Supplemental Table S1. Details of neutron and X-ray data collections and refinements of kernite.

T (K)	20	293
Crystal shape	Prism	Prism
Crystal volume (mm)	3 x 2 x 2	0.22 x 0.12 x 0.11
Crystal colour	White	White
Unit-cell parameters	a = 6.996(1) Å	a = 6.9983(3) Å
	b = 9.128(3) Å	b = 9.1375(3) Å
	c = 15.608(3) Å	c = 15.6389(7) Å
	β = 109.06(3)°	β = 108.832(5)°
	V = 942.0(4) Å^3	V = 946.53(7) Å^3
Chemical formula	$Na_2B_4O_6(OH)_2{\cdot}3H_2O$	$Na_2B_4O_6(OH)_2{\cdot}3H_2O$
Space Group	$P\,2_1/c$	$P\,2_1/c$
Z	4	4
Radiation type, λ (Å)	Neutron CW, 0.8347	X-ray, Mo$K\alpha$
Diffractometer	D9 four-circle - ILL	Rigaku XtaLABSynergy-i
Data-collection method	ω-scans, ω-2θ scans	ω-scans
$d_{min.}$ (Å)	0.59	0.71
	$-10 \leq h \leq +10$	$-9 \leq h \leq +8$
	$0 \leq k \leq +18$	$-12 \leq k \leq +12$
	$-23 \leq l \leq +24$	$-19 \leq l \leq +20$
Measured reflections	3434	13010
Unique reflections	3161	2296
Unique reflections with F_o >4σ(F_o)	2656	1908
Refined parameters	226	193
Extinction coeff.	0.014(2)	0.001(1)
R_{Int}	0.0488	0.0361
R_σ	0.0557	0.0259
R_1 (F) with $F_o > 4\sigma(F_o)$	0.0723	0.0324
R_1 (F) for all reflections	0.0884	0.0412
$wR_2(F^2)$	0.1491	0.0655
GooF	1.636	1.519
Residuals (fm/Å^3, e^-/Å^3)	-1.9/+2.5	-0.3/+0.5

Note: Statistical parameters according to the Shelxl-97 definition (Sheldrick 1997, 2008).

Supplemental Table S2. Refined fractional atomic coordinates and equivalent/isotropic displacement factors (Å^2) of kernite, based on the X-ray structure refinement at 293 K and neutron refinement at 20 K. U_{eq} is defined as one third of the trace of the orthogonalised U_{ij} tensor.

			X-ray	***293 K***				***Neutron***	***20 K***	
Site	*s.o.f.*	*x/a*	*y/b*	*z/c*	U_{eq}	*s.o.f.*	*x/a*	*y/b*	*z/c*	U_{eq}/U_{iso}
Na1	1	0.31944(12)	0.46480(8)	0.31093(6)	0.0245(2)	1	0.3190(4)	0.4638(2)	0.3102(2)	0.0067(7)
Na2	1	0.18563(14)	0.36644(9)	0.07250(6)	0.0353(2)	1	0.1869(4)	0.3681(2)	0.0703(2)	0.0073(8)
O1	1	0.4874(2)	0.52527(13)	0.10281(8)	0.0182(3)	1	0.4865(2)	0.52517(13)	0.10184(13)	0.0050(4)
O2	1	0.55971(19)	0.59894(13)	0.25905(8)	0.0157(3)	1	0.5610(2)	0.59800(12)	0.25950(12)	0.0038(4)
O3	1	0.23252(19)	0.70586(14)	0.23145(9)	0.0192(3)	1	0.2321(2)	0.70429(13)	0.23132(13)	0.0046(4)
O4	1	0.46514(18)	0.35087(12)	0.20889(8)	0.0138(3)	1	0.4642(2)	0.34976(12)	0.20771(12)	0.0038(4)
O5	1	0.79157(19)	0.44857(14)	0.21541(9)	0.0200(3)	1	0.7920(2)	0.44738(13)	0.21481(13)	0.0046(4)
O6	1	0.0623(2)	0.29066(16)	0.24061(11)	0.0293(4)	1	0.0648(2)	0.28819(15)	0.24073(14)	0.0062(4)
O7	1	0.4154(2)	0.70621(16)	-0.00985(10)	0.0301(4)	1	0.4169(3)	0.70779(14)	-0.01111(14)	0.0074(5)
O8	1	0.2249(3)	0.53337(18)	0.43187(11)	0.0338(4)	1	0.2223(3)	0.53220(17)	0.43146(15)	0.0105(5)
O9	1	0.5654(2)	0.27258(13)	0.36300(9)	0.0188(3)	1	0.5643(2)	0.27324(13)	0.36308(13)	0.0050(4)
O10	1	-0.0389(2)	0.56220(18)	0.08468(11)	0.0311(4)	1	-0.0380(3)	0.55883(16)	0.08588(15)	0.0080(5)
O11	1	0.1674(2)	0.11763(17)	0.07646(11)	0.0294(4)	1	0.1662(3)	0.11800(15)	0.07555(14)	0.0074(5)
B1	1	0.4469(3)	0.6680(2)	0.07836(14)	0.0173(4)	1	0.4480(2)	0.66898(13)	0.07755(14)	0.00330(18)
B2	1	0.5532(3)	0.2325(2)	0.26885(13)	0.0137(4)	1	0.5530(2)	0.23179(13)	0.26849(13)	0.00260(18)
B3	1	0.5736(3)	0.4804(2)	0.19976(14)	0.0141(4)	1	0.5738(2)	0.48006(13)	0.19901(13)	0.00272(17)
B4	1	0.1323(3)	0.8137(2)	0.25825(15)	0.0184(4)	1	0.1300(2)	0.81241(13)	0.25821(13)	0.00304(18)
H1	1	0.264(4)	0.100(4)	0.1327(16)	0.072(10)	1	0.2679(5)	0.1025(4)	0.1359(3)	0.0207(10)
H2	1	0.106(4)	0.1942(16)	0.2510(19)	0.056(9)	1	0.1110(6)	0.1887(4)	0.2510(3)	0.0202(8)
H3	1	0.048(4)	0.622(3)	0.1249(19)	0.067(10)	1	0.0591(5)	0.6211(4)	0.1296(3)	0.0195(9)
H4	1	0.431(5)	0.626(2)	-0.0447(19)	0.072(10)	1	0.4388(6)	0.6245(4)	-0.0462(3)	0.0195(9)
H5	1	-0.109(4)	0.523(3)	0.120(2)	0.071(10)	1	-0.1151(7)	0.5161(5)	0.1215(3)	0.0247(10)
H6	1	0.293(5)	0.620(3)	0.454(2)	0.088(12)	1	0.2962(6)	0.6219(4)	0.4549(3)	0.0214(8)
H71	0.40(3)	0.197(10)	0.058(6)	0.033(4)	0.046(8)	0.361(14)	0.2060(18)	0.0590(12)	0.0305(11)	0.023(3)
H72	0.60(3)	0.252(7)	0.478(4)	0.485(2)	0.046(8)	0.639(14)	0.2305(10)	0.4714(6)	0.4858(6)	0.0192(17)
H81	0.60(3)	0.048(5)	0.082(5)	0.081(3)	0.046(8)	0.639(14)	0.0370(9)	0.0838(7)	0.0774(5)	0.0208(14)
H82	0.40(3)	0.092(5)	0.568(7)	0.418(5)	0.046(8)	0.361(14)	0.0729(19)	0.5631(12)	0.4193(9)	0.024(2)

