Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Shedding Light on Intrinsic Characteristics and Optical Properties of Novel Selenite and Tellurite Crystals $ZrSe_2O_6$, $HfSe_2O_6$ and $HfTe_3O_8$

Junai Lv, [a] Qi Li, [a] Xin Guan, [a] Na Lin, *[a] Jian Zhang, *[a] Zhitai Jia, [a,b] Xutang Tao. [a]

[a]State Key laboratory of Crystal Material, Shandong University, Jinan, 250100, PR China.
[b]Shandong Research Institute of Industrial Technology, Jinan, Shandong, 250100, PR China.
E-mail: linnakth@gmail.com, Jian.zhang@sdu.edu.cn.

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Table S1 $ZrSe_2O_6$ of Geometric parameters (Å^2)

$O5^{i}$—Zr01—O5	180.0 (3)	O5—Zr01—$O3^{v}$	93.6 (2)
$O5^{i}$—Zr01—$O4^{ii}$	89.1 (2)	$O4^{ii}$—Zr01—$O3^{v}$	89.4 (2)
O5—Zr01—$O4^{ii}$	90.9 (2)	$O4^{iii}$—Zr01—$O3^{v}$	90.6 (2)
$O5^{i}$—Zr01—$O4^{iii}$	90.9 (2)	$O3^{iv}$—Zr01—$O3^{v}$	180.0
O5—Zr01—$O4^{iii}$	89.1 (2)	O3—Se2—O4	102.6 (3)
$O4^{ii}$—Zr01—$O4^{iii}$	180.0 (3)	O3—Se2—O5	100.3 (3)
$O5^{i}$—Zr01—$O3^{iv}$	93.6 (2)	O4—Se2—O5	98.6 (3)
O5—Zr01—$O3^{iv}$	86.4 (2)	Se2—O3—$Zr01^{vi}$	142.5 (3)
$O4^{ii}$—Zr01—$O3^{iv}$	90.6 (2)	Se2—O4—$Zr01^{vii}$	134.0 (3)
$O4^{iii}$—Zr01—$O3^{iv}$	89.4 (2)	Se2—O5—Zr01	151.0 (4)

O5^{i}—Zr01—O3^{v}	86.4 (2)		

Symmetry codes: (i) -*x*, -*y*+1, -*z*+1; (ii) *x*-1, -*y*+1/2, *z*-1/2; (iii) -*x*+1, *y*+1/2, -*z*+3/2; (iv) -*x*, *y*+1/2, -*z*+3/2; (v) *x*, -*y*+1/2, *z*-1/2; (vi) -*x*, *y*-1/2, -*z*+3/2; (vii) -*x*+1, *y*-1/2, -*z*+3/2.

Table S2 $ZrSe_2O_6$ of Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zr01	0.0078 (4)	0.0077 (4)	0.0102 (4)	0.0005 (3)	0.0005 (3)	-0.0001 (3)
Se2	0.0137 (4)	0.0138 (4)	0.0119 (4)	0.0027 (3)	0.0052 (3)	0.0018 (3)
O3	0.024 (3)	0.022 (3)	0.018 (3)	-0.007 (2)	0.009 (2)	0.002 (2)
O4	0.015 (2)	0.019 (3)	0.024 (3)	0.004 (2)	0.001 (2)	0.004 (2)
O5	0.023 (3)	0.017 (3)	0.023 (3)	0.010 (2)	0.001 (2)	0.009 (2)

Table S3 $HfSe_2O_6$ of Geometric parameters (Å^2)

O005^{i}—Hf01—O005	180.0	O005—Hf01—O004^{v}	90.41 (19)
O005^{i}—Hf01—O003^{ii}	93.8 (2)	O003^{ii}—Hf01—O004^{v}	90.8 (2)
O005—Hf01—O003^{ii}	86.2 (2)	O003^{iii}—Hf01—O004^{v}	89.2 (2)
O005^{i}—Hf01—O003^{iii}	86.2 (2)	O004^{iv}—Hf01—O004^{v}	180.0
O005—Hf01—O003^{iii}	93.8 (2)	O005—Se02—O003	100.2 (3)
O003^{ii}—Hf01—O003^{iii}	180.0	O005—Se02—O004	97.9 (2)
O005^{i}—Hf01—O004^{iv}	90.41 (19)	O003—Se02—O004	102.8 (3)
O005—Hf01—O004^{iv}	89.59 (19)	Se02—O003—Hf01^{vi}	142.1 (3)
O003^{ii}—Hf01—O004^{iv}	89.2 (2)	Se02—O004—Hf01^{vii}	132.3 (3)
O003^{iii}—Hf01—O004^{iv}	90.8 (2)	Se02—O005—Hf01	150.3 (3)
O005^{i}—Hf01—O004^{v}	89.59 (19)		

Symmetry codes: (i) -x+2, -y+1, -z+1; (ii) -x+2, y+1/2, -z+1/2; (iii) x, -y+1/2, z+1/2; (iv) -x+1, y+1/2, -z+1/2; (v) x+1, -y+1/2, z+1/2; (vi) -x+2, y-1/2, -z+1/2; (vii) -x+1, y-1/2, -z+1/2.

Table S4 $HfSe_2O_6$ of Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hf01	0.0082 (3)	0.0016 (2)	0.0064 (2)	-0.00045 (9)	0.00021 (15)	-0.00002 (9)
Se02	0.0128 (3)	0.0053 (3)	0.0065 (3)	-0.0025 (2)	0.0042 (2)	-0.0015 (2)
O003	0.021 (3)	0.016 (2)	0.012 (2)	0.005 (2)	0.008 (2)	-0.0016 (19)
O004	0.013 (2)	0.011 (2)	0.018 (2)	-0.0051 (17)	-0.0020 (18)	-0.0006 (18)
O005	0.019 (2)	0.008 (2)	0.018 (2)	-0.0062 (18)	0.001 (2)	-0.0062 (18)

Table S5 $HfTe_3O_8$ of Geometric parameters.

