

Supplementary Information for

**Quaternary Cerium(IV) Containing Fluorides Exhibiting  
Ce<sub>3</sub>F<sub>16</sub> Sheets and Ce<sub>6</sub>F<sub>30</sub> Frameworks**

Gyanendra B. Ayer, Vladislav V. Klepov, Kristen A. Pace, and Hans-Conrad zur Loye\*

Department of Chemistry and Biochemistry, University of South Carolina, 631 Sumter  
Street, Columbia, SC, United States

\*e-mail: [zurloye@mailbox.sc.edu](mailto:zurloye@mailbox.sc.edu)

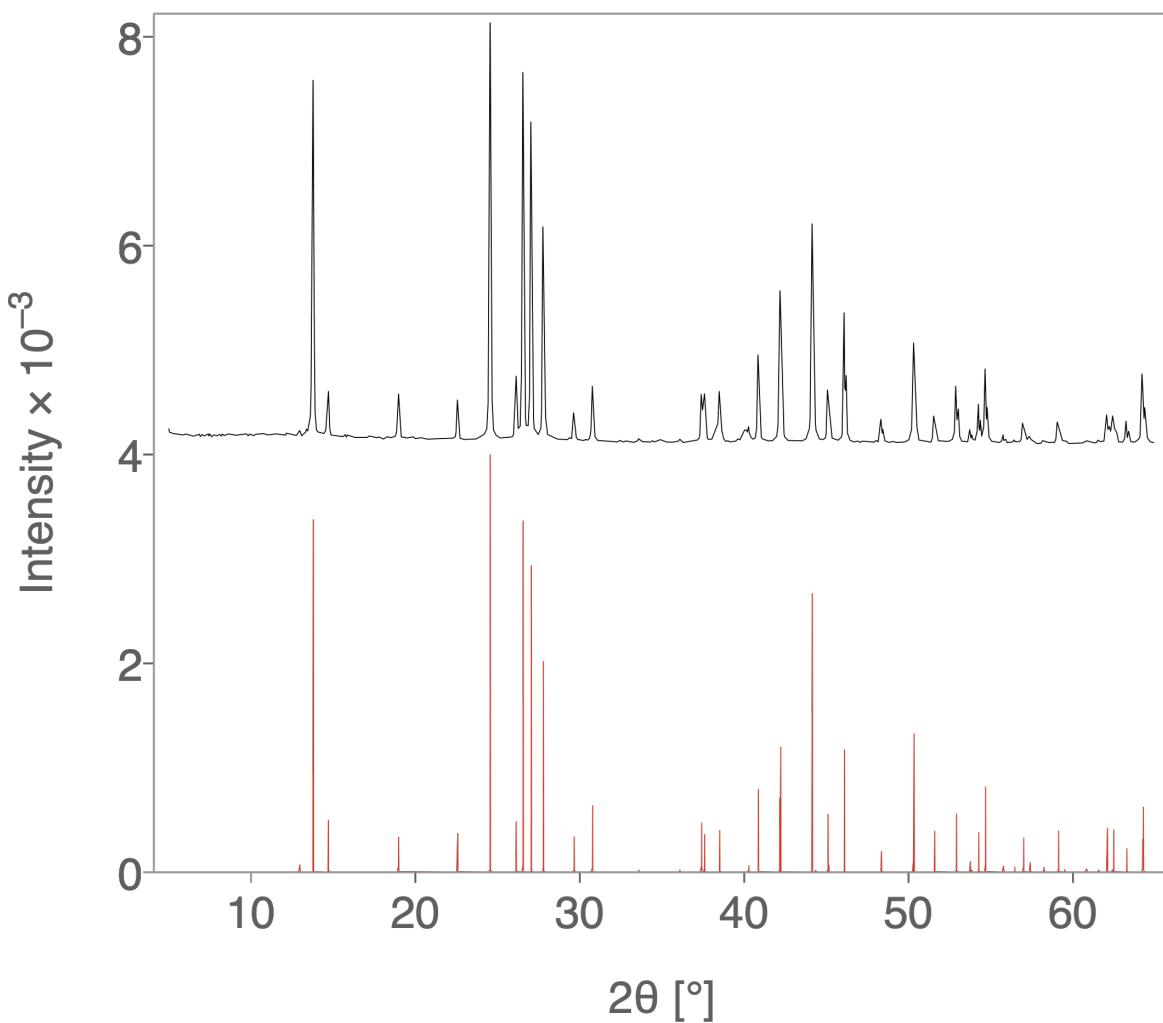


Figure S1. Experimental and calculated powder patterns of  $\text{Cs}_2\text{NiCe}_3\text{F}_{16}$  indicated by the black and red lines respectively. The preferred orientation effects (plate-like crystal morphology along (001) planes) were taken into account for the calculated pattern to bring the intensities on the same scale. The refined unit cell parameters from PXRD are  $a = 7.875(1)$ ,  $c = 12.844(1)$  Å and agree well with the parameters from single crystal X-ray diffraction,  $a = 7.8687(2)$ ,  $c = 12.8302(3)$  Å.

