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A commensurately modulated structure of parabutlerite, $Fe^{3+}SO4(OH)\cdot 2H2O$

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Table S1 Atom coordinates and equivalent displacement parameters in the commensurate structure of parabutlerite (*Pnma*(0β0)*s*0*s*).

Atom	*x/a*	*y/b*	*z/c*	U_{eq}
Fe1	0.375062(12)	–0.00005(3)	0.21143(4)	0.01047(9)
S1	0.37768(3)	0.25	0.57746(9)	0.01163(18)
S2	0.37334(3)	–0.25	–0.15860(9)	0.01083(18)
O1	0.33547(9)	0.25	0.7387(2)	0.0195(6)
O2	0.30588(9)	–0.25	–0.2170(3)	0.0274(7)
O3	0.47584(7)	0.01074(16)	0.2304(2)	0.0283(5)
O4	0.41800(9)	–0.25	–0.3120(3)	0.0210(6)
O5	0.44696(9)	0.25	0.6243(3)	0.0282(7)
O6	0.27525(7)	–0.01426(16)	0.1790(2)	0.0272(5)
O7	0.37696(8)	–0.25	0.3040(2)	0.0137(5)
O8	0.36230(6)	0.08811(16)	0.46558(18)	0.0172(4)
O9	0.38552(6)	–0.08887(16)	–0.04695(18)	0.0203(4)
O10	0.37494(9)	0.25	0.1178(2)	0.0154(5)
H1	0.2482(6)	-0.1067(13)	0.195(3)	0.03263
H2	0.2505(6)	0.0837(13)	0.205(3)	0.03263
H3	0.4994(7)	–0.0871(13)	0.270(3)	0.03397
H4	0.4995(7)	0.1063(13)	0.268(3)	0.03397
H5	0.3765(12)	–0.25	0.4299(8)	0.016465
H6	0.3672(12)	0.25	–0.0063(10)	0.018465

Table S2 Amplitudes of displacive modulations in the commensurate structure of parabutlerite (*Pnma*(0β0)*s*0*s*).

Fe1	sin (0,1,0)	0.005712(15)	–0.00183(4)	−0.00004(5)
	cos (0,1,0)	–0.002614(16)	–0.00040(4)	–0.00593(5)
	sin (0,2,0)	0.002375(18)	0.00045(5)	–0.00091(7)
	cos (0,2,0)	–0.00061(2)	–0.00094(6)	0.00159(7)
S1	sin (0,1,0)	0	–0.01466(11)	0

	cos (0,1,0)	–0.00240(4)	0	0.00371(12)
	sin (0,2,0)	0	0.00223(15)	0
	cos (0,2,0)	–0.00314(5)	0	0.00143(17)
S2	sin (0,1,0)	0	0.00809(10)	0
	cos (0,1,0)	0.00015(4)	0	0.00016(12)
	sin (0,2,0)	0	0.00064(14)	0
	cos (0,2,0)	0.00207(5)	0	–0.00179(16)
		0	–0.0080(3)	0
O1	sin (0,1,0)			
		–0.01131(12)	0	–0.0129(3)
	cos (0,1,0)			
		0	0.0069(4)	0
	sin (0,2,0)			
		–0.00403(15)	0	–0.0026(4)
	cos (0,2,0)			
		0	0.0462(4)	0
O2	sin (0,1,0)			
		–0.00640(12)	0	0.0471(4)
	cos (0,1,0)			
		0	0.0137(4)	0
	sin (0,2,0)			
		0.00523(15)	0	–0.0280(5)
	cos (0,2,0)			
		0.00435(8)	–0.0087(3)	0.0276(3)
O3	sin (0,1,0)			
		–0.00193(8)	0.0309(3)	–0.0099(3)
	cos (0,1,0)			
		0.00252(10)	–0.0030(3)	–0.0025(3)
	sin (0,2,0)			
		–0.00093(10)	–0.0012(3)	0.0059(3)
	cos (0,2,0)			
		0	–0.0029(3)	0
O4	sin (0,1,0)			
		–0.01092(12)	0	–0.0259(3)
	cos (0,1,0)			
		0	–0.0039(4)	0
	sin (0,2,0)			
		0.00732(15)	0	0.0126(4)
	cos (0,2,0)			
		0	–0.0463(3)	0
O5	sin (0,1,0)			
		–0.00567(12)	0	0.0367(4)
	cos (0,1,0)			
		0	0.0065(4)	0
	sin (0,2,0)			
		–0.00363(15)	0	0.0037(5)
	cos (0,2,0)			
		0.00624(8)	–0.0090(2)	–0.0357(3)
O6	sin (0,1,0)			
		–0.00209(8)	–0.0300(2)	–0.0002(3)
	cos (0,1,0)			
		0.00192(10)	0.0009(3)	0.0026(4)
	sin (0,2,0)			
		–0.00115(10)	0.0006(3)	0.0095(3)
	cos (0,2,0)			
		0	–0.0047(3)	0
O7	sin (0,1,0)			