Supplemental Table S3. Refined displacement parameters (Å^2) of kernite in the expression: $-2\pi^2[(ha^*)^2U_{11} + \ldots + 2hka^*b^*U_{12} + \ldots + 2klb^*c^*U_{23}]$, based on the X-ray refinement at 293 and neutron structure refinement at 20 K.

T = 293 K	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Na1	0.0299(5)	0.0193(4)	0.0302(5)	0.0008(3)	0.0177(4)	0.0011(3)
Na2	0.0352(5)	0.0245(5)	0.0360(5)	0.0007(4)	-0.0027(4)	-0.0016(4)
O1	0.0291(7)	0.0128(6)	0.0134(6)	0.0002(5)	0.0078(5)	0.0018(5)
O2	0.0222(7)	0.0105(6)	0.0136(6)	-0.0005(5)	0.0048(5)	0.0020(5)
O3	0.0171(7)	0.0162(6)	0.0249(7)	-0.0048(5)	0.0078(5)	-0.0035(5)
O4	0.0146(6)	0.0103(6)	0.0165(6)	0.0013(5)	0.0052(5)	0.0007(4)
O5	0.0174(6)	0.0165(6)	0.0288(7)	0.0020(5)	0.0112(5)	-0.0001(5)
O6	0.0191(7)	0.0249(8)	0.0462(9)	0.0009(6)	0.0138(6)	0.0025(6)
O7	0.0527(8)	0.0212(7)	0.0172(6)	0.0021(5)	0.0126(6)	0.0074(6)
O8	0.0398(8)	0.0335(8)	0.0306(7)	-0.0049(6)	0.0150(6)	-0.0050(6)
O9	0.0286(7)	0.0131(6)	0.0148(6)	-0.0013(5)	0.0073(5)	-0.0028(5)
O10	0.0331(8)	0.0358(8)	0.0249(8)	-0.0046(7)	0.0103(7)	-0.0087(7)
O11	0.0310(7)	0.0292(7)	0.0248(7)	-0.0015(6)	0.0048(6)	-0.0006(6)
B1	0.0216(11)	0.0154(10)	0.0152(10)	0.0008(8)	0.0064(8)	0.0006(8)
B2	0.0167(10)	0.0112(9)	0.0133(10)	0.0007(7)	0.0051(8)	0.0002(7)
B3	0.0177(10)	0.0113(9)	0.0148(10)	0.0002(7)	0.0073(8)	0.0005(7)
B4	0.0181(10)	0.0190(10)	0.0191(10)	0.0016(8)	0.0071(8)	-0.0004(8)

Note: All the H sites were modelled isotropically in the X-ray structure refinement at 293 K