

Supplementary Materila: Hydrothermal Synthesis and Structural Investigation of a Crystalline Uranyl Borosilicate

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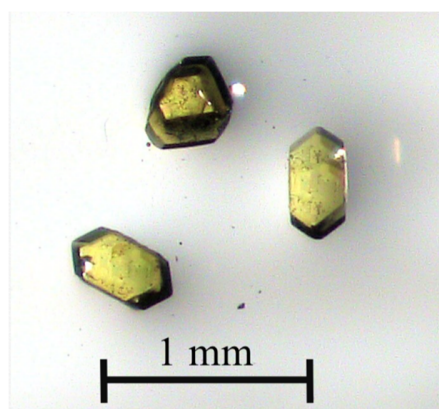


Figure S1: Optical image of single crystals of $K_{1.7}Na_{1.3}[(UO_2)BSi_4O_{12}]$.

Table S1: $K_{1.70}Na_{1.30}[(UO_2)BSi_4O_{12}]$ Crystal Data and Structure Refinement

Formula	$K_{1.70}Na_{1.30}[(UO_2)BSi_4O_{12}]$
space group	<i>Cmca</i>
formula weight (g/mol)	681.56
temperature (K)	300(2)
<i>a</i> (Å)	15.5159(5)
<i>b</i> (Å)	14.3091(4)
<i>c</i> (Å)	11.6961(4)
volume (Å ³)	2596.75(14)
<i>Z</i>	8
density (g cm ⁻³)	3.487
crystal dimensions (mm ³)	0.07 × 0.04 × 0.03
absorption coefficient (mm ⁻¹)	13.536
data collection and refinement	
collected reflections	84652
independent reflections	1671
<i>R</i> _{int}	0.0261

refined restraints/parameters	1/121
goodness-of-fit on F^2	0.972
final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0408$
	$wR_2 = 0.1071$
final R indices (all data)	$R_1 = 0.0413$
	$wR_2 = 0.1077$
largest diff. peak and hole ($e/\text{\AA}^3$)	10.353 and -1.056

Table S2: Selected Interatomic Distances for $K_{1.8}Na_{1.2}[(UO_2)BSi_4O_{12}]$ (\AA)

U(1)-O(1)	1.819(4)	Si(1)-O(5)	1.629(3)	Na(1)/K(2)-O(1)	2.780(3)
U(1)-O(2)	1.813(4)	Si(1)-O(7)	1.614(3)	Na(1)/K(2)-O(2)	2.622(3)
U(1)-O(3) $\times 2$	2.233(3)	Si(1)-O(8)	1.602(3)	Na(1)/K(2)-O(3)	2.834(3)
U(1)-O(8) $\times 2$	2.245(3)	Si(1)-O(9)	1.6268(16)	Na(1)/K(2)-O(4)	2.725(3)
		Si(2)-O(3)	1.587(3)	Na(1)/K(2)-O(5)	2.872(3)
B(1)-O(6) $\times 2$	1.469(4)	Si(2)-O(4)	1.643(2)	Na(1)/K(2)-O(7)	2.590(3)
B(1)-O(7) $\times 2$	1.472(4)	Si(2)-O(5)	1.624(3)	Na(1)/K(2)-O(7)	2.685(4)
		Si(2)-O(6)	1.614(3)	Na(1)/K(2)-O(8)	2.605(3)
				K(2)-O(6)	3.083(3)

Table S3. Selected Interatomic Distances for $K_{1.7}Na_{1.3}[(UO_2)BSi_4O_{12}]$ (\AA)

U(1)-O(1)	1.827(5)	Si(1)-O(5)	1.628(4)	Na(1)/K(2)-O(1)	2.773(4)
U(1)-O(2)	1.813(5)	Si(1)-O(7)	1.611(4)	Na(1)/K(2)-O(2)	2.626(4)
U(1)-O(3) $\times 2$	2.230(4)	Si(1)-O(8)	1.601(4)	Na(1)/K(2)-O(3)	2.825(4)
U(1)-O(8) $\times 2$	2.245(3)	Si(1)-O(9)	1.625(2)	Na(1)/K(2)-O(4)	2.715(4)
		Si(2)-O(3)	1.580(4)	Na(1)/K(2)-O(5)	2.869(4)
B(1)-O(6) $\times 2$	1.467(5)	Si(2)-O(4)	1.639(3)	Na(1)/K(2)-O(7)	2.574(5)
B(1)-O(7) $\times 2$	1.483(6)	Si(2)-O(5)	1.616(4)	Na(1)/K(2)-O(7)	2.675(6)
		Si(2)-O(6)	1.611(4)	Na(1)/K(2)-O(8)	2.584(4)
				K(2)-O(6)	3.074(4)