

Supplementary Materials

Magnetic, Optical, and Thermic Properties of SrLnCuSe₃ (Ln = Dy, Ho, Er, Tm) Compounds

Navruzbek N. Habibullayev ^{1,*}, Nikolay G. Naumov ², Alexander N. Lavrov ², Natalia V. Kuratieva ², Aleksandr S. Aleksandrovsky ^{3,4}, Aleksandr S. Oreshonkov ^{3,4}, Maxim S. Molokeev ^{5,6,7}, Irina V. Palamarchuk ¹, Ilya. O. Yurev ^{1,8}, Yuriy. G. Denisenko ^{1,9}, Oleg V. Andreev ^{1,10} and Alena D. Zakharova ¹

- ¹ Institute of Chemistry, University of Tyumen, 625003 Tyumen, Russia; i.v.palamarchuk@utmn.ru (I.V.P.); i.o.yurev@utmn.ru (I.O.Y.); yu.g.denisenko@gmail.com (Y.G.D.); o.v.andreev@utmn.ru (O.V.A.); a.d.zakharova@utmn.ru (A.D.Z.)
- ² Nikolaev Institute of Inorganic Chemistry SB RAS, 630090 Novosibirsk, Russia; naumov@niic.nsc.ru (N.G.N.); lavrov@niic.nsc.ru (A.N.L.); kuratieva@gmail.com (N.V.K.)
- ³ Kirensky Institute of Physics, Federal Research Center, KSC, SB RAS, 660036 Krasnoyarsk, Russia; aleksandrovsky@kirensky.ru (A.S.A.); oreshonkov@iph.krasn.ru (A.S.O.)
- ⁴ Department of Photonics and Laser Technology, Siberian Federal University, 660036 Krasnoyarsk, Russia
- ⁵ Laboratory of Crystal Physics, Kirensky Institute of Physics, Federal Research Center, KSC, SB RAS, 660036 Krasnoyarsk, Russia; msmolokeev@mail.ru
- ⁶ Laboratory of Theory and Optimization of Chemical and Technological Processes, University of Tyumen, 625003 Tyumen, Russia
- ⁷ Department of Physics, Far Eastern State Transport University, 680021 Khabarovsk, Russia
- ⁸ Department of Physical and Applied Chemistry, Kurgan State University, 640020 Kurgan, Russia
- ⁹ Department of General and Special Chemistry, Industrial University of Tyumen, 625000 Tyumen, Russia
- ¹⁰ Institute of Solid State Chemistry, UB RAS, 620990 Ekaterinburg, Russia
- * Correspondence: habibullayev_navruzbek@mail.ru

Table S1. Main parameters of processing and refinement of the SrTmCuSe₃ samples

Compound	SrTmCuSe ₃
Sp. Gr.	<i>Cmcm</i>
<i>a</i> (Å)	4.06935(6)
<i>b</i> (Å)	13.4758(2)
<i>c</i> (Å)	10.46441(15)
<i>V</i> (Å ³)	573.844(15)
<i>Z</i>	2
2θ-interval, °	10-108
<i>R</i> _{wp} , %	4.6
<i>R</i> _p , %	3.35
χ ²	1.99
<i>R</i> _B , %	2.56

