

Hf₁₈[SO₄]₁₃O₁₀[OH]₂₆[H₂O]₃₃

hP930

(176) $P6_3/m - i^{64}h^{27}$ **Hf₁₈(SO₄)₁₃O₁₀(OH)₂₆·33H₂O [1]**

Structural features: Hf₁₈O₁₀(OH)₂₆(SO₄)₁₃(H₂O)₂₀ units (eighteen interconnected Hf(O,OH,OH₂)₇ and Hf(O,OH,OH₂)₈ polyhedra sharing vertices with surrounding SO₄ tetrahedra).

Mark W., Hansson M. (1975) [1]

H₂₆Hf₁₈O₁₂₁S₁₃ $a = 3.409$, $c = 1.7664$ nm, $c/a = 0.518$, $V = 17.7776$ nm³, $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
(OH ₂)1	12i	1	0.0033	0.5783	0.1065		single atom O
S2	12i	1	0.0087	0.2267	0.1245		tetrahedron O ₄
O3	12i	1	0.0133	0.3682	0.0883		single atom Hf
O4	12i	1	0.0214	0.1997	0.1746		single atom S
O5	12i	1	0.0225	0.4992	0.0944		single atom S
O6	12i	1	0.0495	0.441	0.1718		single atom Hf
O7	12i	1	0.0543	0.2631	0.0878		single atom S
O8	12i	1	0.0606	0.1529	0.0251	0.5	single atom S
O9	12i	1	0.064	0.3354	0.1625		non-coplanar triangle Hf ₃
O10	12i	1	0.0654	0.16	0.1786		single atom S
O11	12i	1	0.0828	0.5756	0.1541		single atom Hf
Hf12	12i	1	0.08517	0.40546	0.14954		square antiprism O ₈
Hf13	12i	1	0.09025	0.51315	0.14552		8-vertex polyhedron O ₈
O14	12i	1	0.0919	0.1168	0.1098	0.5	single atom S
O15	12i	1	0.094	0.5005	0.0274		non-colinear Hf ₂
S16	12i	1	0.0972	0.1569	0.11	0.5	tetrahedron O ₄
O17	12i	1	0.0992	0.413	0.0329		non-colinear Hf ₂
Hf18	12i	1	0.11547	0.31801	0.15096		square antiprism O ₈
O19	12i	1	0.1195	0.2596	0.1686		non-coplanar triangle Hf ₃
O20	12i	1	0.1292	0.3311	0.0337		non-colinear Hf ₂
O21	12i	1	0.1373	0.4835	0.1123		single atom Hf
O22	12i	1	0.143	0.1989	0.0916		single atom S
O23	12i	1	0.154	0.4002	0.1398		single atom Hf
O24	12i	1	0.1579	0.5729	0.1252		single atom S
O25	12i	1	0.1793	0.2727	0.0303		non-colinear Hf ₂
O26	12i	1	0.1812	0.6205	0.0017		single atom S
Hf27	12i	1	0.18162	0.26398	0.14568		square antiprism O ₈
O28	12i	1	0.1855	0.3327	0.1186		non-coplanar triangle Hf ₃
O29	12i	1	0.1927	0.5524	0.0187		single atom S
S30	12i	1	0.1943	0.5925	0.0627		tetrahedron O ₄
O31	12i	1	0.2013	0.4798	0.0318		non-colinear Hf ₂
O32	12i	1	0.2173	0.227	0.1514		single atom Hf
O33	12i	1	0.2186	0.4897	0.1794		single atom S
O34	12i	1	0.2198	0.0196	0.0672		single atom S
O35	12i	1	0.2228	0.4126	0.0368		non-colinear Hf ₂
(OH ₂)36	12i	1	0.224	0.163	0.0521		tetrahedron O ₄
O37	12i	1	0.2372	0.4214	0.1808		single atom S
O38	12i	1	0.2386	0.6159	0.1039		single atom S
O39	12i	1	0.2574	0.3132	0.1224		single atom S
O40	12i	1	0.2593	0.0112	0.1712		single atom S
O41	12i	1	0.2649	0.3671	0.0282		single atom S
S42	12i	1	0.2845	0.3408	0.0608		tetrahedron O ₄

