

Supplementary materials

A Synthetic Analogue of the Mineral Ivanyukite: Sorption Behavior to Lead Cations

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Table S1. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for Pb-exchanged ivanyukite. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U(eq)
Ti1	6428(3)	6428(3)	6428(3)	22.7(12)
Si1	5000	10000	5000	26.0(18)
Pb1	5400	10000	10000	116(5)
O2	3823(12)	6177(12)	6177(12)	24(4)
O1	6226(10)	8808(12)	6226(10)	31(3)
O3	1810(30)	8190(30)	8190(30)	140(30)

Table S2. Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for Pb-exchanged ivanyukite. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a \times ^2U_{11} + 2hka \times b \times U_{12} + \dots]$.

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
Ti1	22.7(12)	22.7(12)	22.7(12)	−0.1(12)	−0.1(12)	−0.1(12)
Si1	28(3)	21(4)	28(3)	0	0	0
Pb1	207(14)	71(3)	71(3)	−29(6)	0	0
O2	24(4)	24(4)	24(4)	−4(4)	4(4)	4(4)
O1	35(4)	23(5)	35(4)	0(3)	−1(5)	0(3)
O3	140(30)	140(30)	140(30)	−48(16)	48(16)	48(16)

Table S3. Bond Lengths for Pb-exchanged ivanyukite.

Atom	Atom	Length/ \AA	Atom	Atom	Length/ \AA	Atom	Atom	Length/ \AA
Ti1	O2	2.052(8)	Si1	O1 ²	1.642(10)	O3	Pb1 ¹	2.955(8)
Ti1	O2 ¹	2.052(8)	Si1	O1 ⁶	1.642(10)	O3	Pb1 ²	2.955(8)
Ti1	O2 ²	2.052(8)	Si1	O1	1.642(10)	O3	Pb1 ³	2.955(8)
Ti1	O1 ⁴	1.870(10)	Si1	O1 ⁷	1.642(10)			
Ti1	O1 ⁵	1.870(10)						
Ti1	O1	1.870(10)						

¹ 1−X,1−Y,+Z; ² 1−X,+Y,1−Z; ³ X,1−Y,1−Z; ⁴ +Y,+Z,+X; ⁵ +Z,+X,+Y; ⁶ +X,2−Y,1−Z; ⁷ 1−X,2−Y,+Z.