interconnected via six vertex-linked WO₆ octahedra) in a Mg-type (h.c.p.) arrangement; H₂O between the units. See Fig. IV.86.

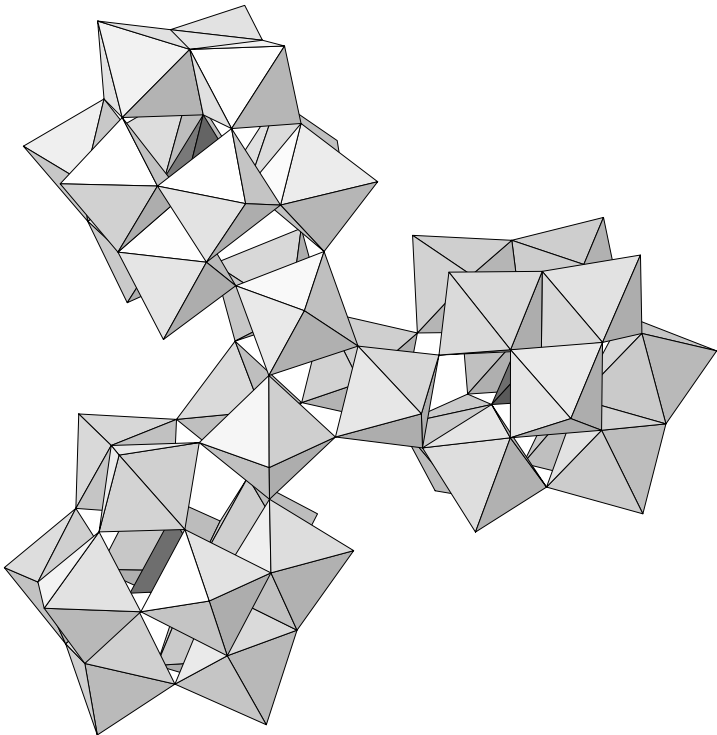


Fig. IV.86. **H₂₁[B₃W₃₉O₁₃₂]·69H₂O**

B₃W₃₉O₁₃₂-unit: three Keggin-related units (a BO₄ tetrahedron (dark) surrounded by eleven WO₆ octahedra (light)) interconnected via six WO₆ octahedra.

Tézé A. et al. (1997) [1]
 $\text{B}_3\text{H}_{36}\text{O}_{150}\text{W}_{39}$
 $a = 2.1626, c = 2.146 \text{ nm}, c/a = 0.992, V = 8.6919 \text{ nm}^3, Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.017	0.271	0.0902		non-colinear W ₂
O2	12 <i>i</i>	1	0.0183	0.5674	0.1218		single atom W
O3	12 <i>i</i>	1	0.024	0.156	0.133		single atom W
O4	12 <i>i</i>	1	0.0239	0.3737	0.0089		single atom W
W5	12 <i>i</i>	1	0.03354	0.36577	0.08667		octahedron O ₆
W6	12 <i>i</i>	1	0.03384	0.51389	0.17061		octahedron O ₆
W7	12 <i>i</i>	1	0.03478	0.23383	0.16453		octahedron O ₆
O8	12 <i>i</i>	1	0.052	0.4565	0.1145		non-colinear W ₂
O9	12 <i>i</i>	1	0.0562	0.347	0.1924		single atom B
O10	12 <i>i</i>	1	0.1323	0.3971	0.0887		non-colinear W ₂
O11	12 <i>i</i>	1	0.1326	0.2944	0.1535		non-colinear W ₂
O12	12 <i>i</i>	1	0.1376	0.5728	0.1776		non-colinear W ₂

W13	12i	1	0.17945	0.39737	0.16524	octahedron O ₆
O14	12i	1	0.1905	0.486	0.1812	non-colinear W ₂
O15	12i	1	0.2021	0.5603	0.0736	single atom W
W16	12i	1	0.2265	0.58669	0.1607	octahedron O ₆
O17	12i	1	0.2608	0.4194	0.1352	single atom W
O18	12i	1	0.2653	0.0619	0.192	non-colinear W ₂
O19	12i	1	0.3171	0.5897	0.143	non-colinear W ₂
(OH ₂)20	12i	1	0.332	0.475	0.023	non-colinear (OH ₂)O
O21	12i	1	0.3941	0.0631	0.1181	non-colinear W ₂
O22	12i	1	0.4015	0.1661	0.1885	non-colinear W ₂
W23	12i	1	0.46074	0.12573	0.17246	octahedron O ₆
O24	12i	1	0.4944	0.0567	0.1764	non-colinear W ₂
(OH ₂)25	12i	1	0.511	0.354	0.095	single atom (OH ₂)
O26	12i	1	0.522	0.187	0.1232	single atom W
(OH ₂)27	12i	1	0.532	0.073	0.013	non-coplanar triangle (OH ₂) ₃
B28	6h	m..	0.027	0.36	¹ / ₄	tetrahedron O ₄
O29	6h	m..	0.027	0.551	¹ / ₄	non-colinear W ₂
O30	6h	m..	0.051	0.226	¹ / ₄	non-colinear W ₂
O31	6h	m..	0.058	0.445	¹ / ₄	single atom B
O32	6h	m..	0.19	0.381	¹ / ₄	non-colinear W ₂
O33	6h	m..	0.2485	0.6027	¹ / ₄	non-colinear W ₂
O34	6h	m..	0.306	0.194	¹ / ₄	single atom W
W35	6h	m..	0.3267	0.1242	¹ / ₄	octahedron O ₆
O36	6h	m..	0.379	0.052	¹ / ₄	single atom B
O37	6h	m..	0.509	0.165	¹ / ₄	non-colinear W ₂

Transformation from published data: $y, x, -z$; origin shift $0\ 0\ \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.049, T = 294 K

Remarks: Part of H₂O not located. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Tézé A., Michelon M., Hervé G. (1997), Inorg. Chem. 36, 505-509.