Table 47A-1-001. $Ca_2B_6O_{11} \cdot 5H_2O$ (colemanite). Crystal structure of phase I [66Hai]. $T = 23$ °C. Fractional coordinates, and isotropic temperature parameters obtained by neutron diffraction. For A, B, C, D sites, see Fig. 47A-1-002, Fig. 47A-1-003. The temperature parameters are defined by Eq. (e) in Introduction.

Atom	*x*	*y*	*z*	*B*
	[10^{-4}]			[Å^2]
H(63)	775(15)	246(12)	6959(26)	1.8(2)
H(83)	–789(11)	830(8)	–1276(26)	1.5(2)
H(54) (C)	3799(35)	–843(31)	6539(69)	3.0(6)
H(54) (D)	3128(26)	–992(30)	6784(49)	1.6(4)
H(99) (A)	232(63)	5037(99)	9336(99)	5.7(11)
H(99) (B)	729(55)	5199(52)	7120(91)	4.0(8)
H(96)	2006(15)	5204(15)	229(32)	3.4(3)
Ca	1349(8)	2884(6)	7340(17)	1.20(9)
B(1)	3345(6)	2117(15)	3104(11)	0.47(7)
B(2)	2204(6)	523(4)	4943(23)	0.44(7)
B(3)	402(5)	1709(5)	1656(11)	0.56(7)
O(1)	3424(6)	1499(5)	5078(12)	0.78(9)
O(2)	1889(5)	2314(4)	1411(10)	0.43(6)
O(3)	880(5)	554(5)	2701(10)	0.43(6)
O(4)	4808(5)	2530(5)	3139(11)	0.59(6)
O(5)	2961(7)	–671(7)	5151(27)	1.11(9)
O(6)	1669(7)	776(5)	6924(12)	0.82(7)
O(8)	–801(6)	1632(5)	–724(13)	0.67(7)
O(9)	1143(7)	4823(6)	9047(15)	1.52(10)

Table 47A-1-002. $Ca_2B_6O_{11} \cdot 5H_2O$ (colemanite). Crystal structure of phase II [66Hai]. $T = –20$ °C. Fractional coordinates and isotropic temperature parameters. A primed atom is related to an unprimed atom by the *a* glide plane in phase I. For A, B, C, D sites, see Fig. 47A-1-002, Fig. 47A-1-003. See also captions of Table 47A-1-003, Table 47A-1-004. The temperature parameters are defined by Eq. (e) in Introduction.

Atom	Unprimed	Primed	Unprimed	Primed	Unprimed	Primed	Unprimed	Primed
	x [10^{-4}]		*y* [10^{-4}]		*z* [10^{-4}]		*B* [Å^2]	
H(63)	3331(40)	8224(34)	198(36)	4711(38)	6922(93)	6989(75)	1.7(6)	1.2(5)
H(83)	1606(27)	6847(26)	878(29)	4180(31)	–1365(55)	–1204(71)	0.7(4)	0.9(4)
H(54) (C)		1322(30)		5769(37)		6574(62)		2.9(5)
H(54) (D)	5645(25)		–937(36)		6823(43)		1.6(4)	
H(99) (A)		7600(69)		52(81)		9312(96)		5.0(7)
H(99) (B)	3293(36)		5229(34)		7232(96)		2.4(6)	
H(96)	4524(52)	9564(33)	5212(76)	–143(55)	66(99)	466(64)	4.3(10)	1.8(5)
Ca	3929(27)	8781(25)	2878(18)	2110(18)	7320(47)	7434(46)	0.97(37)	1.05(34)
B(1)	5821(19)	876(23)	2164(28)	2907(30)	3040(55)	3030(69)	0.23(30)	0.37(32)
B(2)	4704(17)	9715(20)	604(26)	4585(29)	4906(62)	4883(91)	0.18(30)	0.61(38)
B(3)	2938(19)	7868(17)	1784(25)	3361(24)	1640(48)	1614(40)	0.70(30)	0.39(25)
O(1)	5970(20)	883(17)	1473(29)	3495(24)	5054(46)	5063(38)	1.19(32)	0.28(23)
O(2)	4426(18)	9346(19)	2291(30)	2681(32)	1381(31)	1446(37)	0.15(25)	0.69(29)
O(3)	3318(21)	8409(18)	581(29)	4509(29)	2680(48)	2704(37)	0.93(34)	0.24(24)
O(4)	7302(20)	2310(21)	2537(30)	2490(32)	3165(42)	3139(44)	0.51(30)	0.78(33)
O(5)	5481(26)	442(20)	–614(37)	5708(30)	5162(82)	5075(75)	1.81(43)	0.40(29)
O(6)	4104(23)	9238(21)	790(33)	4244(29)	6696(46)	6984(69)	1.50(41)	0.59(29)
O(8)	1705(21)	6705(16)	1568(32)	3329(27)	–691(49)	–781(32)	1.46(33)	0.16(21)
O(9)	3599(18)	8698(27)	4878(23)	256(29)	8974(32)	9155(52)	0.54(22)	2.47(46)

Table 47A-1-003. $Ca_2B_6O_{11} \cdot 5H_2O$ (colemanite). Crystal structures of phases I and II [66Hai]. T = +23 °C (phase I) and T = –20 °C (phase II). Interatomic distances and angles for the hydroxyl groups. A primed atom is related to an unprimed atom by the *a* glide plane in phase I; to a two primed atom by the 2_1 axis in both phases; to a three primed atom by inversion in phase I. For sites C, D, see Fig. 47A-1-002, Fig. 47A-1-003.

