

Mild Hydrothermal Crystal Growth, Structure, and Magnetic Properties of Ternary U(IV) Containing Fluorides; LiUF_5 , KU_2F_9 , $\text{K}_7\text{U}_6\text{F}_{31}$, RbUF_5 , RbU_2F_9 , and $\text{RbU}_3\text{F}_{13}$

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Figure S1. The experimental and calculated powder X-ray diffraction data for LiUF_5 , KU_2F_9 , $\text{K}_7\text{U}_6\text{F}_{31}$, RbUF_5 , and $\text{RbU}_3\text{F}_{13}$

Figure S2. Temperature dependence of the molar inverse susceptibility data for LiUF_5 , KU_2F_9 , $\text{K}_7\text{U}_6\text{F}_{31}$, RbUF_5 , and $\text{RbU}_3\text{F}_{13}$, measured in an applied field of 1000 Oe

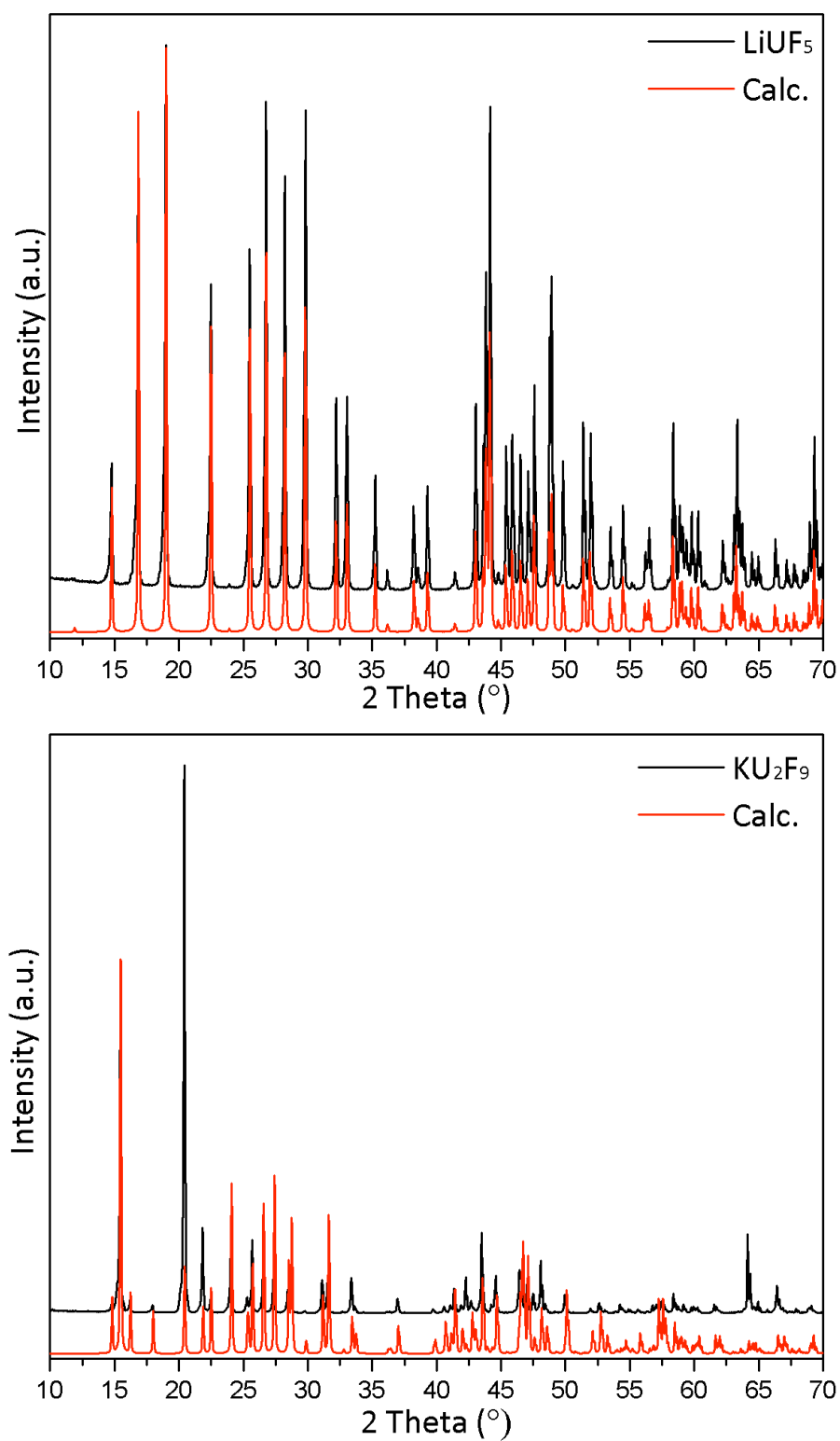
Figure S3. Field dependence of the magnetization for LiUF_5 , KU_2F_9 , $\text{K}_7\text{U}_6\text{F}_{31}$, RbUF_5 , and $\text{RbU}_3\text{F}_{13}$

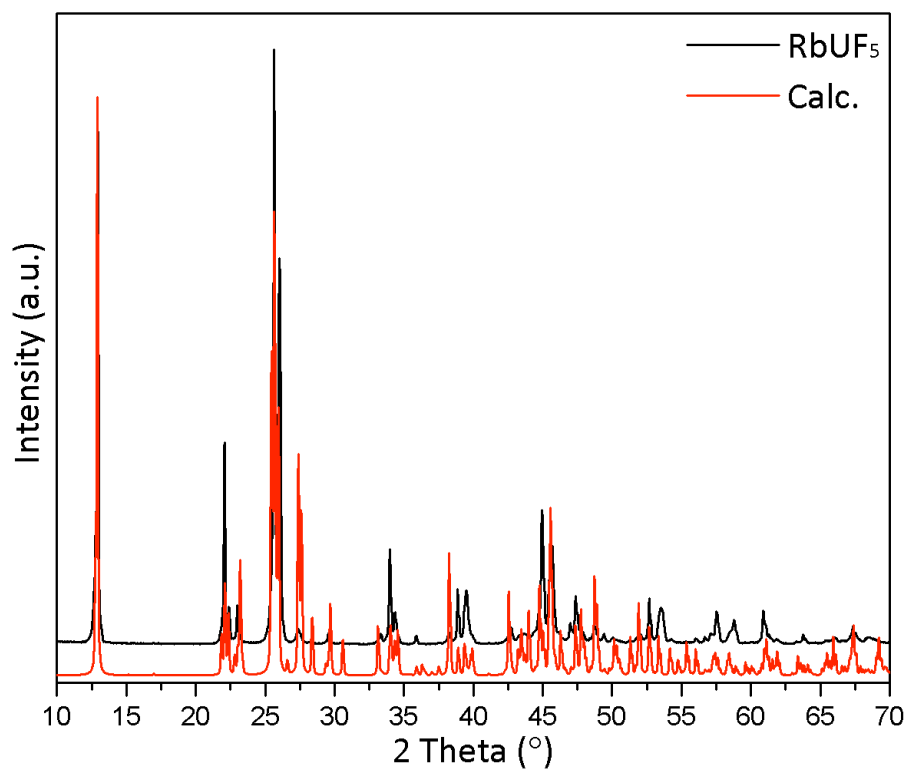
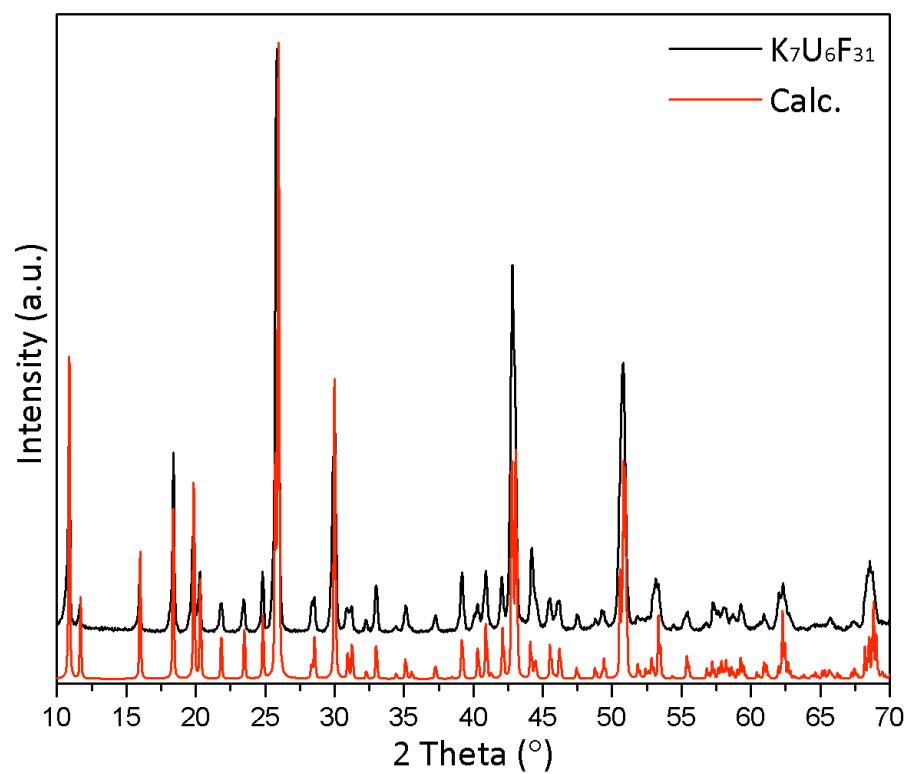
Figure S4. $\chi_m T$ vs T data for LiUF_5 , KU_2F_9 , $\text{K}_7\text{U}_6\text{F}_{31}$, RbUF_5 , and $\text{RbU}_3\text{F}_{13}$, measured in an applied field of 1000 Oe

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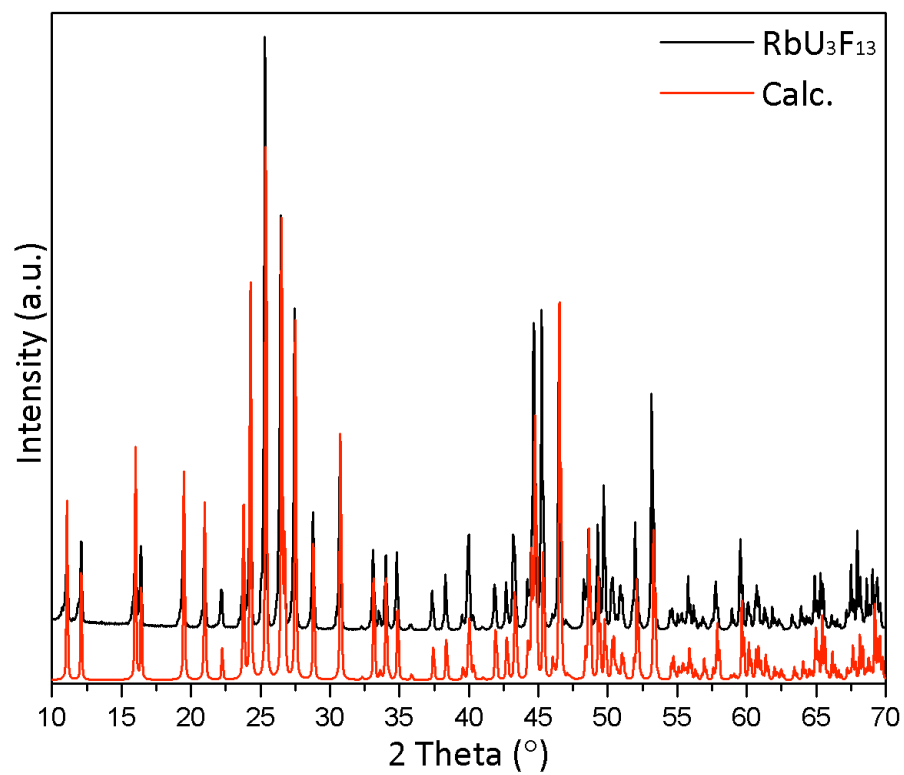


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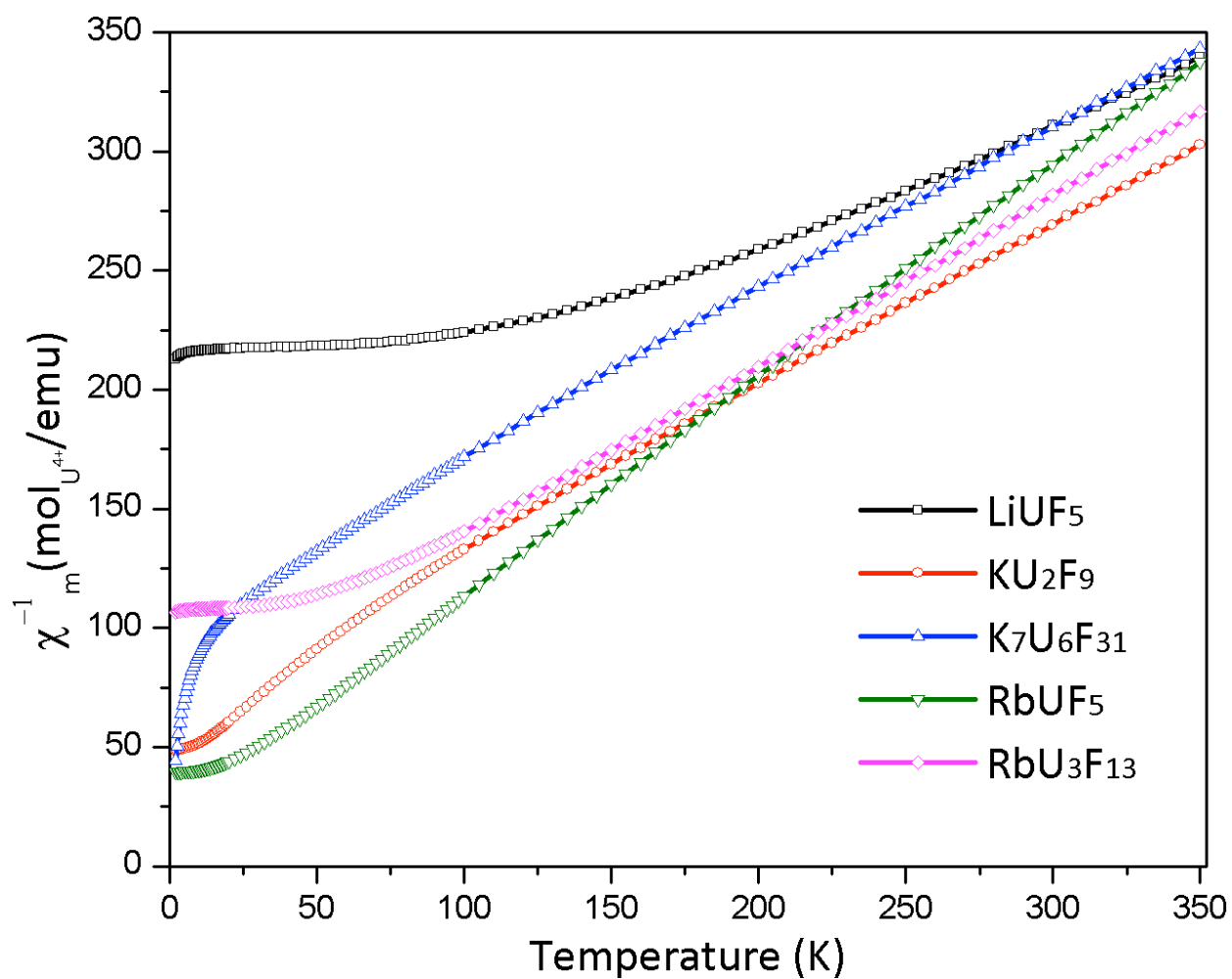