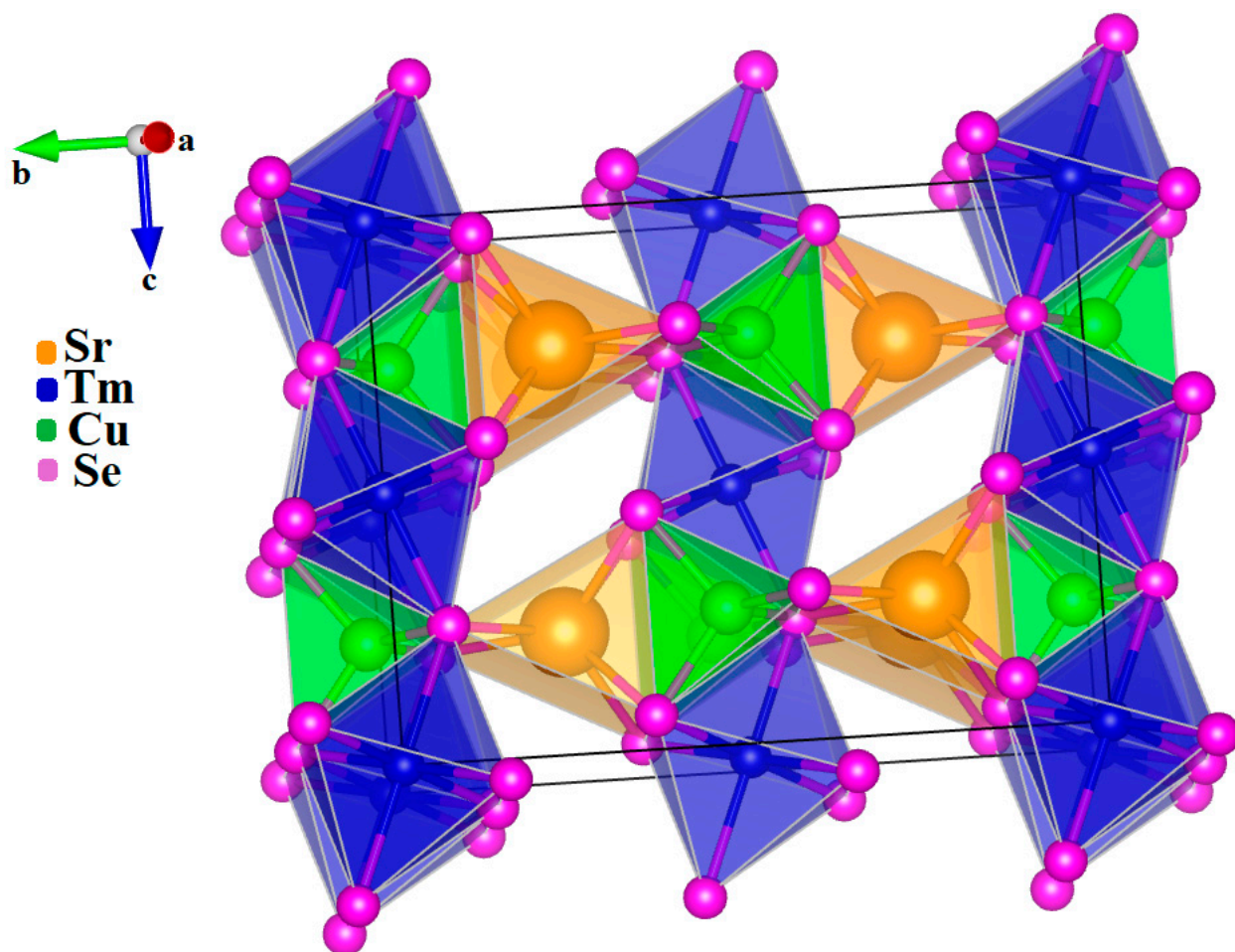
Table S2. Fractional atomic coordinates and isotropic displacement parameters (\AA^2) of SrTmCuSe_3

Ato m	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{iso}	<i>Occ.</i>
Tm	0	0	0	1.99(14)	1
Sr	0	0.74970(18)	0.25	1.99(15)	1
Cu	0	0.4692(3)	0.25	2.47(19)	1
Se1	0	0.0763(2)	0.25	2.22(17)	1
Se2	0	0.36198(18)	0.06490(18)	2.11(15)	1

Table S3. Main bond lengths (\AA) of SrTmCuSe_3 .

