Supplementary Information for

Gowerite $Ca[B_5O_8(OH)][B(OH)_3]\cdot 3H_2O$:

Revisiting the crystal structure and exploring its formation context

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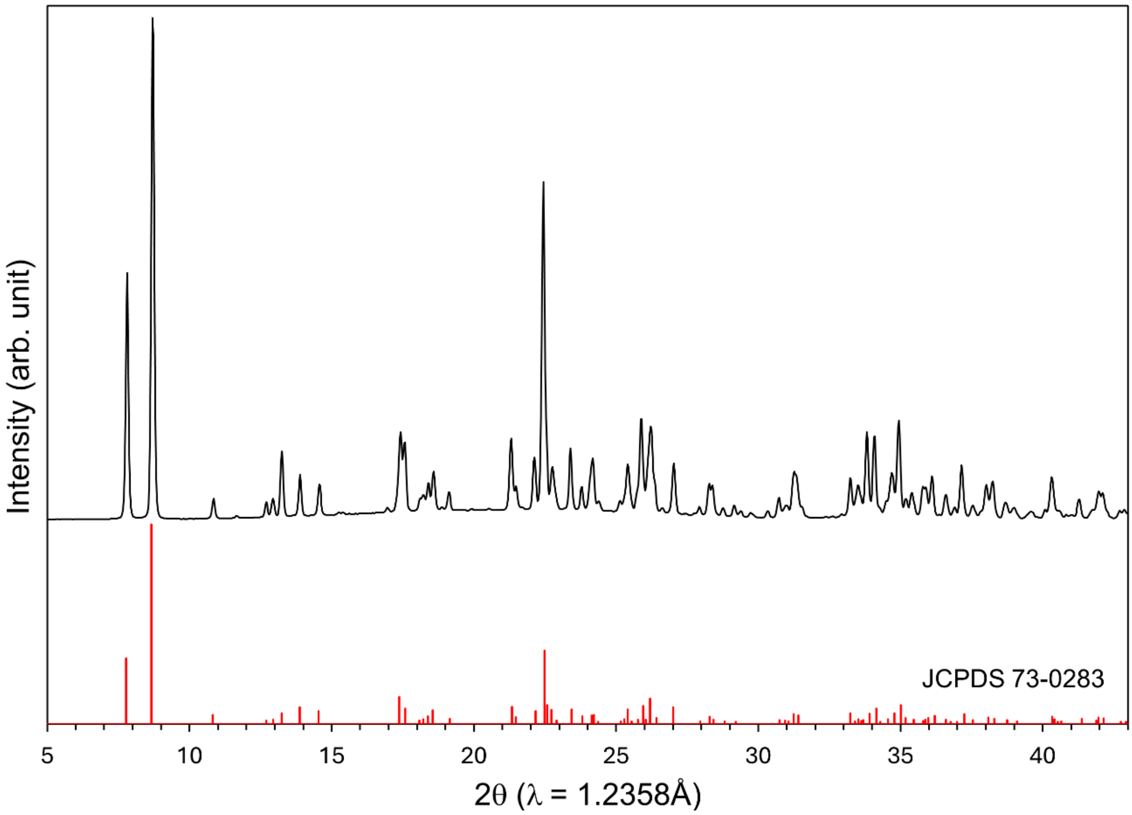

Figure S1. The synchrotron powder XRD pattern of the product obtained from a mixture with a molar ratio of 5.0 H_3BO_3, 1.0 $CaCl_2 \cdot 2H_2O$, and 1.0 NaOH by heating at 120 °C.

Table S1. Crystal data and summary of parameters describing data collection and refinement for gowerite.

Diffractometer	Bruker AXS Smart Apex II Ultra
X-ray radiation (Å)	Mo*K*α (λ = 0.71073)
Temperature (K)	296(2)
Formula	$Ca[B_5O_8(OH)][B(OH)_3]\cdot 3H_2O$
Colour	colourless
Crystal size (mm)	0.10 × 0.05 × 0.05
Crystal system	monoclinic
Space group	$P2_1/a$
a (Å)	12.872(4)
b (Å)	16.326(4)
c (Å)	6.5634(18)
β (°)	121.319(3)
V (Å^3)	1178.3(6)
Z	4
Maximum observed 2θ (°)	49.27
Measured reflections	5319
Unique reflections	1970
Reflections $F_o > 4\sigma(F_o)$, R_{int}	1730, 0.0300
Range of *h*, *k*, *l*	$-11 \le h \le 15$
	$-18 \le k \le 19$
	$-7 \le l \le 6$
$R1$ [$F_o > 4\sigma(F_o)$]	0.0413
*wR*2	0.1161
GoF	1.478
Number of l.s. parameters	240
Residual highest peak (e/Å^3) [distance from the nearest atom]	0.64 [1.12 Å from Ca]
Residual deepest hole (e/Å^3) [distance from the nearest atom]	-0.37 [0.90 Å from B2]

Note: $R_{int} = \Sigma|F_o^2 - F_o^2(mean)|/\Sigma[F_o^2]$. GoF = $S = \{\Sigma[w(F_o^2 - F_c^2)^2]/(n-p)\}^{1/2}$. $R1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. $wR2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$. $w = 1/[\sigma^2(F_o^2)+(aP)^2]$ where a is 0.0510, b is 2.6403, and P is $[\mathrm{Max}(F_o^2, 0)+2F_c^2]/3$.