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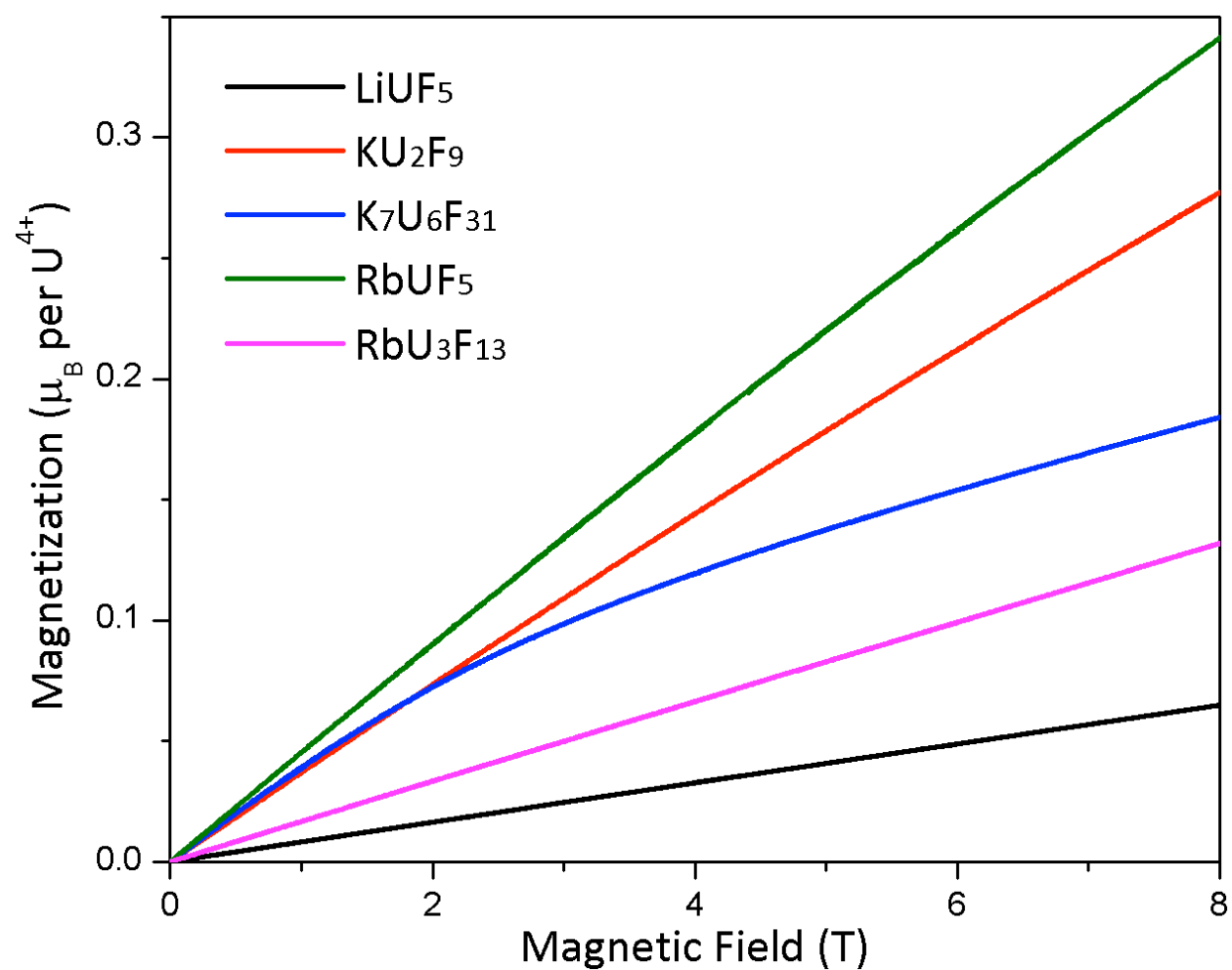


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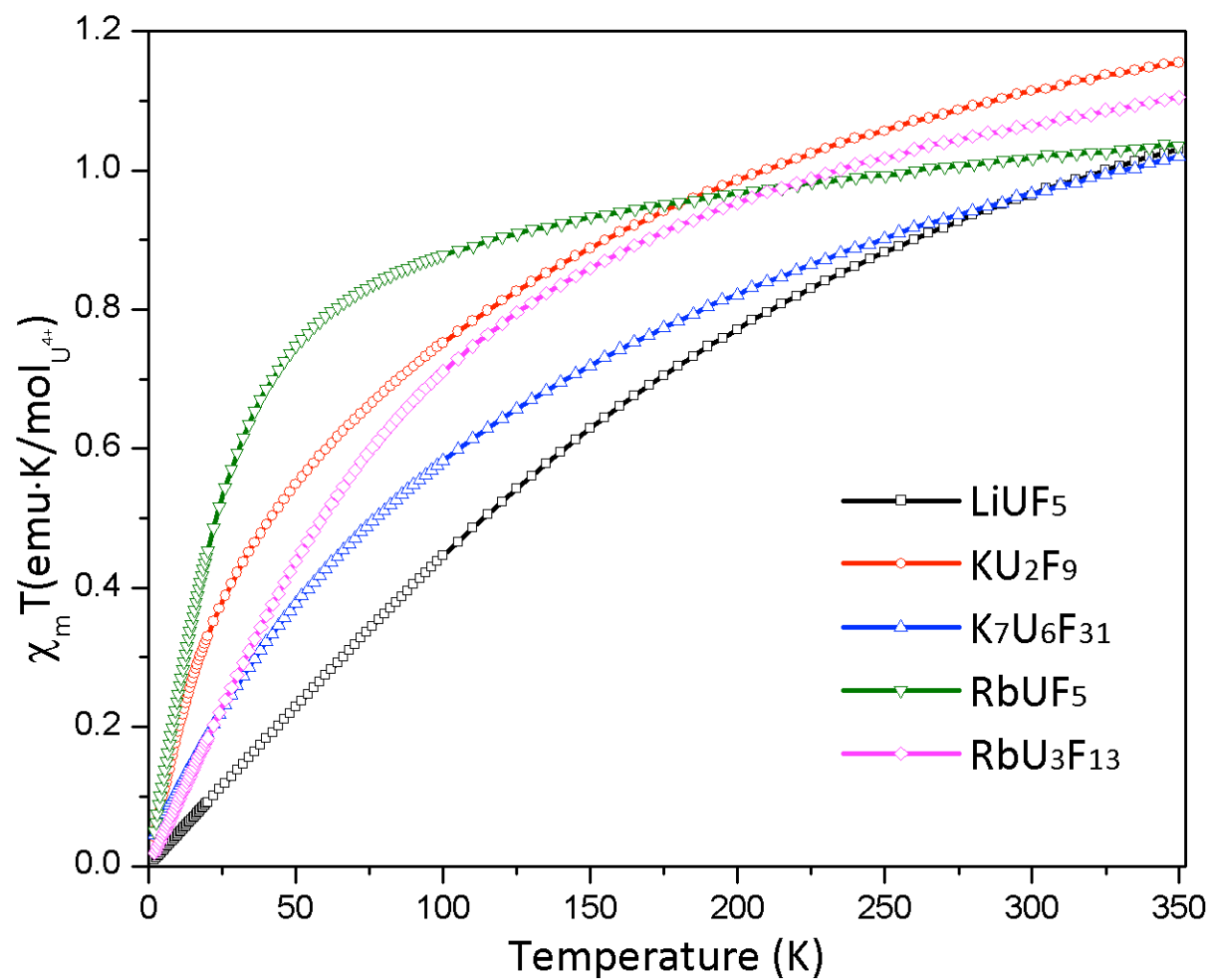


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	Structure			Product	Year
	Space group	Dimension	Connectivity between UF _x polyhedra		
LiUF ₅	<i>I4₁/a</i>	3-D	corner- and edge-shared UF ₉	single crystal	1966
Li ₄ UF ₈	<i>Pnma</i>	0-D	isolated UF ₈	single crystal	1967
β ₂ -Na ₂ UF ₆	<i>P321</i>	1-D	face-shared UF ₉	powder	1948
δ-Na ₂ UF ₆	<i>P3</i>	2-D	edge-shared UF ₉	single crystal	1979
γ-Na ₂ UF ₆	<i>Immm</i>	1-D	edge-shared UF ₈	powder	1948
Na ₃ UF ₇	<i>I4/mmm</i>	0-D	isolated UF ₈	single crystal	1948
