Supplement for

Kahlenbergite KAl11O17, a new β-alumina mineral and Fe-rich hibonite from the Hatrurim Basin, Negev Desert, Israel

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Table S1. Experimental parameter

Mineral	kahlenbergite	Hibonite
Refined formula	$KAl_{9.621}Fe_{1.379}O_{17}$	$Ca\ Al_{10.166}\ Fe_{1.554}\ O_{19}\ Ti0.28$
Unit cell dimensions(Å)	$a = b = 5.6486(1)$ $c = 22.8970(3)$ $\alpha = \beta = 90°\ \gamma = 120°$ V = 632.690(12)	$a = b = 5.6420(2)$ $c = 22.1749(7)$ $\alpha = \beta = 90°\ \gamma = 120°$ V = 611.31(4)
Z	2	2
Space group	$P6_3/mmc$ (no.194)	$P6_3/mmc$ (no.194)
Density (calculated) g/cm^3	3.40	3.9037
Crystal size (μm)	30 × 25 × 20	60 × 30 × 15
Data collection		
Diffractometer	beamline X06DA, SLS, λ= 0.70849Å	
Detector / det. distance	PILATUS 2M-F / 80 mm	
Exposure time (sec.) / step size	0.1 / 0.1	
Number of frames	1800	
Max. θ°-range for data	34.04	32.52
Index ranges	$-8 \leq h \leq 8$ $-8 \leq k \leq 8$ $-33 \leq l \leq 35$	$-8 \leq h \leq 8$ $-7 \leq k \leq 8$ $-31 \leq l \leq 32$
No. of measured reflections	525	506
No. of unique reflections	494	481
Refinement of the structure		
no. of parameters	39	46
no. of constraints	9	0
R_{int}	0.0165	0.0306
R1 (obs) / *R*1 (all)	0.0455 / 0.0465	0.0228 /0.0235
*wR*2(obs) / *wR*2 (all)	0.0926 /0.0928	0.0820 /0.0823
GOF (obs) /GOF (all)	0.0747/0.0724	0.0302 /0.0294
Δρ min (-e. Å^{-3})	3.10 (2.58 Å from O5)	0.68
Δρ max (e. Å^{-3})	-0.91 (0.49 Å from K1)	-0.42

Table S2. Anisotropic displacement parameters ($Å^2$x 10^3) for kahlenbergite.

Site	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
A	0.0299(8)	0.0299(8)	0.0109(9)	0.0150(4)	0	0
M1	0.0057(5)	0.0052(5)	0.0074(6)	0.0026(3)	0.00010(13)	0.0002(2)
M2	0.0033(5)	0.0033(5)	0.0042(6)	0.0016(2)	0	0
M3	0.0050(6)	0.0050(6)	0.0045(8)	0.0025(3)	0	0
M4	0.0045(7)	0.0045(7)	0.0032(9)	0.0023(3)	0	0
O1	0.0072(8)	0.0065(10)	0.0064(10)	0.0033(5)	-0.0008(3)	-0.0015(7)
O2	0.0050(8)	0.0045(10)	0.0085(10)	0.0023(5)	0.0003(3)	0.0006(6)
O3	0.0074(10)	0.0074(10)	0.0058(17)	0.0037(5)	0	0
O4	0.0044(10)	0.0044(10)	0.0078(15)	0.0022(5)	0	0
O5	0.045(3)	0.045(3)	0.005(3)	0.0223(16)	0	0

Table S3. Anisotropic displacement parameters ($Å^2$x 10^3) for hibonite.

Site	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
A	0.0299(3)	0.0299(3)	0.0277(5)	0.01493(17)	0	0
M1	0.0082(3)	0.0082(3)	0.0086(4)	0.00411(16)	0	0
M2	0.0064(3)	0.0064(3)	0.033(7)	0.00322(13)	0	0
M3	0.0066(3)	0.0066(3)	0.0078(3)	0.00331(13)	0	0
M4	0.0072(2)	0.0072(2)	0.0073(3)	0.00361(12)	0	0
M5	0.0064(2)	0.0058(3)	0.0083(3)	0.00291(13)	0.00001(5)	0.00002(10)
O1	0.0090(4)	0.0090(4)	0.0113(7)	0.0045(2)	0	0
O2	0.0085(5)	0.0085(5)	0.0104(7)	0.0043(2)	0	0
O3	0.0200(6)	0.0200(6)	0.0117(7)	0.0136(7)	0	0
O4	0.0098(3)	0.0114(4)	0.0096(4)	0.0057(2)	-0.00081(14)	-0.0016(3)
O5	0.0092(3)	0.0092(3)	0.0108(4)	0.0038(3)	-0.00086(14)	0.00086(14)