O003^{i}—Hf01—O003^{ii}	180.00 (19)	O003^{iv}—Hf01—O003	91.50 (15)
O003^{i}—Hf01—O003^{iii}	91.50 (15)	O003^{v}—Hf01—O003	88.50 (15)
O003^{ii}—Hf01—O003^{iii}	88.50 (15)	O003—Te02—O003^{vi}	102.2 (3)
O003^{i}—Hf01—O003^{iv}	88.50 (15)	O003—Te02—O004^{vi}	86.4 (2)
O003^{ii}—Hf01—O003^{iv}	91.50 (15)	O003^{vi}—Te02—O004^{vi}	80.13 (13)
O003^{iii}—Hf01—O003^{iv}	88.50 (15)	O003—Te02—O004	80.13 (13)
O003^{i}—Hf01—O003^{v}	91.50 (15)	O003^{vi}—Te02—O004	86.4 (2)
O003^{ii}—Hf01—O003^{v}	88.50 (15)	O004^{vi}—Te02—O004	158.5 (2)
O003^{iii}—Hf01—O003^{v}	91.50 (15)	Te02—O003—Hf01	137.4 (2)
O003^{iv}—Hf01—O003^{v}	180.00 (19)	Te02^{vii}—O004—Te02^{viii}	117.29 (9)
O003^{i}—Hf01—O003	88.50 (15)	Te02^{vii}—O004—Te02	117.29 (9)
O003^{ii}—Hf01—O003	91.50 (15)	Te02^{viii}—O004—Te02	117.29 (9)
O003^{iii}—Hf01—O003	180.0		

Symmetry codes: (i) -y+1, -z+1, -x+1; (ii) y, z, x; (iii) -x+1, -y+1, -z+1; (iv) z, x, y; (v) -z+1, -x+1, -y+1; (vi) x, -y+1, -z+3/2; (vii) -y+1, z-1/2, -x+3/2; (viii) z, -x+1, -y+3/2.

Table S6 $HfTe_3O_8$ of Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Hf01	0.00683 (19)	0.00683 (19)	0.00683 (19)	-0.00059 (10)	-0.00059 (10)	-0.00059 (10)
Te02	0.0043 (3)	0.0314 (4)	0.0080 (3)	0	0	-0.00933 (19)
O003	0.018 (2)	0.0118 (19)	0.0138 (19)	-0.0028 (15)	-0.0103 (16)	0.0003 (15)
O004	0.0075 (12)	0.0075 (12)	0.0075 (12)	-0.0027 (14)	-0.0027 (14)	0.0027 (14)

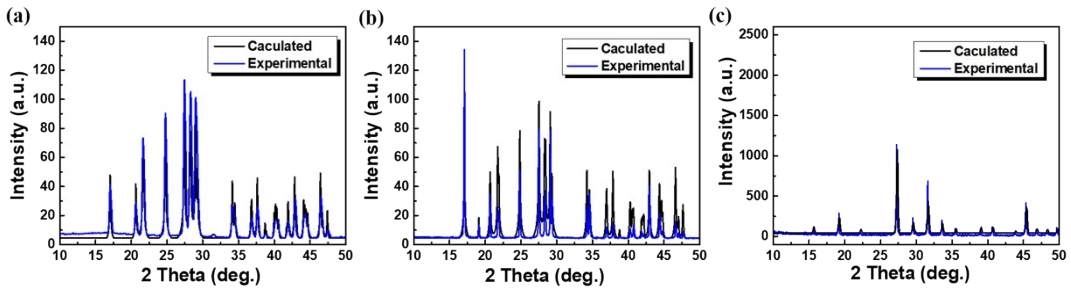

Figure S1. Experimental (blue) and calculated (black) PXRD patterns confirming the phase purity of (a) $ZrSe_2O_6$, (b) $HfSe_2O_6$, and (c) $HfTe_3O_8$.

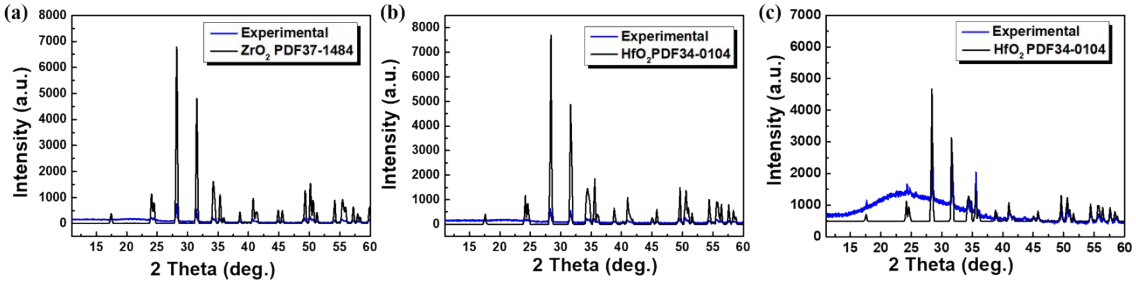

Figure S2. PXRD pattern of the final residual of (a) $ZrSe_2O_6$, (b) $HfSe_2O_6$, and (c) $HfTe_3O_8$ obtained by DSC measurement.