Bond system	T [°C]	Distances [Å]			Angles [deg]		
O (6)–H (63)		O (6)···O (3)	O (6)–H (63)	H (63)···O (3)	B (2)–O (6)···O (3)	B (2)–O (6)–H (63)	O (6)–H (63)···O (3)
B (2)–O (6)–H (63)···O‴ (3)	+23	2.76 (1)	1.01 (2)	1.79 (2)	117	112	172
B (2)–O (6)–H (63)···O‴ (3)	–20	2.76 (4)	1.01 (5)	1.79 (5)	124	118	163
B (2)–O′ (6)–H′ (63)···O″ (3)	–20	2.76 (4)	1.05 (5)	1.73 (5)	113	111	173
O (8)–H (83)		O (8)···O (3)	O (8)–H (83)	H (83)···O (3)	B (3)–O (8)···O (3)	B (3)–O (8)–H (83)	O (8)–H (83)···O (3)
B (3)–O (8)–H (83)···O‴ (3)	+23	2.73 (1)	0.99 (2)	1.79 (2)	113	108	172
B (3)–O (8)–H (83)···O‴ (3)	–20	2.61 (4)	0.89 (5)	1.74 (5)	117	122	175
B (3)–O′ (8)–H′ (83)···O″ (3)	–20	2.79 (3)	1.02 (4)	1.80 (4)	108	97	165
O (5)–H (54), site C		O (5)···O (4)	O (5)–H (54)	H (54)···O (4)	B (2)–O (5)···O (4)	B (2)–O (5)–H (54)	O (5)–H (54)···O (4)
B (2)–O (5)–H (54)···O‴ (4)	+23	2.81 (1)	0.98 (4)	2.25 (4)	160	117	120
B′ (2)–O′ (5)–H′ (54)···O″ (4)	–20	2.80 (5)	1.01 (5)	2.30 (4)	161	109	111
O (5)–H (54), site D		O (5)···O (2)	O (5)–H (54)	H (54)···O (2)	B (2)–O (5)···O (2)	B (2)–O (5)–H (54)	O (5)–H (54)···O (2)
B (2)–O (5)–H (54)···O″ (2)	+23	3.06 (1)	1.04 (3)	2.21 (3)	130	108	140
B (2)–O (5)–H (54)···O″ (2)	–20	3.15 (4)	1.06 (5)	2.29 (4)	131	109	139

Table 47A-1-004. $Ca_2B_6O_{11} \cdot 5H_2O$ (colemanite). Crystal structures of phases I and II [66Hai]. Interatomic distances and angles for water molecules at different sites. See captions of Table 47A-1-002, Table 47A-1-003 for primed atoms. For sites A, B, see Fig. 47A-1-002, Fig. 47A-1-003.

Distances [Å]			Angles [deg]		
T:	+23 °C	−20 °C		+23 °C	−20 °C
Site:	A or A′	A		A or A′	A′
O‴ (9)···O′ (6)	2.77 (1)	2.68 (4)	O (9)···O‴ (9)···O (6)	87	86
O‴ (9)–H‴ (96)	0.99 (4)	1.06 (5)	O‴ (9)–H‴ (99)···O (9)	158	150
H‴ (96)···O′ (6)	1.86 (3)	1.71 (5)	O‴ (9)–H‴ (96)···O′ (6)	163	157
O‴ (99)···O (9)	2.67 (1)	2.66 (4)	H‴ (96)–O‴ (9)–H‴ (99)	105	104
O‴ (9)–H‴ (99)	0.99 (8)	1.05 (5)			
H‴ (99)···O (9)	1.85 (9)	1.74 (5)			
Ca‴–H‴ (99)	3.02 (8)	2.93 (7)			
Ca‴–O‴ (9)	2.45 (1)	2.35 (4)			
Site:	B or B′	B		B or B′	B
O (9)···O″ (6)	2.77 (1)	2.90 (4)	O″ (5)···O (9)···O″ (6)	122	123
O (9)–H (96)	0.99 (2)	0.96 (7)	O (9)–H (99)···O″ (5)	114	118
H 96···O″ (6)	1.86 (3)	2.03 (7)	O (9)–H (96)···O″ (6)	163	165
O (9)–H (99)	1.23 (7)	1.11 (5)	H (96)–O (9)–H (99)	119	119
Ca···H (99)	2.66 (6)	2.70 (5)			
Ca···O (9)	2.45 (1)	2.53 (4)			