

Electronic Supplementary Information (ESI) for:

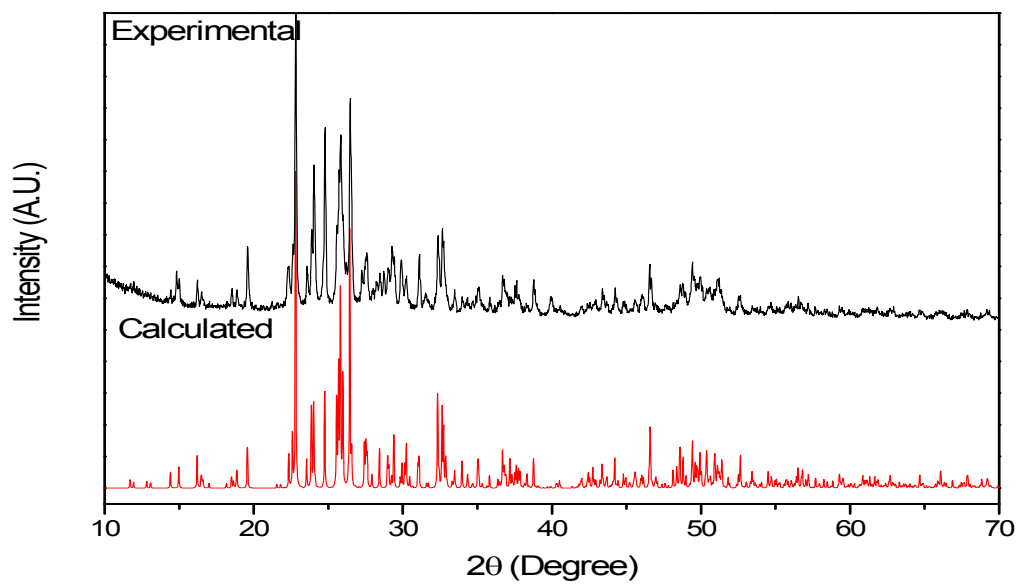
Dimensionality variations in new zirconium iodates:
Hydrothermal syntheses, structure determinations, and
characterizations of $\text{BaZr}(\text{IO}_3)_6$ and $\text{K}_2\text{Zr}(\text{IO}_3)_6$

Hyun Sun Ahn, Dong Woo Lee, and Kang Min Ok*

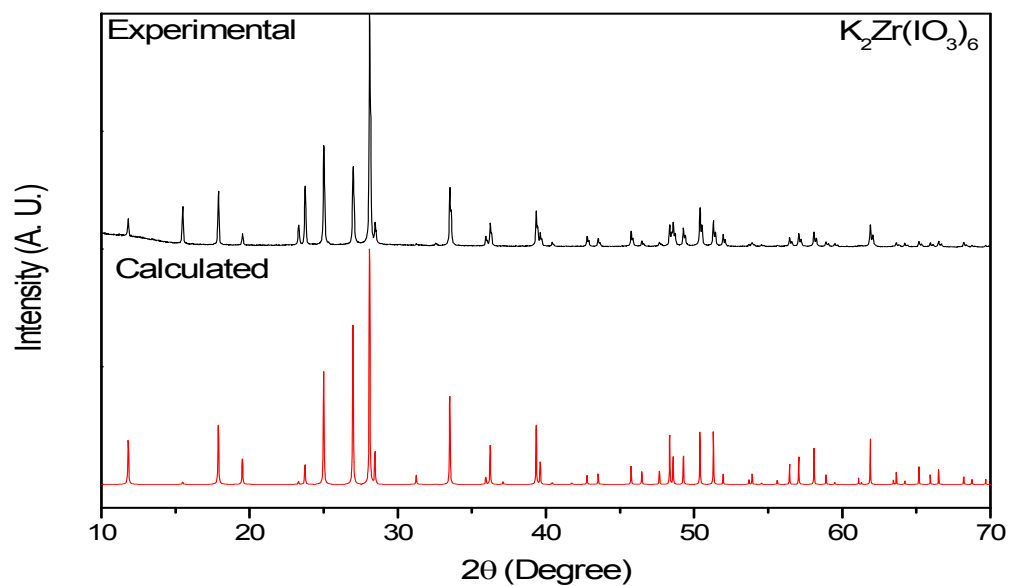
Department of Chemistry, Chung-Ang University, 84 Heukseok-ro, Dongjak-gu, Seoul 156-756,
Republic of Korea

