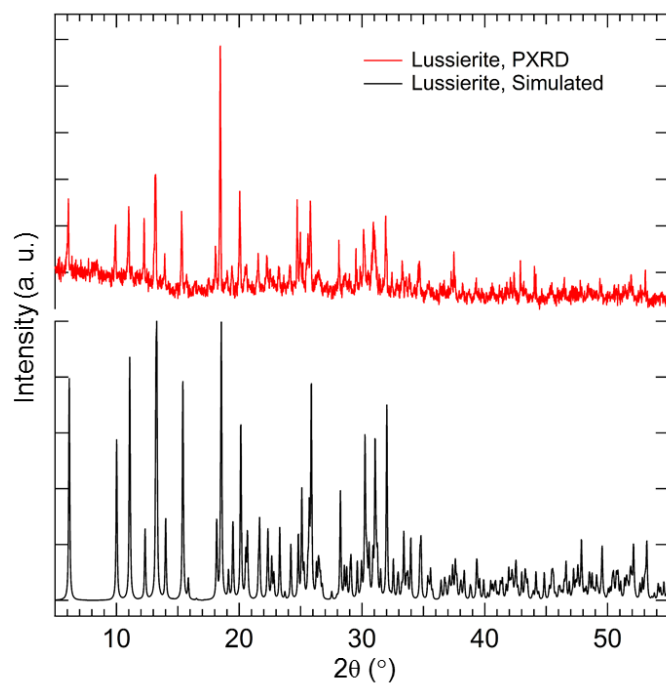
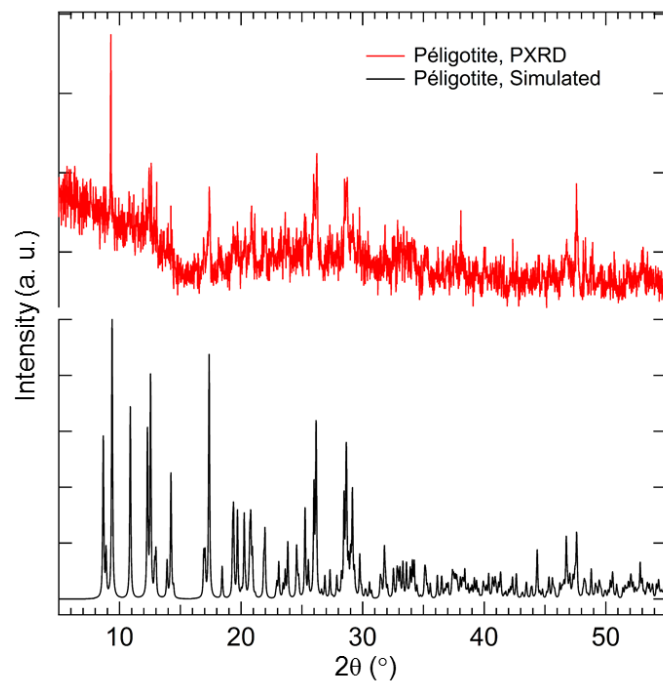


## Supplemental Material

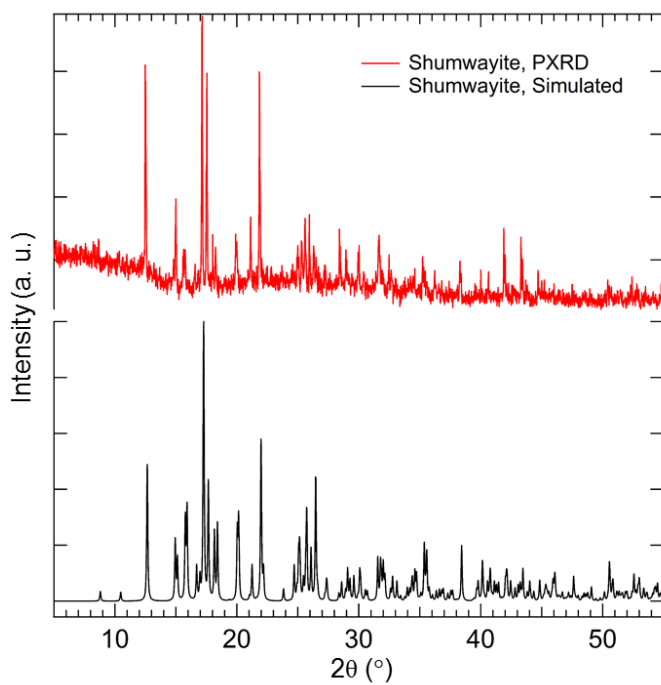
**Figure S1.** PXRD diffractogram and simulated diffractograms of synthetic lussierite.