Table S2. The fractional atomic coordinates, isotropic displacement parameters, and anisotropic displacement parameters for gowerite.

	x	y	z	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	U_{eq}
Ca	0.19017(5)	0.25205(3)	0.08245(11)	0.0053(3)	0.0102(4)	0.0055(4)	0.0001(2)	0.0031(3)	-0.0006(2)	0.0069(2)
B(1)	0.6289(3)	0.23940(18)	0.5725(6)	0.0059(16)	0.0068(17)	0.0061(17)	-0.0021(12)	0.0054(14)	-0.0034(12)	0.0052(7)
B(2)	0.4396(3)	0.30885(19)	0.4935(6)	0.0045(15)	0.0121(18)	0.0054(16)	0.0012(13)	0.0028(14)	0.0010(12)	0.0072(7)
B(3)	0.4769(3)	0.27536(19)	0.1681(6)	0.0081(17)	0.0063(16)	0.0069(17)	-0.0011(12)	0.0046(14)	-0.0022(12)	0.0067(7)
B(4)	0.3451(3)	0.31314(19)	0.7323(6)	0.0039(15)	0.0098(17)	0.0049(16)	0.0010(12)	0.0022(13)	0.0013(12)	0.0062(6)
B(5)	0.4185(3)	0.4408(2)	0.6527(6)	0.0026(15)	0.0167(19)	0.0065(16)	0.0007(12)	0.0026(14)	0.0006(12)	0.0085(7)
B(6)	0.2308(3)	0.0731(2)	0.0509(6)	0.0079(17)	0.0159(19)	0.0114(18)	0.0022(13)	0.0049(15)	0.0010(13)	0.0118(7)
O(1)	0.23635(16)	0.29336(11)	0.7392(3)	0.0041(10)	0.0104(11)	0.0058(10)	-0.0010(7)	0.0027(9)	-0.0009(8)	0.0067(5)
O(2)	0.55331(18)	0.26207(11)	0.6476(4)	0.0040(10)	0.0113(11)	0.0044(11)	0.0004(7)	0.0022(9)	0.0012(7)	0.0065(5)
O(3)	0.59500(18)	0.24999(11)	0.3362(4)	0.0048(10)	0.0142(12)	0.0063(11)	0.0007(8)	0.0037(9)	0.0021(7)	0.0081(5)
O(4)	0.39844(16)	0.29591(11)	0.2393(3)	0.0055(10)	0.0116(11)	0.0041(11)	-0.0008(7)	0.0031(9)	0.0001(7)	0.0068(5)
O(5)	0.46724(17)	0.39696(11)	0.5465(3)	0.0068(10)	0.0082(11)	0.0098(11)	-0.0011(7)	0.0062(9)	0.0000(7)	0.0073(5)
O(6)	0.34149(16)	0.28214(12)	0.5220(3)	0.0050(10)	0.0106(11)	0.0060(11)	-0.0009(8)	0.0043(9)	-0.0004(8)	0.0065(4)
O(7)	0.45374(17)	0.27828(12)	-0.0558(3)	0.0040(10)	0.0126(11)	0.0051(11)	0.0006(8)	0.0026(9)	0.0010(8)	0.0071(5)
O(8)	0.35599(17)	0.40425(11)	0.7446(3)	0.0085(10)	0.0087(11)	0.0092(11)	-0.0011(8)	0.0063(9)	-0.0008(7)	0.0080(5)
O(9)	0.42893(18)	0.52460(12)	0.6689(4)	0.0186(12)	0.0087(11)	0.0207(12)	-0.0012(8)	0.0185(10)	-0.0020(8)	0.0121(5)
O(10)	0.18242(18)	0.11082(12)	0.1676(4)	0.0156(12)	0.0123(12)	0.0192(13)	0.0009(8)	0.0121(10)	0.0010(8)	0.0143(5)
O(11)	0.28345(19)	0.12873(12)	-0.0225(4)	0.0179(12)	0.0127(12)	0.0215(13)	0.0016(9)	0.0146(11)	0.0004(8)	0.0153(5)
O(12)	0.22779(19)	-0.00899(12)	0.0108(4)	0.0205(12)	0.0119(12)	0.0264(14)	0.0011(9)	0.0181(11)	0.0003(9)	0.0168(5)
O(13)	0.12680(19)	0.38902(12)	0.0561(4)	0.0135(12)	0.0127(12)	0.0158(12)	0.0003(8)	0.0090(10)	-0.0007(8)	0.0133(5)
O(14)	0.0964(2)	0.44711(15)	0.4065(4)	0.0216(15)	0.0161(16)	0.0151(15)	0.0010(10)	0.0027(13)	0.0022(11)	0.0185(6)
O(15)	0.38485(19)	0.10910(13)	0.7035(4)	0.0133(12)	0.0201(13)	0.0156(13)	0.0004(9)	0.0072(11)	-0.0016(9)	0.0164(5)
H(9)	0.462(3)	0.5486(19)	0.590(6)							0.025(10)
H(10)	0.142(4)	0.079(3)	0.226(8)							0.076(17)
H(11)	0.315(3)	0.116(2)	-0.122(6)							0.044(12)
H(12)	0.194(4)	-0.038(3)	0.085(7)							0.070(16)
H(13A)	0.171(3)	0.4306(19)	0.037(7)							0.054(14)
H(13B)	0.113(4)	0.409(2)	0.175(6)							0.060(15)
H(14A)	0.106(4)	0.5046(13)	0.391(8)							0.071(16)
H(14B)	0.167(4)	0.431(3)	0.549(7)							0.081(17)
H(15A)	0.367(3)	0.1601(17)	0.625(7)							0.061(15)
H(15B)	0.4700(18)	0.109(2)	0.808(6)							0.057(14)