KU ₂ F ₉	<i>Pnma</i>	3-D	corner- and edge-shared UF ₉	single crystal	1969
β ₁ -K ₂ UF ₆	<i>P62m</i>	1-D	face-shared UF ₉	single crystal	1969
β ₂ -K ₂ UF ₆	<i>P321</i>	1-D	face-shared UF ₉	powder	1948
Lt-K ₃ UF ₇	<i>I4₁/a</i>	0-D	isolated UF ₇	powder	1954
Ht-K ₃ UF ₇	<i>Fm3m</i>	0-D	unusual isolated UF _x	powder	1954
K ₇ U ₆ F ₃₁	N/A			powder	1996
RbUF ₅	N/A			powder	1996
Rb ₂ UF ₆	<i>Cmcm</i>	1-D	edge-shared UF ₈	single crystal	1971
CsU ₂ F ₉	<i>C2/c</i>	2-D	corner- and edge-shared UF ₉	single crystal	1973
CsU ₆ F ₂₅	<i>P6₃/mmc</i>	3-D	corner- and edge-shared UF ₉	single crystal	1971
TlUF ₅	<i>P2₁/c</i>	2-D	corner-, edge-, and face-shared UF ₉	single crystal	1980
U ₂ AuF ₁₁	<i>I4/mcm</i>	3-D	corner-shared UF ₉	single crystal	2004
(NH ₄) ₄ UF ₈	<i>C2/c</i>	0-D	isolated UF ₈	single crystal	1970
(NH ₄) ₇ U ₆ F ₃₁	<i>R3</i>	3-D	corner- and edge-shared UF ₈	single crystal	2001
(NH ₄)U ₃ F ₁₃	<i>Pm2₁b</i>	3-D	corner- and edge-shared UF ₉	single crystal	2001
β -(NH ₄)UF ₅	<i>P2₁/c</i>	2-D	corner- and edge-shared UF ₉	single crystal	1974

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for LiUF_5 , KU_2F_9 , $\text{K}_7\text{U}_6\text{F}_{31}$, RbUF_5 , RbU_2F_9 and $\text{RbU}_3\text{F}_{13}$. $U(eq)$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
LiUF_5				
U(1)	619(1)	562(1)	2480(1)	5(1)