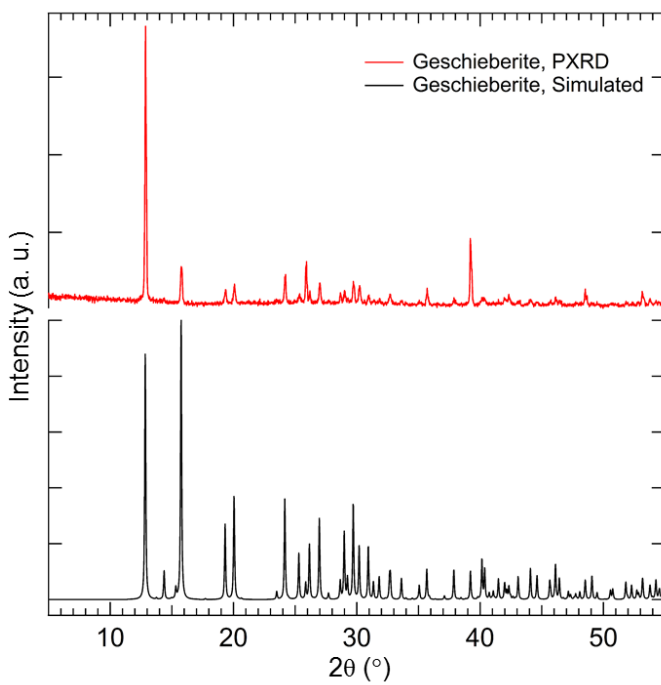
**Figure S2.** PXRD diffractogram and simulated diffractograms of synthetic péligotite.



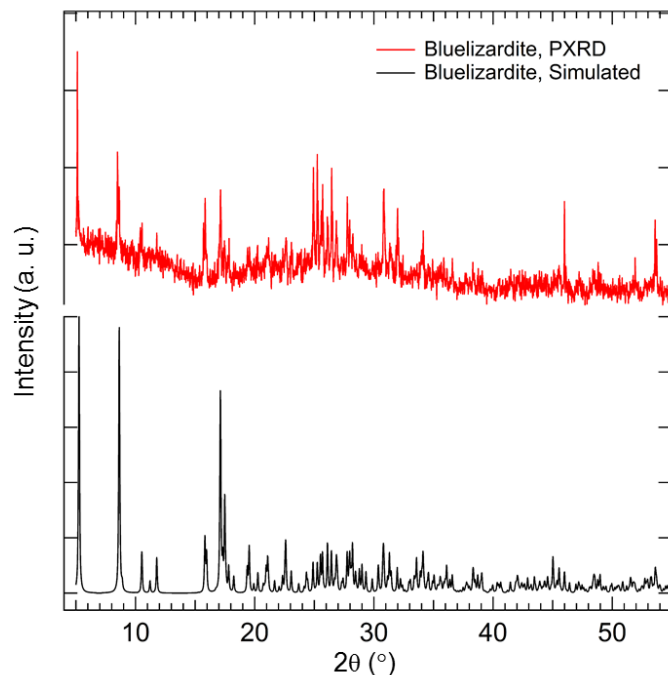
**Figure S3.** PXRD diffractogram and simulated diffractograms of synthetic shumwayite.



**Figure S4.** PXRD diffractogram and simulated diffractograms of synthetic geschieberite.



**Figure S5.** PXRD diffractogram and simulated diffractograms of synthetic blueizardite.



**Table S1.** The ICP-OES determined ratios of the cations of the synthetic analogs. Error is two standard deviations of the mean.