O43	12i	1	0.2904	0.3134	0.0023	single atom S
O44	12i	1	0.2916	0.4977	0.0372	single atom Hf
O45	12i	1	0.2952	0.1549	0.0965	single atom Hf
(OH ₂)46	12i	1	0.2983	0.5961	0.0221	non-coplanar triangle O ₃
O47	12i	1	0.327	0.0991	0.1033	single atom Hf
O48	12i	1	0.3285	0.3751	0.0941	single atom S
(OH ₂)49	12i	1	0.3338	0.266	0.0562	non-coplanar triangle O ₃
Hf50	12i	1	0.34126	0.1488	0.00845	square antiprism O ₈
(OH ₂)51	12i	1	0.3626	0.4717	0.015	non-coplanar triangle O ₃
O52	12i	1	0.3875	0.1883	0.0971	non-colinear Hf ₂
O53	12i	1	0.3943	0.1007	0.1788	single atom S
O54	12i	1	0.4439	0.0186	0.0357	single atom S
O55	12i	1	0.4535	0.1614	0.0916	single atom Hf
O56	12i	1	0.4539	0.2844	0.0922	non-colinear Hf ₂
O57	12i	1	0.4564	0.3625	0.1048	single atom Hf
Hf58	12i	1	0.45797	0.22708	0.05534	square antiprism O ₈
O59	12i	1	0.4639	0.229	0.1688	single atom S
O60	12i	1	0.4671	0.0341	0.1723	single atom S
S61	12i	1	0.4777	0.0223	0.0941	tetrahedron O ₄
Hf62	12i	1	0.48318	0.34003	0.00835	pentagonal bipyramid O ₇
O63	12i	1	0.5242	0.0559	0.0788	single atom S
O64	12i	1	0.5302	0.2625	0.0941	non-colinear HfO
Hf65	6h	m..	0.00774	0.42024	¹ / ₄	monocapped trigonal prism O ₇
Hf66	6h	m..	0.02433	0.30629	¹ / ₄	monocapped trigonal prism O ₇
O67	6h	m..	0.0359	0.3766	¹ / ₄	non-colinear Hf ₂
O68	6h	m..	0.0457	0.5011	¹ / ₄	non-colinear Hf ₂
O69	6h	m..	0.0723	0.2791	¹ / ₄	tetrahedron Hf ₄
Hf70	6h	m..	0.07879	0.21755	¹ / ₄	square antiprism O ₈
O71	6h	m..	0.1223	0.4273	¹ / ₄	non-coplanar triangle Hf ₃
O72	6h	m..	0.1249	0.5231	¹ / ₄	non-colinear Hf ₂
O73	6h	m..	0.1484	0.3498	¹ / ₄	non-coplanar triangle Hf ₃
O74	6h	m..	0.1487	0.2169	¹ / ₄	non-colinear Hf ₂
Hf75	6h	m..	0.18144	0.42117	¹ / ₄	square antiprism O ₈
O76	6h	m..	0.209	0.2969	¹ / ₄	non-colinear Hf ₂
O77	6h	m..	0.2163	0.5538	¹ / ₄	single atom S
S78	6h	m..	0.2342	0.5211	¹ / ₄	tetrahedron O ₄
S79	6h	m..	0.2702	0.4246	¹ / ₄	tetrahedron O ₄
(OH ₂)80	6h	m..	0.2761	0.1154	¹ / ₄	non-colinear O ₂
O81	6h	m..	0.2793	0.3834	¹ / ₄	single atom S
O82	6h	m..	0.2833	0.5479	¹ / ₄	single atom S
O83	6h	m..	0.3129	0.4688	¹ / ₄	single atom S
O84	6h	m..	0.3353	0.0436	¹ / ₄	single atom S
(OH ₂)85	6h	m..	0.3471	0.3685	¹ / ₄	single atom O
S86	6h	m..	0.3872	0.0782	¹ / ₄	tetrahedron O ₄
O87	6h	m..	0.3943	0.2041	¹ / ₄	single atom S
O88	6h	m..	0.4116	0.0554	¹ / ₄	single atom S
S89	6h	m..	0.4489	0.2357	¹ / ₄	tetrahedron O ₄
O90	6h	m..	0.4606	0.2829	¹ / ₄	single atom S
(OH ₂)91	6h	m..	0.5439	0.0086	¹ / ₄	non-coplanar triangle O(OH ₂) ₂

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.075

Remarks: OH and non-zeolitic H₂O not identified. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Mark W., Hansson M. (1975), Acta Crystallogr. B 31, 1101-1108.