

Appendix 1

Selected bond lengths (Å) and angles(°) for MgSO₄·2.5H₂O.

Mg(1)-O(1)	2.029(5)	Mg(2)-O(4w)	2.120(6)
Mg(1)-O(2)#1	2.049(6)	Mg(2)-O(5w)	2.091(6)
Mg(1)-O(5)#2	2.043(5)	S(1)-O(1)	1.446(6)
Mg(1)-O(1w)	2.094(6)	S(1)-O(2)	1.471(6)
Mg(1)-O(2w)	2.098(6)	S(1)-O(3)	1.473(7)
Mg(1)-O(3w)	2.067(6)	S(1)-O(4)	1.469(6)
Mg(2)-O(4)	2.046(5)	S(2)-O(5)	1.494(7)
Mg(2)-O(6)	2.079(5)	S(2)-O(6)	1.469(6)
Mg(2)-O(7)#3	2.064(5)	S(2)-O(7)	1.462(6)
Mg(2)-O(8)#4	2.071(5)	S(2)-O(8)	1.454(6)
O(1)-Mg(1)-O(2)#1	84.4(3)	O(4)-Mg(2)-O(6)	79.6(3)
O(1)-Mg(1)-O(5)#2	175.4(3)	O(4)-Mg(2)-O(7)#3	173.4(3)
O(1)-Mg(1)-O(1w)	90.0(3)	O(4)-Mg(2)-O(8)#4	91.9(3)
O(1)-Mg(1)-O(2w)	88.7(3)	O(4)-Mg(2)-O(4w)	95.1(3)
O(1)-Mg(1)-O(3w)	93.2(3)	O(4)-Mg(2)-O(5w)	91.9(3)
O(2)#1-Mg(1)-O(5)#2	100.0(3)	O(6)-Mg(2)-O(7)#3	97.7(3)
O(2)#1-Mg(1)-O(1w)	92.2(3)	O(6)-Mg(2)-O(8)#4	94.8(3)
O(2)#1-Mg(1)-O(2w)	172.1(3)	O(6)-Mg(2)-O(4w)	172.9(3)
O(2)#1-Mg(1)-O(3w)	84.0(3)	O(6)-Mg(2)-O(5w)	86.8(3)
O(5)#2-Mg(1)-O(1w)	90.8(3)	O(7)#3-Mg(2)-O(8)#4	82.1(2)
O(5)#2-Mg(1)-O(2w)	86.7(3)	O(7)#3-Mg(2)-O(4w)	87.9(3)
O(5)#2-Mg(1)-O(3w)	86.1(3)	O(7)#3-Mg(2)-O(5w)	93.9(3)
O(1w)-Mg(1)-O(2w)	91.7(3)	O(8)#4-Mg(2)-O(4w)	90.2(3)
O(1w)-Mg(1)-O(3w)	174.7(3)	O(8)#4-Mg(2)-O(5w)	176.0(3)
O(2w)-Mg(1)-O(3w)	92.4(3)	O(4w)-Mg(2)-O(5w)	88.5(3)
O(1)-S(1)-O(2)	112.8(4)	O(5)-S(2)-O(6)	109.1(4)
O(1)-S(1)-O(3)	111.9(5)	O(5)-S(2)-O(7)	105.9(4)
O(1)-S(1)-O(4)	111.5(4)	O(5)-S(2)-O(8)	113.7(4)
O(2)-S(1)-O(3)	108.0(4)	O(6)-S(2)-O(7)	110.3(5)
O(2)-S(1)-O(4)	107.0(5)	O(6)-S(2)-O(8)	113.9(4)
O(3)-S(1)-O(4)	105.1(4)	O(7)-S(2)-O(8)	103.3(4)

Symmetry transformations used to generate equivalent atoms: #1 x,1-y,0.5+z #2 1-x,1-y,1-z #3 1-x,-y,1-z #4 1-x,y,0.5-z