- S1. Experimental and calculated powder X-ray diffraction patterns for $\text{BaZr}(\text{IO}_3)_6$
- S2. Experimental and calculated powder X-ray diffraction patterns for $\text{K}_2\text{Zr}(\text{IO}_3)_6$
- S3. Atomic positions and isotropic displacement parameters for $\text{K}_2\text{Zr}(\text{IO}_3)_6$
- S4. Powder XRD pattern for calcined product of $\text{BaZr}(\text{IO}_3)_6$
- S5. Powder XRD pattern for calcined product of $\text{K}_2\text{Zr}(\text{IO}_3)_6$

S1. Experimental and calculated powder X-ray diffraction patterns for $\text{BaZr}(\text{IO}_3)_6$



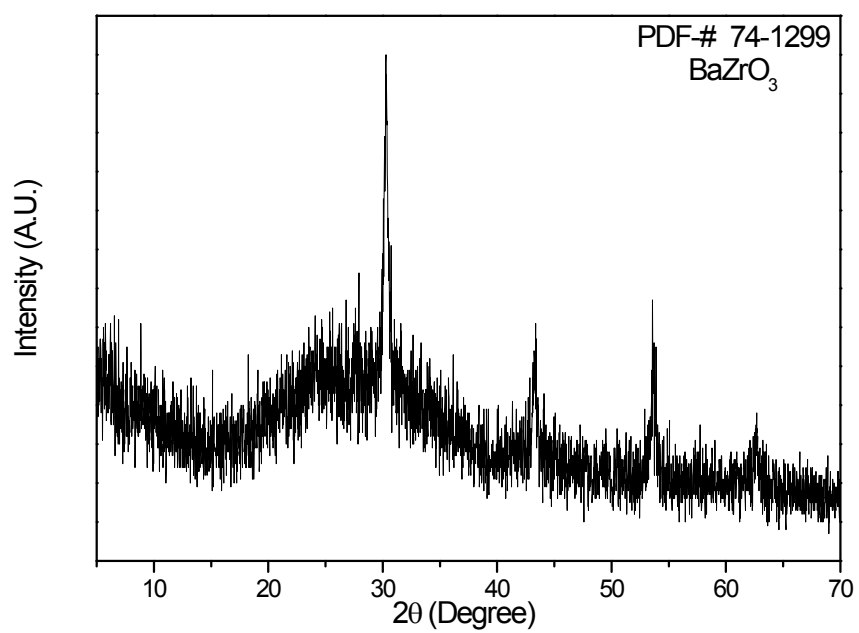
S2. Experimental and calculated powder X-ray diffraction patterns for $\text{K}_2\text{Zr}(\text{IO}_3)_6$



S3. Atomic positions and isotropic displacement parameters for $\text{K}_2\text{Zr}(\text{IO}_3)_6$

Atom	x	y	z	$U_{\text{iso}}(\text{\AA}^2)$
K(1)	0	0	0.8312(7)	0.033(3)
I(1)	0.39452(14)	0.38246(14)	0.71894(16)	0.028(3)
Zr(1)	0.66667	0.33333	0.83333	0.035(2)
O(1)	0.5532(10)	0.3819(11)	0.7208(8)	0.029(5)
O(2)	0.4484(10)	0.5206(11)	0.6227(8)	0.027(5)
O(3)	0.4272(11)	0.4691(10)	0.8566(9)	0.042(5)

S4. Powder XRD pattern for calcined product of $\text{BaZr}(\text{IO}_3)_6$



S5. Powder XRD pattern for calcined product of $\text{K}_2\text{Zr}(\text{IO}_3)_6$

