STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

Volume 74 (2018)

Supporting information for article:

The puzzling structure of Cu5FeS4 (bornite) at low temperature

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Figures S1 and S2 illustrate the polarization vector of the distortion modes Γ_4^+ and Γ_1^-; representative displacements observed in the first two slabs of the crystallographic cell are drawn.

Table S1 and S2 list the structural data obtained using the monoclinic $P2_1/c$ and the orthorhombic $P2_12_12_1$ structural models (XRPD data collected at 10 K).

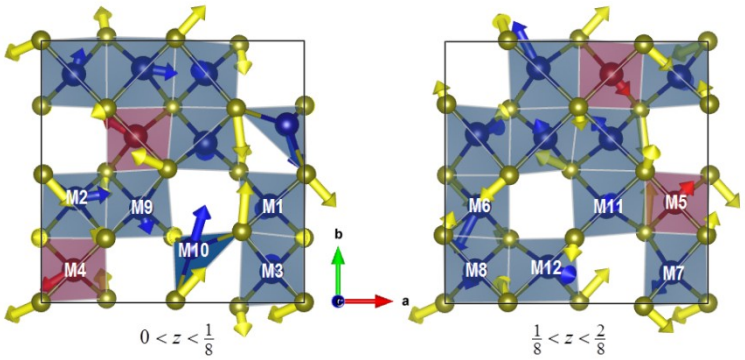

Figure S1. Structural layers of bornite projected along [001]; atom displacements are represented, corresponding to the Γ_4^+ *irrep* determining the *Pbca* → $P2_1/c$ structural transition; selected cationic sites are labelled.

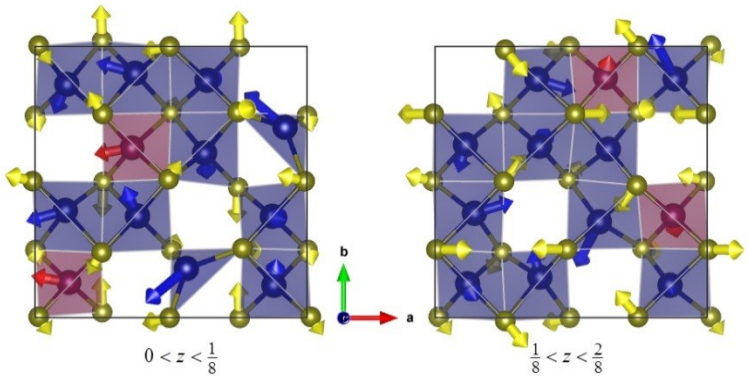

Figure S2. Structural layers of bornite projected along [001]; atom displacements are represented, corresponding to the Γ_1^- *irrep* determining the *Pbca* → $P2_12_12_1$ structural transition; cationic sites as in figure S1.

Table S1. Structural model for bornite at 10 K according to the space group $P2_1/c$.

a (Å)	*b* (Å)	*c* (Å)	β (deg)
10.9382(1)	10.8816(1)	21.7462(1)	90.02(1)