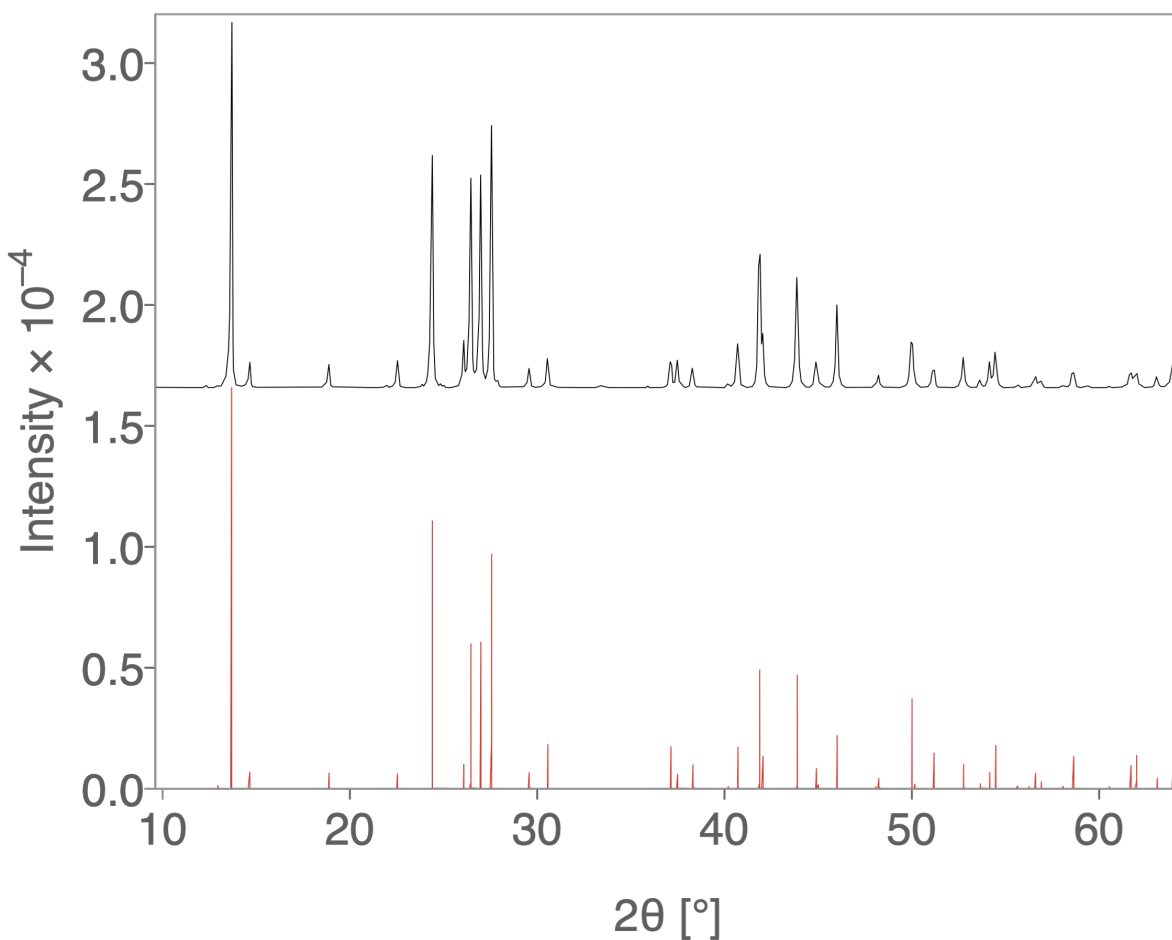
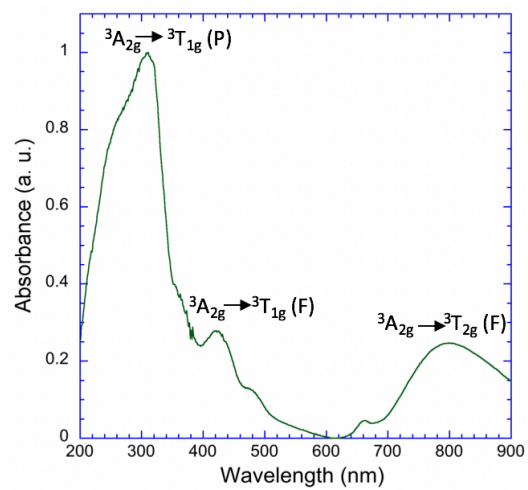
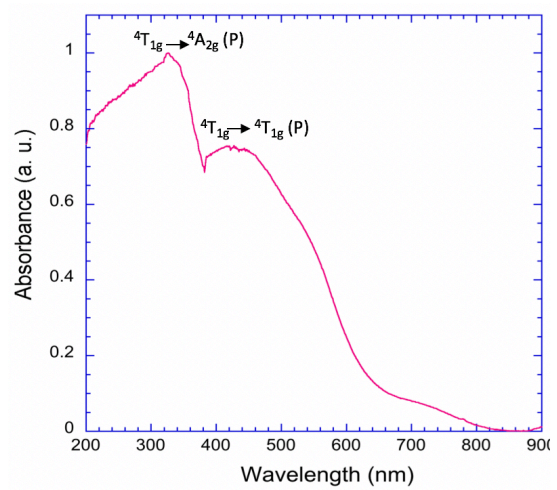