Tm—Se1	2.81090(98)	Tm—Se2 ⁱ	2.8391(16)
Sr—Se1 ⁱⁱ	3.0984(27)	Sr—Se2 ⁱⁱ	3.1907(19)
Cu—Se1 ⁱⁱ	2.4945(28)	Cu—Se2	2.4165(31)

Symmetry codes: (i) $x+1/2, y+1/2, z$; (ii) $x+1/2, y+1/2, z$

**Figure S1.** Polyhedral structure of SrTmCuSe_3 .

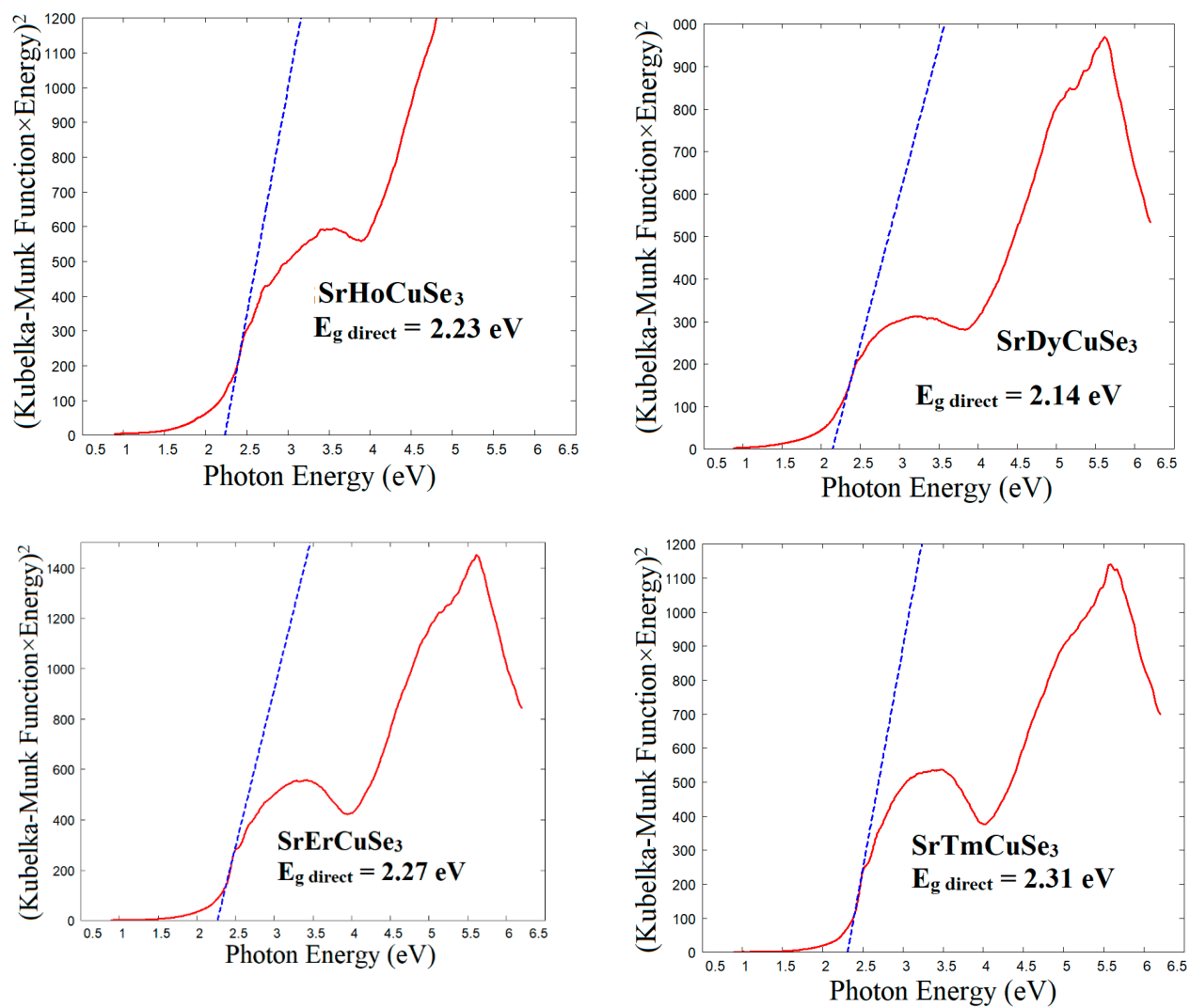


Figure S2. Kubelka-Munk Functions for determination of direct bandgaps in SrLnCuSe₃ crystals.