site	Atom	position	coordinates		
			x	*y*	*z*
S1a	S(1)	4*e*	0.2477(4)	0.0155(3)	0.9950(1)
S1b	S(2)	4*e*	0.2492(4)	0.0014(3)	0.4996(1)
S2a	S(3)	4*e*	0.2440(3)	0.4895(4)	0.2512(1)
S2b	S(4)	4*e*	0.2388(3)	0.4951(4)	0.7486(1)
S3a	S(5)	4*e*	0.2589(3)	0.2421(3)	0.3769(2)
S3b	S(6)	4*e*	0.2372(3)	0.7272(3)	0.8755(2)
S4a	S(7)	4*e*	0.9982(3)	0.2475(3)	0.0035(2)
S4b	S(8)	4*e*	0.4995(3)	0.7527(3)	0.5014(2)
S5a	S(9)	4*e*	0.4894(3)	0.5096(4)	0.3726(2)
S5b	S(10)	4*e*	0.9927(3)	0.5100(4)	0.8745(2)
S6a	S(11)	4*e*	0.9987(3)	0.0015(4)	0.1194(1)
S6b	S(12)	4*e*	0.4795(3)	0.9887(4)	0.6263(1)
S7a	S(13)	4*e*	0.2446(4)	0.2456(3)	0.1239(2)
S7b	S(14)	4*e*	0.2490(4)	0.7577(3)	0.6256(2)
S8a	S(15)	4*e*	0.4926(3)	0.2499(4)	0.2500(2)
S8b	S(16)	4*e*	0.0058(3)	0.7387(4)	0.7478(2)
M1a	Cu(1)	4*e*	0.3744(1)	0.3731(2)	0.4416(1)
M1b	Cu(2)	4*e*	0.1307(1)	0.6302(2)	0.9467(1)
M2a	Cu(3)	4*e*	0.1242(1)	0.8823(2)	0.9372(1)
M2b	Cu(4)	4*e*	0.3801(2)	0.3607(2)	0.0658(1)
M3a	Cu(5)	4*e*	0.3760(1)	0.1100(2)	0.4418(1)
M3b	Cu(6)	4*e*	0.1242(1)	0.8823(2)	0.9372(1)
M4a	Fe(1)	4*e*	0.1228(2)	0.1243(2)	0.0612(1)
M4b	Fe(2)	4*e*	0.3588(2)	0.8645(2)	0.5582(1)
M5a	Fe(3)	4*e*	0.3672(2)	0.3753(2)	0.3113(1)
M5b	Fe(4)	4*e*	0.1243(2)	0.6148(2)	0.8098(1)
M6a	Cu(7)	4*e*	0.1302(1)	0.3709(2)	0.1856(1)
M6b	Cu(8)	4*e*	0.3552(1)	0.6012(1)	0.6851(1)
M7a	Cu(9)	4*e*	0.3696(1)	0.1292(2)	0.3108(1)
M7b	Cu(10)	4*e*	0.1395(1)	0.8816(2)	0.8139(1)
M8a	Cu(11)	4*e*	0.1146(2)	0.1255(2)	0.1915(1)
M8b	Cu(12)	4*e*	0.3820(2)	0.8676(2)	0.6930(1)
M9a	Cu(13)	4*e*	0.3801(2)	0.3607(2)	0.0658(1)
M9b	Cu(14)	4*e*	0.1236(2)	0.6279(2)	0.5652(1)
M10a	Cu(15)	4*e*	0.0663(2)	0.1797(1)	0.4074(1)
M10b	Cu(16)	4*e*	0.4263(1)	0.7950(1)	0.9028(1)
M11a	Cu(17)	4*e*	0.1094(1)	0.3663(2)	0.3237(1)
M11b	Cu(18)	4*e*	0.3864(1)	0.6302(2)	0.8149(1)
M12a	Cu(19)	4*e*	0.3935(1)	0.1403(2)	0.1883(1)
M12b	Cu(20)	4*e*	0.1218(1)	0.8537(2)	0.6781(1)

Table S2. Structural model for bornite at 10 K according to the space group $P2_12_12_1$.

a (Å)	*b* (Å)	*c* (Å)
10.9393(1)	10.8784(1)	21.7496(1)

