$Zr_{18}[SO_4]_{12.6}O_4[OH]_{38.8}[H_2O]_{33}$	*hP*966	(176) $P6_3/m$ – $i^{65}h^{31}$

$Zr_{18}O_4(OH)_{38.8}(SO_4)_{12.6}\cdot 33H_2O$ [1]
Structural features: $Zr_{18}O_4(OH)_{38.8}(SO_4)_{12.6}(H_2O)_{16}$ units consisting of eighteen interconnected ZrO_7 and ZrO_8 polyhedra (H ignored) sharing vertices with surrounding SO_4 tetrahedra; partial disorder SO_4/2OH.

Squattrito P.J. et al. (1987) [1]
$H_{70.90}O_{127.06}S_{12.55}Zr_{18}$
a = 3.3779, c = 1.7522 nm, c/a = 0.519, V = 17.3144 nm^3, Z = 6

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	12*i*	1	0.0098	0.2279	0.1213		tetrahedron O_4
O2	12*i*	1	0.0149	0.3689	0.0902		single atom Zr
O3	12*i*	1	0.0206	0.1996	0.1741		single atom S
O4	12*i*	1	0.0254	0.5009	0.097		single atom S
O5	12*i*	1	0.0525	0.2631	0.0854		single atom S
(OH)6	12*i*	1	0.0571	0.4474	0.1617		non-coplanar triangle Zr_3
M7	12*i*	1	0.0641	0.156	0.177		single atom S
(OH)8	12*i*	1	0.0689	0.3402	0.1586		non-coplanar triangle Zr_3
O9	12*i*	1	0.07	0.159	0.01	0.54	single atom S
O10	12*i*	1	0.0879	0.5801	0.158		single atom Zr
Zr11	12*i*	1	0.08834	0.40852	0.1482		square antiprism $(OH)_6O_2$
Zr12	12*i*	1	0.09283	0.5166	0.1449		square antiprism $(OH)_5O_3$
S13	12*i*	1	0.0945	0.1579	0.0965	0.54	tetrahedron O_4
O14	12*i*	1	0.098	0.115	0.095	0.54	single atom S
(OH)15	12*i*	1	0.1006	0.5102	0.0255		non-colinear Zr_2
(OH)16	12*i*	1	0.1034	0.42	0.0272		non-colinear Zr_2
Zr17	12*i*	1	0.11814	0.31944	0.15043		square antiprism $(OH)_6O_2$
(OH)18	12*i*	1	0.1213	0.259	0.1632		non-coplanar triangle Zr_3
(OH)19	12*i*	1	0.1327	0.3313	0.0289		non-colinear Zr_2
(OH)20	12*i*	1	0.1385	0.4846	0.1192		non-coplanar triangle Zr_3
M21	12*i*	1	0.1413	0.1945	0.0918		single atom S
(OH)22	12*i*	1	0.1532	0.4014	0.1358		non-coplanar triangle Zr_3
M23	12*i*	1	0.161	0.5795	0.124		single atom S
Zr24	12*i*	1	0.18294	0.26339	0.1445		square antiprism $(OH)_5O_3$
(OH)25	12*i*	1	0.1829	0.276	0.0251		non-colinear Zr_2
(OH)26	12*i*	1	0.1907	0.3337	0.1207		non-coplanar triangle Zr_3
O27	12*i*	1	0.1918	0.6222	0.012		single atom S
S28	12*i*	1	0.1996	0.5965	0.0698	0.76	tetrahedron O_4
M29	12*i*	1	0.2008	0.5592	0.032		single atom S
(OH)30	12*i*	1	0.2061	0.4829	0.0295		non-coplanar triangle $Zr_2(OH)$
O31	12*i*	1	0.22	0.2237	0.1591		single atom Zr
O32	12*i*	1	0.2203	0.492	0.1856		single atom S
O33	12*i*	1	0.2209	0.0223	0.0661		single atom S
(OH)34	12*i*	1	0.2223	0.4119	0.0332		non-coplanar triangle $Zr_2(OH)$
(OH_2)35	12*i*	1	0.2299	0.1676	0.0557		tetrahedron O_4
O36	12*i*	1	0.2434	0.4244	0.1855		single atom S
O37	12*i*	1	0.2435	0.6237	0.111		single atom S
O38	12*i*	1	0.2581	0.31	0.1233		single atom S
O39	12*i*	1	0.2607	0.009	0.1669		single atom S
O40	12*i*	1	0.2659	0.3657	0.0301		single atom S
S41	12*i*	1	0.2876	0.3406	0.0618		tetrahedron O_4
O42	12*i*	1	0.2921	0.4996	0.0389		single atom Zr