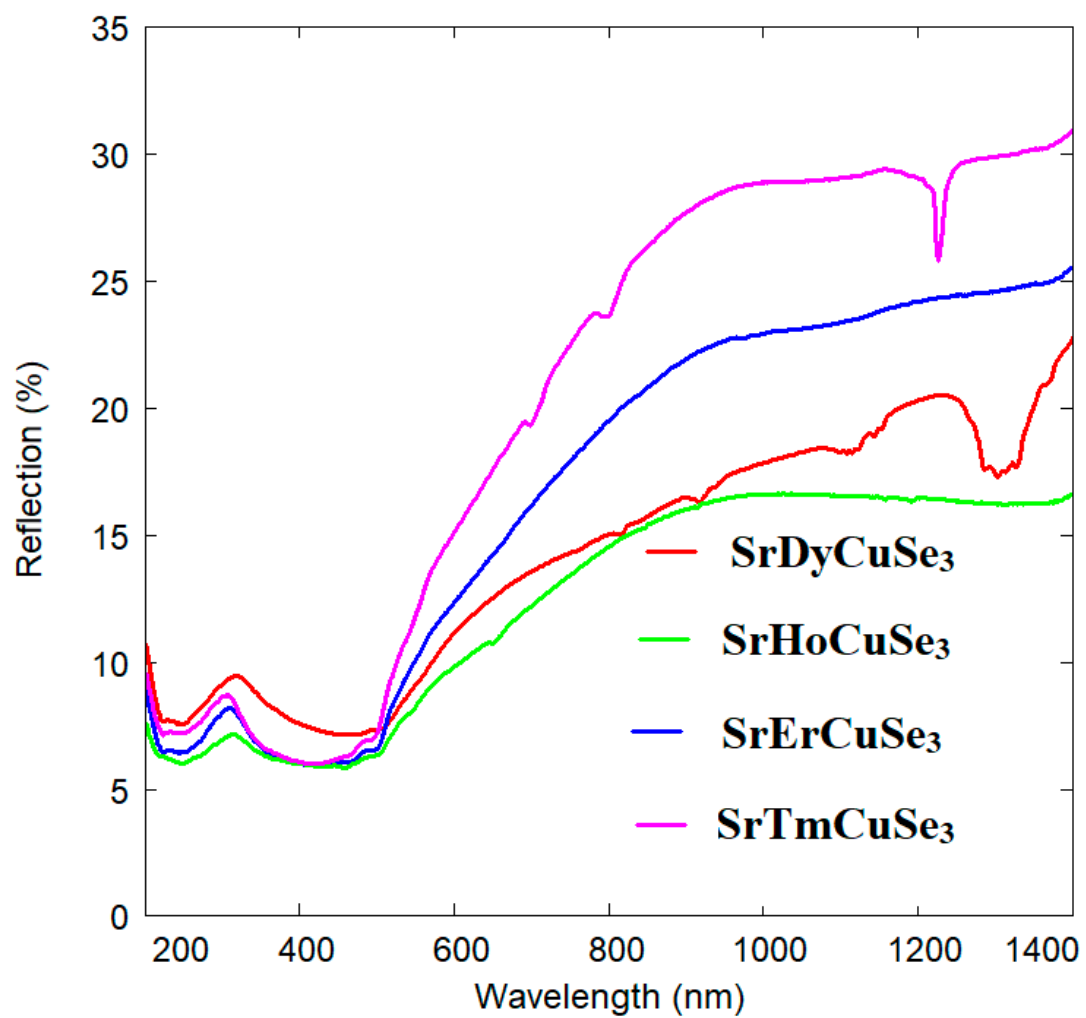


Figure S3. UV-vis-NIR diffuse reflectance spectra of quaternary rare earth selenides.