site	atom	position	coordinates		
			x	*y*	*z*
S1a	S(1)	4*a*	0.2469(4)	0.0204(3)	0.9999(2)
S1b	S(2)	4*a*	0.7523(4)	0.9990(3)	0.0030(2)
S2a	S(3)	4*a*	0.2536(3)	0.5020(3)	0.2470(2)
S2b	S(4)	4*a*	0.7583(3)	0.5124(3)	0.7487(2)
S3a	S(5)	4*a*	0.2549(3)	0.2581(4)	0.3702(2)
S3b	S(6)	4*a*	0.7373(3)	0.7443(4)	0.6220(2)
S4a	S(7)	4*a*	0.0019(4)	0.2499(5)	0.0044(2)
S4b	S(8)	4*a*	0.9999(4)	0.7444(5)	0.9973(2)
S5a	S(9)	4*a*	0.5051(3)	0.4999(4)	0.3747(2)
S5b	S(1)	4*a*	0.5088(3)	0.4968(4)	0.6297(2)
S6a	S(1)	4*a*	0.0137(3)	0.0032(4)	0.1221(2)
S6b	S(12)	4*a*	0.9912(3)	0.9893(4)	0.8778(2)
S7a	S(13)	4*a*	0.2451(3)	0.2405(4)	0.1235(2)
S7b	S(14)	4*a*	0.7487(3)	0.7493(4)	0.8750(2)
S8a	S(1)	4*a*	0.4850(3)	0.2517(4)	0.2519(2)
S8b	S(2)	4*a*	0.4948(3)	0.7486(4)	0.7551(2)
M1a	Cu(1)	4*a*	0.3676(1)	0.3752(2)	0.4453(1)
M1b	Cu(2)	4*a*	0.6276(1)	0.6261(2)	0.5586(1)
M2a	Cu(3)	4*a*	0.1119(1)	0.3954(2)	0.0584(1)
M2b	Cu(4)	4*a*	0.8680(1)	0.5989(2)	0.9435(1)
M3a	Cu(5)	4*a*	0.3768(2)	0.1071(2)	0.4419(1)
M3b	Cu(6)	4*a*	0.6220(2)	0.8805(2)	0.5628(1)
M4a	Fe(1)	4*a*	0.1247(2)	0.1296(2)	0.0615(1)
M4b	Fe(2)	4*a*	0.8563(2)	0.8738(2)	0.9403(1)
M5a	Fe(3)	4*a*	0.3735(2)	0.3848(2)	0.3087(1)
M5b	Fe(4)	4*a*	0.6249(2)	0.6242(2)	0.6882(1)
M6a	Cu(7)	4*a*	0.1449(1)	0.3849(2)	0.1850(1)
M6b	Cu(8)	4*a*	0.8751(1)	0.6213(2)	0.8162(1)
M7a	Cu(9)	4*a*	0.3629(2)	0.1215(2)	0.3142(1)
M7b	Cu(1)	4*a*	0.6363(2)	0.8805(2)	0.6875(1)
M8a	Cu(1)	4*a*	0.1198(2)	0.1248(1)	0.1940(1)
M8b	Cu(12)	4*a*	0.8840(2)	0.8681(1)	0.8100(1)
M9a	Cu(13)	4*a*	0.3769(2)	0.3746(1)	0.0669(1)
M9b	Cu(14)	4*a*	0.6171(2)	0.6394(1)	0.9361(1)
M10a	Cu(1)	4*a*	0.0809(1)	0.2018(1)	0.4096(1)
M10b	Cu(2)	4*a*	0.9432(1)	0.8187(1)	0.6011(1)
M11a	Cu(2)	4*a*	0.1178(1)	0.3802(1)	0.3129(1)
M11b	Cu(2)	4*a*	0.8958(1)	0.6464(1)	0.6761(1)
M12a	Cu(2)	4*a*	0.3853(2)	0.1498(2)	0.1846(1)
M12b	Cu(2)	4*a*	0.6117(2)	0.8621(2)	0.8163(1)

Table S3. Structure parameters of bornite at 80 K (space group *Pbca*).

a (Å)	*b* (Å)	*c* (Å)
10.9404(1)	10.9169(1)	21.7947(1)

site	atom	position	Coordinates		
			x	*y*	*z*
S1	S(1)	8*c*	0.2524(1)	0.0027(1)	0.0005(1)
S2	S(2)	8*c*	0.2513(1)	0.4955(1)	0.2494(1)
S3	S(3)	8*c*	0.2557(1)	0.2535(1)	0.3748(1)
S4	S(4)	8*c*	0.0056(1)	0.2463(1)	0.0014(1)
S5	S(5)	8*c*	0.4946(1)	0.4965(1)	0.3728(1)
S6	S(6)	8*c*	0.0060(1)	0.0047(1)	0.1228(1)
S7	S(7)	8*c*	0.2458(1)	0.2436(1)	0.1216(1)
S8	S(8)	8*c*	0.4946(1)	0.2530(1)	0.2523(1)
M1	Cu(1)	8*c*	0.3677(1)	0.3729(1)	0.4400(1)
M2	Cu(2)	8*c*	0.1211(1)	0.4007(1)	0.0591(1)
M3	Cu(3)	8*c*	0.3697(1)	0.1148(1)	0.4379(1)
M4	Fe(1)	8*c*	0.1259(1)	0.1207(1)	0.0598(1)
M5	Fe(2)	8*c*	0.3668(1)	0.3781(1)	0.3099(1)
M6	Cu(4)	8*c*	0.1428(1)	0.3812(1)	0.1843(1)
M7	Cu(5)	8*c*	0.3577(1)	0.1283(1)	0.3066(1)
M8	Cu(6)	8*c*	0.1158(1)	0.1256(1)	0.1906(1)
M9	Cu(7)	8*c*	0.3906(1)	0.3618(1)	0.0670(1)
M10	Cu(8)	8*c*	0.0951(1)	0.1636(1)	0.4182(1)
M11	Cu(9)	8*c*	0.1002(1)	0.3651(1)	0.3211(1)
M12	Cu(10)	8*c*	0.3979(1)	0.1565(1)	0.1743(1)