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_audit_creation_method 'Created with Materials Studio'
_audit_creation_date 2010-26-02
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_chemical_name_systematic 'Iron oxyhydroxysulfate'
_chemical_formula_structural 'Fe16 O28 (SO4)4 H16'
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_atom_site_occupancy
Fe1 Fe 0.345(5) 0 0.152(3) 0.002(2) 1.00

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Fe2	Fe	0.140(5)	0	0.645(4)	0.002(2)	1.00
O1	O	0.288(8)	0	0.322(7)	0.009(1)	1.00
O2	O	0.043(8)	0	0.336(9)	0.009(1)	1.00
O3	O	0.335(9)	0	0.690(1)	0.009(1)	1.00
O4	O	0.325(6)	0	0.946(5)	0.009(1)	1.00
Fe3	Fe	0.857(7)	0.25	0.611(6)	0.002(2)	1.00
Fe4	Fe	0.700(4)	0.25	0.093(5)	0.002(2)	1.00
O5	O	0.787(5)	0.25	0.796(7)	0.009(1)	1.00
O6	O	0.540(1)	0.25	0.810(4)	0.009(1)	1.00
O7	O	0.861(6)	0.25	0.159(7)	0.009(1)	1.00
O8	O	0.824(6)	0.25	0.419(7)	0.009(1)	1.00
Fe5	Fe	0.669(5)	0	0.811(4)	0.002(2)	1.00
Fe6	Fe	0.866(4)	0	0.320(3)	0.002(2)	1.00
O9	O	0.711(5)	0	0.626(6)	0.009(1)	1.00
O10	O	0.956(6)	0	0.612(8)	0.009(1)	1.00
O11	O	0.664(5)	0	0.260(7)	0.009(1)	1.00
O12	O	0.674(7)	0	0.002(8)	0.009(1)	1.00
Fe7	Fe	0.151(4)	0.25	0.352(4)	0.002(2)	1.00
Fe8	Fe	0.344(3)	0.25	0.840(5)	0.002(2)	1.00
O13	O	0.211(6)	0.25	0.152(7)	0.009(1)	1.00
O14	O	0.456(7)	0.25	0.138(7)	0.009(1)	1.00
O15	O	0.165(6)	0.25	0.786(7)	0.009(1)	1.00
O16	O	0.175(7)	0.25	0.527(8)	0.009(1)	1.00
Fe9	Fe	0.337(5)	0.5	0.142(4)	0.002(2)	1.00
Fe10	Fe	0.144(4)	0.5	0.648(5)	0.002(2)	1.00
O17	O	0.288(5)	0.5	0.322(5)	0.009(1)	1.00
O18	O	0.043(7)	0.5	0.336(7)	0.009(1)	1.00
O19	O	0.335(8)	0.5	0.690(1)	0.009(1)	1.00
O20	O	0.325(3)	0.5	0.946(5)	0.009(1)	1.00
Fe11	Fe	0.846(3)	0.75	0.606(4)	0.002(2)	1.00
Fe12	Fe	0.696(4)	0.75	0.095(3)	0.002(2)	1.00
O21	O	0.787(6)	0.75	0.796(8)	0.009(1)	1.00
O22	O	0.542(7)	0.75	0.810(6)	0.009(1)	1.00
O23	O	0.857(1)	0.75	0.157(1)	0.009(1)	1.00
O24	O	0.824(7)	0.75	0.419(7)	0.009(1)	1.00
Fe13	Fe	0.666(4)	0.5	0.804(3)	0.002(2)	1.00
Fe14	Fe	0.865(5)	0.5	0.322(3)	0.002(2)	1.00
O25	O	0.711(6)	0.5	0.626(8)	0.009(1)	1.00
O26	O	0.956(7)	0.5	0.612(7)	0.009(1)	1.00
O27	O	0.664(6)	0.5	0.260(6)	0.009(1)	1.00
O28	O	0.674(6)	0.5	0.002(7)	0.009(1)	1.00
Fe15	Fe	0.153(5)	0.75	0.338(5)	0.002(2)	1.00
Fe16	Fe	0.363(4)	0.75	0.835(5)	0.002(2)	1.00
O29	O	0.211(6)	0.75	0.150(1)	0.009(1)	1.00
O30	O	0.456(6)	0.75	0.138(6)	0.009(1)	1.00
O31	O	0.165(7)	0.75	0.786(6)	0.009(1)	1.00
O32	O	0.175(6)	0.75	0.528(7)	0.009(1)	1.00

#Positions of 16 elements of H are undetermined

#Positions of 12 elements of O are undetermined

#Positions of 4 elements of S are undetermined

#End of data_Schw1