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data_Schw2
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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'
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Fe1 Fe 0.345(1) 0.00 0.122(3) 0.003(2) 1.00

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Fe2	Fe	0.150(6)	0.00	0.626(9)	0.003(2)	1.00
O1	O	0.288(3)	0.00	0.307(4)	0.009(6)	1.00
O2	O	0.052(1)	0.00	0.334(5)	0.009(6)	1.00
O3	O	0.334(5)	0.00	0.67(1)	0.009(6)	1.00
O4	O	0.324(1)	0.00	0.929(3)	0.009(6)	1.00
Fe3	Fe	0.883(7)	0.25	0.560(2)	0.003(2)	1.00
Fe4	Fe	0.710(2)	0.25	0.054(9)	0.003(2)	1.00
O5	O	0.786(2)	0.25	0.756(2)	0.009(6)	1.00
O6	O	0.541(5)	0.25	0.782(4)	0.009(6)	1.00
O7	O	0.866(6)	0.25	0.126(3)	0.009(6)	1.00
O8	O	0.822(3)	0.25	0.378(1)	0.009(6)	1.00
Fe5	Fe	0.688(6)	0.00	0.770(1)	0.003(2)	1.00
Fe6	Fe	0.897(3)	0.00	0.266(5)	0.003(2)	1.00
O9	O	0.709(7)	0.00	0.590(1)	0.009(6)	1.00
O10	O	0.964(8)	0.00	0.563(9)	0.009(6)	1.00
O11	O	0.690(2)	0.00	0.208(5)	0.009(6)	1.00
O12	O	0.691(2)	0.00	0.959(9)	0.009(6)	1.00
Fe7	Fe	0.158(7)	0.25	0.323(8)	0.003(2)	1.00
Fe8	Fe	0.338(4)	0.25	0.835(8)	0.003(2)	1.00
O13	O	0.211(2)	0.25	0.141(3)	0.009(6)	1.00
O14	O	0.455(7)	0.25	0.115(1)	0.009(6)	1.00
O15	O	0.164(2)	0.25	0.777(7)	0.009(6)	1.00
O16	O	0.174(6)	0.25	0.519(4)	0.009(6)	1.00
Fe9	Fe	0.328(5)	0.50	0.117(1)	0.003(2)	1.00
Fe10	Fe	0.155(9)	0.50	0.624(1)	0.003(2)	1.00
O17	O	0.287(6)	0.50	0.307(4)	0.009(6)	1.00
O18	O	0.042(6)	0.50	0.333(6)	0.009(6)	1.00
O19	O	0.335(5)	0.50	0.671(3)	0.009(6)	1.00
O20	O	0.324(2)	0.50	0.929(3)	0.009(6)	1.00
Fe11	Fe	0.841(3)	0.75	0.554(3)	0.003(2)	1.00
Fe12	Fe	0.845(1)	0.75	0.956(6)	0.003(2)	1.00
O21	O	0.786(1)	0.75	0.765(7)	0.009(6)	1.00
O22	O	0.541(5)	0.75	0.782(4)	0.009(6)	1.00
O23	O	0.854(2)	0.75	0.138(2)	0.009(6)	1.00
O24	O	0.822(6)	0.75	0.378(1)	0.009(6)	1.00
Fe13	Fe	0.668(5)	0.50	0.771(1)	0.003(2)	1.00
Fe14	Fe	0.867(8)	0.50	0.271(7)	0.003(2)	1.00
O25	O	0.709(8)	0.50	0.590(1)	0.009(6)	1.00
O26	O	0.964(6)	0.50	0.563(6)	0.009(6)	1.00
O27	O	0.691(5)	0.50	0.959(9)	0.009(6)	1.00
Fe15	Fe	0.147(4)	0.75	0.322(1)	0.003(2)	1.00
Fe16	Fe	0.353(3)	0.75	0.821(1)	0.003(2)	1.00
O28	O	0.211(4)	0.75	0.141(3)	0.009(6)	1.00
O29	O	0.455(2)	0.75	0.115(1)	0.009(6)	1.00
O30	O	0.164(1)	0.75	0.777(7)	0.009(6)	1.00
O31	O	0.174(7)	0.75	0.519(4)	0.009(6)	1.00
O32	O	0.969(5)	0.50	0.958(5)	0.009(6)	1.00
O33	O	0.969(8)	0.00	0.958(5)	0.009(6)	1.00
O34	O	0.690(6)	0.50	0.213(6)	0.009(6)	1.00

#Positions of 20 elements of H are undetermined

#Positions of 12 elements of O are undetermined

#Positions of 4 elements of S are undetermined

#End of data_Schw2