F(1)	3018(2)	2128(2)	1259(6)	7(1)
F(2)	4272(2)	422(2)	41(6)	10(1)
F(3)	1075(2)	1832(2)	750(5)	6(1)
F(4)	2036(2)	929(2)	3614(6)	7(1)
F(5)	484(2)	1696(2)	4799(5)	7(1)
Li(1)	4164(8)	1853(8)	220(18)	14(2)
KU_2F_9				
U1	3257.7(2)	4496.7(1)	1532.0(2)	9.24(6)
K1	4659(2)	2500	6407(2)	15.3(2)
F1	4963(3)	5990(2)	761(4)	13.2(4)
F2	2910(3)	4040(2)	4712(4)	12.4(4)
F3	2835(3)	6070(2)	3553(3)	13.6(5)
F4	656(3)	4199(3)	1973(4)	13.8(4)
F5	3258(4)	2500	1622(5)	11.3(7)
$\text{K}_7\text{U}_6\text{F}_{31}$				
U1	4693.2(2)	6144.2(2)	4895.9(3)	16.8(1)
K1	4176(1)	4381(1)	1625(2)	23.6(4)
K2	3333	6667	1667	29.8(9)
F1	4261(3)	4473(3)	4257(4)	18.7(9)
F2	4611(4)	6126(3)	2797(5)	25(1)