Mineral Analog	Ideal M:U	Actual M:U	Ideal S:U	Actual S:U
Lussierite	10	$9.8 \pm 1.1$	6	$5.4 \pm 0.7$
Péligotite	6	$5.9 \pm 0.3$	4	$3.98 \pm 0.19$
Shumwayite	N/A	N/A	1	$1.02 \pm 0.03$
Geschieberite	2	$2.0 \pm 0.13$	2	$1.84 \pm 0.12$
Blueizardite	7	$7.5 \pm 1.0$	4	$4.1 \pm 0.6$

**Table S2.** The water and Cl moles per formula unit of the uranyl sulfate phases calculated from the mass loss during TGA analysis.

Mineral Analog	Ideal H <sub>2</sub> O	Actual H <sub>2</sub> O	Ideal Cl	Actual Cl
Lussierite	3	3.07	N/A	N/A
Péligotite	4	4.06	N/A	N/A
Shumwayite	5	5.00	N/A	N/A
Geschieberite	2	2.04	N/A	N/A
Blueizardite	2	2.14	1	0.99

**Table S3.** Atomic coordinates and equivalent isotropic displacement parameters ( $\text{\AA}^2$ ) for synthetic lussierite.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	$U(\text{eq})$
U(1)	0.89883(3)	0.17264(2)	0.59519(3)	0.010(1)
S(1)	1.16426(16)	0.34080(6)	0.85644(15)	0.010(1)
S(2)	0.74595(14)	0.16482(4)	0.94349(13)	0.010(1)
S(3)	0.66811(17)	0.33815(6)	0.36555(16)	0.011(1)
S(4)	1.25112(14)	0.16360(4)	0.44648(13)	0.011(1)
S(5)	2.00060(14)	0.03160(4)	1.19165(13)	0.013(1)
S(6)	1.56578(14)	0.03417(4)	0.76984(13)	0.012(1)
Na(1)	0.9043(7)	0.32340(6)	0.6065(6)	0.016(1)
Na(2)	1.2109(2)	0.06282(7)	0.6645(2)	0.022(1)
Na(3)	1.2653(3)	0.24689(10)	0.6871(3)	0.026(1)
Na(4)	1.5212(3)	0.25002(10)	0.4783(3)	0.022(1)
Na(5)	1.4963(3)	0.13854(9)	0.6908(3)	0.023(1)
Na(6)	1.8988(3)	0.06458(8)	0.8519(2)	0.022(1)
Na(7)	1.6664(2)	0.06528(8)	1.1169(2)	0.023(1)
Na(8)	1.7796(3)	-0.04080(8)	0.9758(2)	0.022(1)
Na(9)	1.3588(2)	-0.06790(8)	0.8081(2)	0.024(1)
Na(10)	2.0044(3)	0.13934(8)	1.1797(3)	0.022(1)
O(1)	0.8691(4)	0.23373(12)	0.5801(5)	0.019(1)
O(2)	0.9260(4)	0.11140(11)	0.6037(5)	0.017(1)
O(3)	1.1499(4)	0.33683(12)	1.0107(3)	0.014(1)
O(4)	1.3240(4)	0.33770(12)	0.8450(4)	0.015(1)
O(5)	0.7638(5)	0.16547(14)	0.7893(4)	0.031(1)
O(6)	0.5673(4)	0.30748(12)	0.2732(4)	0.021(1)
O(7)	1.1019(4)	0.17997(15)	0.4749(5)	0.036(1)
O(8)	1.0957(4)	0.30080(12)	0.7855(4)	0.018(1)
O(9)	1.1065(4)	0.38514(14)	0.8057(4)	0.021(1)
O(10)	0.8050(7)	0.12172(16)	0.9995(5)	0.039(1)
O(11)	0.8216(5)	0.20366(14)	1.0096(5)	0.034(1)
O(12)	0.5925(5)	0.1676(2)	0.9570(6)	0.051(2)
O(13)	1.2730(6)	0.11713(14)	0.5024(5)	0.033(1)
O(14)	1.3512(4)	0.19562(13)	0.5163(4)	0.022(1)
O(15)	1.2594(6)	0.16396(17)	0.2966(4)	0.042(1)