		0.00775(11)	0	–0.0048(3)
	cos (0,1,0)			
		0	0.0002(4)	0
	sin (0,2,0)			
		0.00198(14)	0	–0.0010(4)
	cos (0,2,0)			
		–0.01051(8)	–0.00197(20)	–0.0083(2)
O8	sin (0,1,0)			
		–0.00063(8)	–0.00124(19)	–0.0041(2)
	cos (0,1,0)			
		0.00232(11)	0.0005(3)	0.0007(3)
	sin (0,2,0)			
		–0.00124(10)	–0.0011(3)	0.0036(3)
	cos (0,2,0)			
		0.01390(9)	–0.0040(2)	0.0052(2)
O9	sin (0,1,0)			
		0.00367(9)	0.00052(20)	–0.0052(2)
	cos (0,1,0)			
		0.00028(11)	–0.0006(3)	–0.0006(3)
	sin (0,2,0)			
		–0.00365(11)	0.0023(3)	–0.0010(3)
	cos (0,2,0)			
		0	–0.0008(3)	0
O10	sin (0,1,0)			
		–0.01678(13)	0	–0.0058(3)
	cos (0,1,0)			
		0	–0.0027(4)	0
	sin (0,2,0)			
		–0.00260(15)	0	0.0039(4)
	cos (0,2,0)			
		0.0074(8)	0.0006(16)	–0.026(3)
H1	sin (0,1,0)			
		–0.0005(8)	–0.0218(18)	0.023(3)
	cos (0,1,0)			
		–0.0031(9)	0.0155(18)	0.008(3)
	sin (0,2,0)			
		–0.0017(9)	0.0078(18)	0.021(3)
	cos (0,2,0)			
		0.0083(8)	–0.0131(16)	–0.033(3)
H2	sin (0,1,0)			
		–0.0014(8)	–0.0197(17)	–0.007(3)
	cos (0,1,0)			
		0.0068(9)	0.0144(18)	–0.002(2)
	sin (0,2,0)			
		–0.0055(9)	–0.0086(18)	0.0151(19)
	cos (0,2,0)			
		0.0049(8)	–0.0129(16)	0.0348(19)
H3	sin (0,1,0)			
		–0.0017(7)	0.0243(17)	–0.0087(19)
	cos (0,1,0)			
		0.0041(9)	0.000(2)	–0.0036(17)
	sin (0,2,0)			
		0.0033(8)	0.0041(19)	0.0100(17)
	cos (0,2,0)			
		0.0060(9)	0.0007(17)	0.014(3)
H4	sin (0,1,0)			
		–0.0053(9)	0.0278(17)	0.006(3)
	cos (0,1,0)			

		–0.0003(11)	0.006(2)	–0.007(4)
	sin (0,2,0)			
		0.0001(11)	0.001(2)	–0.008(4)
	cos (0,2,0)			
		0	–0.001(4)	0
H5	sin (0,1,0)			
		0.0079(15)	0	–0.0047(11)
	cos (0,1,0)			
		0	0.008(5)	0
	sin (0,2,0)			
		–0.0010(18)	0	–0.0011(12)
	cos (0,2,0)			
		0	0.001(4)	0
H6	sin (0,1,0)			
		–0.0134(15)	0	–0.0069(13)
	cos (0,1,0)			
		0	–0.001(5)	0
	sin (0,2,0)			
		0.0012(18)	0	0.0029(15)
	cos (0,2,0)			

Table S3 Harmonic atomic displacement parameters in the commensurate structure of parabutlerite (*Pnma*(0β0)*s*0*s*).

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.01311(16)	0.00660(15)	0.01170(16)	–0.00007(9)	0.00002(10)	–0.00089(10)
S1	0.0147(3)	0.0098(3)	0.0104(3)	0	–0.0019(2)	0
S2	0.0123(3)	0.0091(3)	0.0111(3)	0	–0.0005(2)	0
O1	0.0317(11)	0.0174(10)	0.0093(10)	0	0.0056(8)	0
O2	0.0208(11)	0.0241(11)	0.0374(15)	0	-0.0120(10)	0
O3	0.0159(7)	0.0219(8)	0.0471(10)	-0.0012(6)	-0.0056(7)	0.0051(8)
O4	0.0289(11)	0.0189(10)	0.0151(11)	0	0.0073(9)	0
O5	0.0187(10)	0.0268(11)	0.0390(14)	0	-0.0105(9)	0
O6	0.0125(7)	0.0210(7)	0.0481(10)	0.0003(5)	-0.0018(7)	-0.0078(8)
O7	0.0256(10)	0.0074(8)	0.0081(9)	0	0.0013(8)	0
O8	0.0299(8)	0.0105(6)	0.0111(7)	–0.0027(5)	0.0004(5)	–0.0015(6)
O9	0.0387(9)	0.0105(6)	0.0118(7)	–0.0014(6)	0.0028(6)	–0.0030(6)
O10	0.0290(11)	0.0083(8)	0.0089(9)	0	–0.0014(8)	0