Figure S2. Experimental and calculated powder patterns of  $\text{Cs}_2\text{CoCe}_3\text{F}_{16}$  indicated by the black and red lines respectively. The preferred orientation effects (plate-like crystal morphology along (001) planes) were taken into account for the calculated pattern to bring the intensities on the same scale. The refined unit cell parameters from PXRD are  $a = 7.887(3)$ ,  $c = 12.924(2)$  Å and agree well with the parameters from single crystal X-ray diffraction,  $a = 7.8823(2)$ ,  $c = 12.9303(3)$  Å.

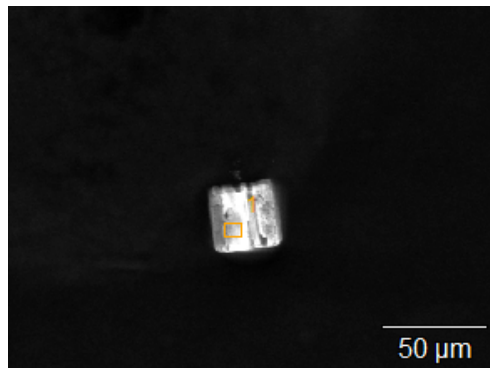


(a)

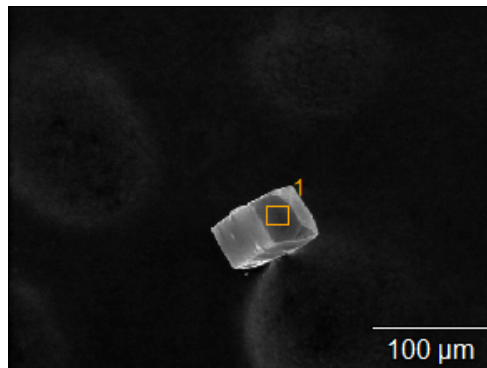


(b)

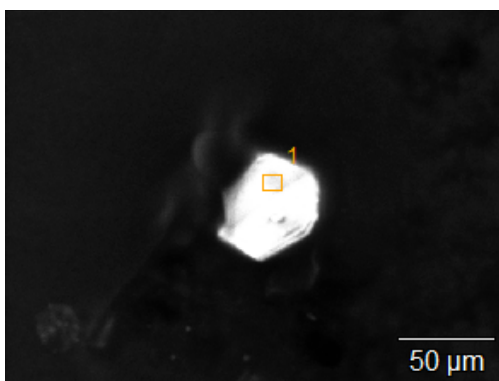
Figure S3. UV-Vis diffuse absorbance spectra of (a)  $\text{Cs}_2\text{NiCe}_3\text{F}_{16}$  and (b)  $\text{Cs}_2\text{CoCe}_3\text{F}_{16}$ .



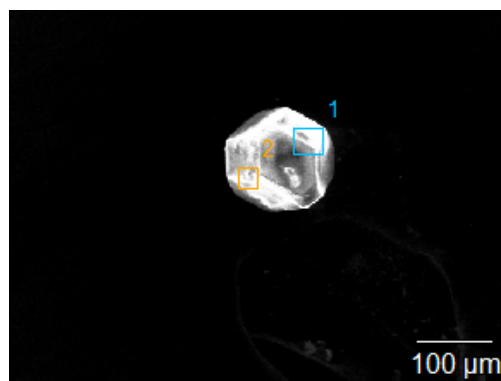
(a)



(b)



(c)

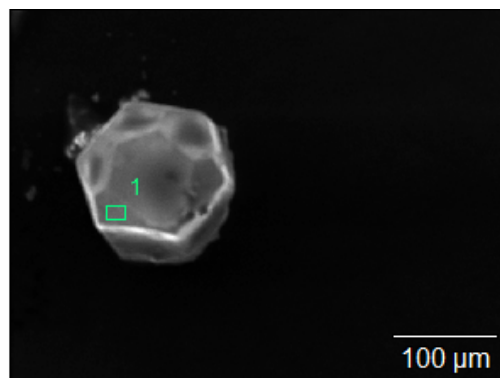


(d)