O(16)	0.6506(4)	0.32311(12)	0.5089(4)	0.018(1)
O(17)	0.8127(4)	0.32758(13)	0.3262(4)	0.023(1)
O(18)	1.8868(4)	0.05301(15)	1.2696(4)	0.026(1)
O(19)	1.0587(4)	0.01043(12)	0.7637(4)	0.018(1)
O(20)	1.4420(4)	0.06574(13)	0.7892(4)	0.021(1)
O(21)	0.6295(4)	0.38671(14)	0.3442(4)	0.019(1)
O(22)	2.1175(4)	0.06584(13)	1.1803(4)	0.025(1)
O(23)	1.5128(5)	-0.01070(14)	0.7149(5)	0.024(1)
O(24)	1.6621(5)	0.05652(14)	0.6740(4)	0.033(1)
O(25)	1.6458(5)	0.02691(15)	0.9041(4)	0.032(1)
O(26)	1.9400(4)	0.01859(14)	1.0531(4)	0.029(1)
O(27)	0.8750(4)	0.40729(13)	0.5596(4)	0.020(1)
O(28)	1.5311(6)	0.24934(15)	0.7405(5)	0.033(1)
O(29)	1.2813(5)	0.01498(15)	0.4802(5)	0.025(1)
H(27A)	0.789(3)	0.414(2)	0.554(6)	0.024
H(27B)	0.896(6)	0.413(2)	0.479(3)	0.024
H(28A)	1.541(8)	0.2296(19)	0.804(5)	0.040
H(28B)	1.595(6)	0.266(2)	0.776(7)	0.040
H(29A)	1.344(6)	-0.003(2)	0.513(7)	0.030
H(29B)	1.221(6)	-0.0063(19)	0.462(7)	0.030

**Table S4.** Atomic coordinates and equivalent isotropic displacement parameters ( $\text{\AA}^2$ ) for synthetic geschieberite.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	$U(\text{eq})$
U(1)	0.24451(2)	0.41382(3)	0.18839(13)	0.009(1)
S(1)	0.1768(2)	0.7443(4)	-0.03169(19)	0.011(1)
S(2)	0.1764(2)	0.7427(4)	0.40863(19)	0.012(1)
O(3)	0.2481(5)	0.7901(16)	0.5007(10)	0.016(2)
O(5)	0.2372(5)	0.6723(13)	0.3121(8)	0.014(2)
O(4)	0.2394(5)	0.6714(13)	0.0650(7)	0.014(2)
O(8)	0.1074(6)	0.6014(9)	-0.0703(8)	0.020(2)
O(9)	0.1280(6)	0.9137(10)	0.0057(7)	0.017(2)
O(10)	0.1081(6)	0.6122(10)	0.4481(7)	0.019(2)

K(1)	0.4299(2)	0.7383(4)	0.4004(3)	0.023(1)
K(2)	0.0701(2)	0.2380(4)	0.4758(3)	0.023(1)
O(1)	0.3738(3)	0.4305(5)	0.1885(15)	0.019(1)
O(7)	0.2340(4)	0.0698(7)	0.1873(15)	0.021(1)
O(2)	0.1148(3)	0.3980(5)	0.1893(14)	0.017(1)
O(12)	0.0702(4)	0.3973(6)	0.6834(12)	0.027(1)
O(11)	0.1282(6)	0.9104(10)	0.3688(7)	0.019(2)
O(6)	0.2485(4)	0.7903(15)	-0.1260(8)	0.013(2)
H(12A)	0.128(5)	0.470(12)	0.711(10)	0.05(3)
H(12B)	0.036(8)	0.510(11)	0.709(15)	0.11(5)
H(7A)	0.199(4)	0.023(9)	0.255(4)	-0.001(14)
H(7B)	0.20(4)	0.00(10)	0.12(4)	0.8(6)