F3	4597(5)	7577(4)	4447(6)	37(1)
F4	6249(3)	7219(4)	4274(5)	22.8(9)
F5	3796(4)	5068(4)	6622(5)	29(1)
F6 (occ. = 1/6)	3310(140)	6460(80)	6010(30)	77(18)

RbUF ₅				
U1	546.0(3)	2468.9(2)	5412.5(3)	12.7(6)
U2	4846.2(3)	2456.7(1)	4110.8(3)	13.45(7)
Rb1	2697.3(9)	5197.2(5)	7702.9(9)	25.8(2)
Rb2	2188.1(9)	5191.7(5)	2927.7(9)	27.2(2)
F1	3234(5)	3184(3)	6475(5)	20.8(8)
F2	180(6)	4007(3)	4946(6)	31(1)
F3	-2301(5)	2651(4)	4767(5)	30.8(1)
F4	-283(5)	1026(3)	5818(5)	25.8(9)
F5	-308(5)	1958(3)	2734(5)	25.7(9)
F6	2728(5)	1493(3)	4870(5)	19.8(8)
F7	2132(5)	3114(3)	3143(5)	20.5(8)
F8	5194(5)	4009(3)	4399(5)	26.6(9)
F9	5657(5)	975(3)	3888(5)	25.6(9)
F10	5797(5)	2094(3)	6820(5)	24.3(9)