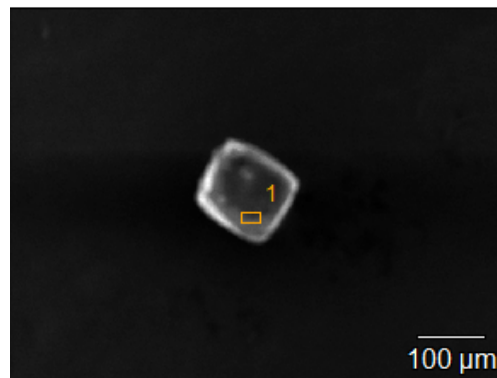
Figure S4. SEM images of crystals of  $\text{Cs}_2\text{NiCe}_3\text{F}_{16}$  (a),  $\text{Cs}_2\text{CoCe}_3\text{F}_{16}$  (b),  $\text{Cs}_2\text{MnCe}_3\text{F}_{16}$  (c), and  $\text{Cs}_2\text{ZnCe}_3\text{F}_{16}$  (d).

Table S1. Elemental composition determined by EDS for  $\text{Cs}_2\text{MCe}_3\text{F}_{16}$  (M= Ni, Co, Mn, and Zn)

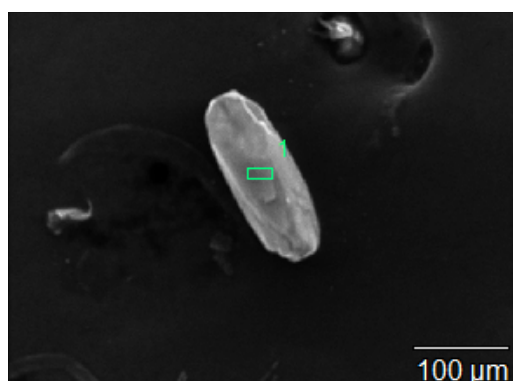
$\text{Cs}_2\text{NiCe}_3\text{F}_{16}$		$\text{Cs}_2\text{CoCe}_3\text{F}_{16}$		$\text{Cs}_2\text{MnCe}_3\text{F}_{16}$		$\text{Cs}_2\text{ZnCe}_3\text{F}_{16}$	
Element	Atom %	Element	Atom %	Element	Atom %	Element	Atom %
Cs	13.64	Cs	10.66	Cs	13.10	Cs	8.88
Ce	21.70	Ce	16.45	Ce	19.04	Ce	13.57
Ni	4.51	Co	3.86	Mn	5.11	Zn	4.10
F	60.15	F	69.03	F	62.76	F	73.45



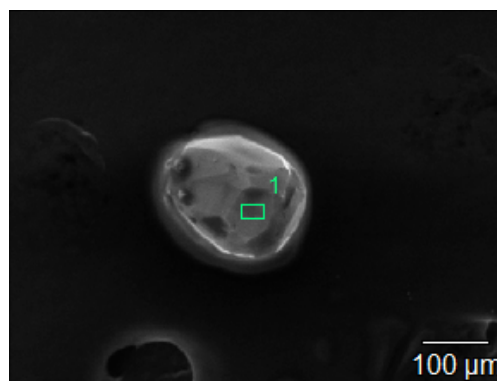
(a)



(b)



(c)



(d)

Figure S4. SEM images of crystals of  $\text{Na}_3\text{AlCe}_6\text{F}_{30}$  (a),  $\text{Na}_3\text{GaCe}_6\text{F}_{30}$  (b),  $\text{Na}_3\text{CrCe}_6\text{F}_{30}$  (c), and  $\text{Na}_3\text{FeCe}_6\text{F}_{30}$  (d)

Table S2. Elemental composition determined by EDS for  $\text{Na}_3\text{M}\text{Ce}_6\text{F}_{30}$  (M = Al, Ga, Fe, and Cr)

$\text{Na}_3\text{AlCe}_6\text{F}_{30}$		$\text{Na}_3\text{GaCe}_6\text{F}_{30}$		$\text{Na}_3\text{FeCe}_6\text{F}_{30}$		$\text{Na}_3\text{CrCe}_6\text{F}_{30}$	
Element	Atom %	Element	Atom %	Element	Atom %	Element	Atom %
Na	9.84	Na	9.88	Na	11.89	Na	12.26
Ce	11.02	Ce	14.43	Ce	17.40	Ce	17.19
Al	2.95	Ga	2.04	Fe	2.58	Cr	2.37
F	76.19	F	73.65	F	68.13	F	68.18