O43	12*i*	1	0.2939	0.3134	0.0028		single atom S
O44	12*i*	1	0.297	0.1533	0.1012		single atom Zr
(OH_2)45	12*i*	1	0.3204	0.616	0.033		single atom O
O46	12*i*	1	0.3289	0.0966	0.1075		single atom Zr
O47	12*i*	1	0.3328	0.3749	0.0939		single atom S
(OH_2)48	12*i*	1	0.3391	0.27	0.0568		non-coplanar triangle $(OH)_2O$
Zr49	12*i*	1	0.34237	0.14678	0.0098		square antiprism $(OH)_5O_3$
(OH_2)50	12*i*	1	0.3546	0.4676	0.056		single atom O
(OH)51	12*i*	1	0.391	0.1869	0.0943		non-colinear Zr_2
O52	12*i*	1	0.3954	0.1028	0.183		single atom S
O53	12*i*	1	0.4455	0.0184	0.0356		single atom S
(OH)54	12*i*	1	0.458	0.2837	0.0907		non-colinear Zr_2
O55	12*i*	1	0.4594	0.3652	0.1037		single atom Zr
O56	12*i*	1	0.46	0.1604	0.0855		single atom Zr
Zr57	12*i*	1	0.46064	0.22528	0.0554		square antiprism $(OH)_4O_4$
O58	12*i*	1	0.4658	0.0307	0.1691		single atom S
M59	12*i*	1	0.4683	0.225	0.1827		single atom S
S60	12*i*	1	0.4788	0.0203	0.0935		tetrahedron O_4
Zr61	12*i*	1	0.48778	0.33993	0.0092		square antiprism $(OH)_5O_3$
O62	12*i*	1	0.5249	0.0554	0.0756		single atom S
O63	12*i*	1	0.5343	0.2611	0.0817		single atom Zr
(OH_2)64	12*i*	1	0.5802	0.0028	0.108		tetrahedron $O_3(OH_2)$
O65	12*i*	1	0.6302	0.17	0.103		single atom Zr
Zr66	6*h*	*m*..	0.01013	0.42282	$^1/_4$		7-vertex polyhedron $(OH)_3O_4$
Zr67	6*h*	*m*..	0.02635	0.30892	$^1/_4$		7-vertex polyhedron $(OH)_2O_5$
O68	6*h*	*m*..	0.0367	0.3773	$^1/_4$		non-colinear Zr_2
(OH)69	6*h*	*m*..	0.0456	0.5009	$^1/_4$		non-coplanar triangle Zr_3
O70	6*h*	*m*..	0.073	0.2811	$^1/_4$		tetrahedron Zr_4
Zr71	6*h*	*m*..	0.07954	0.21766	$^1/_4$		square antiprism $(OH)_3O_5$
(OH)72	6*h*	*m*..	0.1264	0.4288	$^1/_4$		non-coplanar triangle Zr_3
(OH)73	6*h*	*m*..	0.1281	0.5279	$^1/_4$		non-colinear Zr_2
(OH)74	6*h*	*m*..	0.1474	0.2167	$^1/_4$		non-coplanar triangle Zr_3
(OH)75	6*h*	*m*..	0.1534	0.3528	$^1/_4$		non-coplanar triangle Zr_3
(OH_2)76	6*h*	*m*..	0.178	0.072	$^1/_4$		non-coplanar triangle $(OH_2)O_2$
Zr77	6*h*	*m*..	0.1851	0.42437	$^1/_4$		square antiprism $(OH)_4O_4$
(OH)78	6*h*	*m*..	0.2103	0.2958	$^1/_4$		non-colinear Zr_2
O79	6*h*	*m*..	0.2187	0.554	$^1/_4$		single atom S
S80	6*h*	*m*..	0.2388	0.5254	$^1/_4$		tetrahedron O_4
(OH_2)81	6*h*	*m*..	0.2528	0.6372	$^1/_4$		coplanar square O_4
(OH_2)82	6*h*	*m*..	0.2726	0.1058	$^1/_4$		non-coplanar triangle $(OH_2)O_2$
S83	6*h*	*m*..	0.2735	0.4258	$^1/_4$		tetrahedron O_4
O84	6*h*	*m*..	0.276	0.385	$^1/_4$		single atom S
O85	6*h*	*m*..	0.2881	0.553	$^1/_4$		single atom S
O86	6*h*	*m*..	0.3178	0.4671	$^1/_4$		single atom S
O87	6*h*	*m*..	0.3369	0.0434	$^1/_4$		single atom S
(OH_2)88	6*h*	*m*..	0.351	0.364	$^1/_4$		single atom (OH_2)
O89	6*h*	*m*..	0.384	0.195	$^1/_4$	0.95	single atom S
S90	6*h*	*m*..	0.3866	0.0769	$^1/_4$		tetrahedron O_4
O91	6*h*	*m*..	0.4115	0.0513	$^1/_4$		single atom S
(OH_2)92	6*h*	*m*..	0.413	0.337	$^1/_4$		single atom (OH_2)
S93	6*h*	*m*..	0.4554	0.2372	$^1/_4$	0.95	tetrahedron O_4
O94	6*h*	*m*..	0.459	0.282	$^1/_4$	0.95	single atom S
(OH_2)95	6*h*	*m*..	0.548	0.011	$^1/_4$		non-coplanar triangle $(OH)(OH_2)_2$
(OH_2)96	6*h*	*m*..	0.591	0.115	$^1/_4$		non-coplanar triangle $(OH_2)O_2$

M7 = 0.54O + 0.46OH; M21 = 0.54O + 0.46OH; M23 = 0.76O + 0.24OH; M29 = 0.76O + 0.24OH; M59 = 0.95O + 0.05OH
Experimental: single crystal, diffractometer, X-rays, R = 0.083, T = 298 K

Remarks: The authors state that sites O68 and O70 are occupied by O^{2-}; non-zeolitic H_2O and part of OH not identified. Long interatomic distances: d(S93-O89) = 0.210 nm. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Squattrito P.J., Rudolf P.R., Clearfield A. (1987), Inorg. Chem. 26, 4240-4244.