RbU ₂ F ₉				
U1	3250.6(2)	4484.5(2)	1496.5(2)	5.50(8)
Rb1	4671.3(9)	2500	6345(1)	8.9(1)
F1	4935(4)	5967(3)	719(5)	9.6(6)
F2	2871(4)	4067(3)	4650(5)	8.5(5)
F3	2783(4)	6046(3)	3506(4)	9.0(6)
F4	646(4)	4219(3)	1941(5)	10.2(6)
F5	3237(5)	2500	1596(6)	7.5(8)

		RbU ₃ F ₁₃		
U1	2528.1(4)	1044.1(3)	1273.0(7)	5.55(9)
U2	0	3908.1(5)	4637.0(7)	5.3(1)
Rb1	5000	6057.9(2)	2653.9(2)	12.4(3)
F1	1723(8)	1948(7)	5966(6)	9(1)
F2	1958(9)	3898(7)	52(8)	10(1)
F3	2581(6)	3224(8)	3176(8)	10(1)
F4	3018(7)	-486(8)	3665(6)	8(1)
F5	5000	-608(13)	1146(10)	11(1)
F6	5000	2725(11)	896(10)	9(1)
F7	0	979(11)	0(11)	10(2)
F8	0	1380(11)	2833(9)	6(1)
F9	0	5307(11)	2275(11)	10(2)