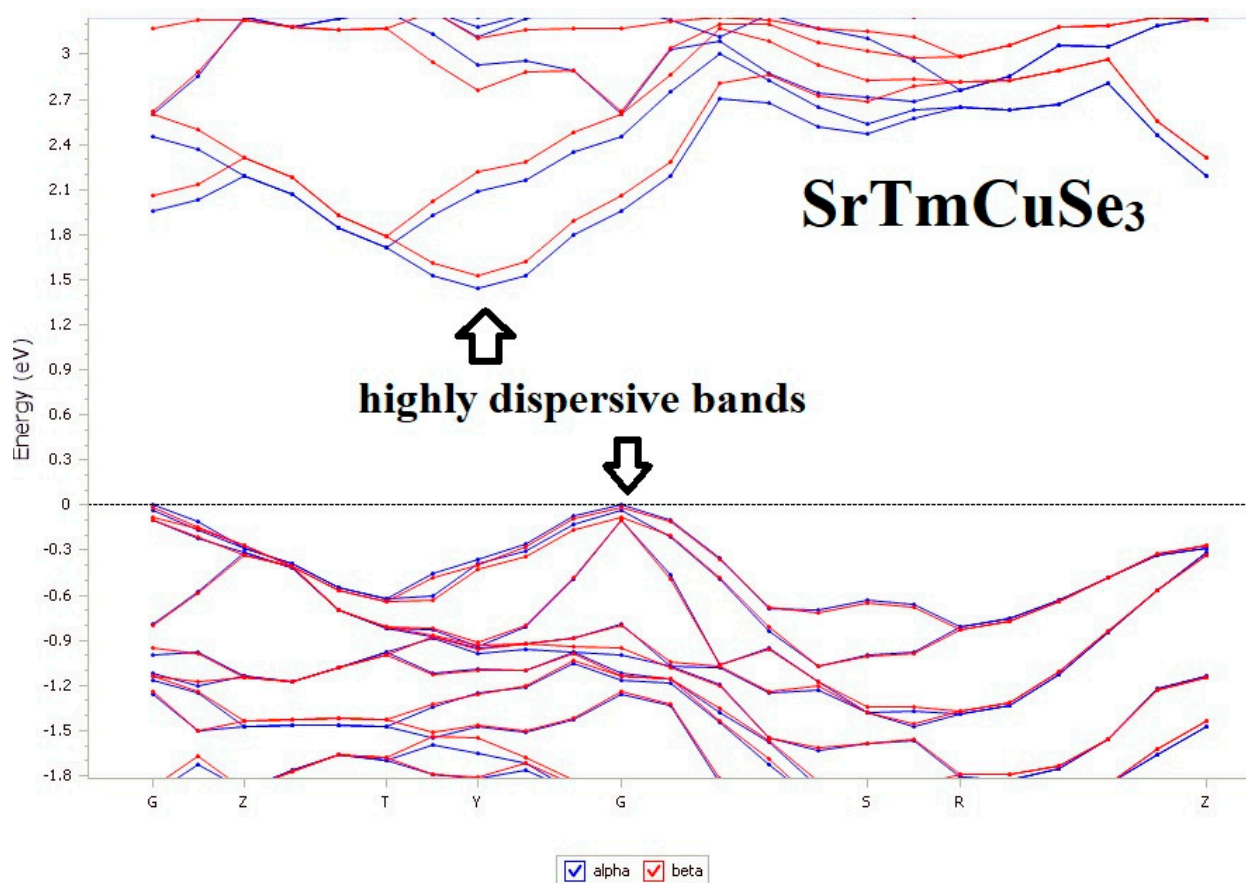


Figure S4. *Ab initio* DFT calculated band structure of SrTmCuSe₃ crystal. Indirect bandgap 1.35 eV.

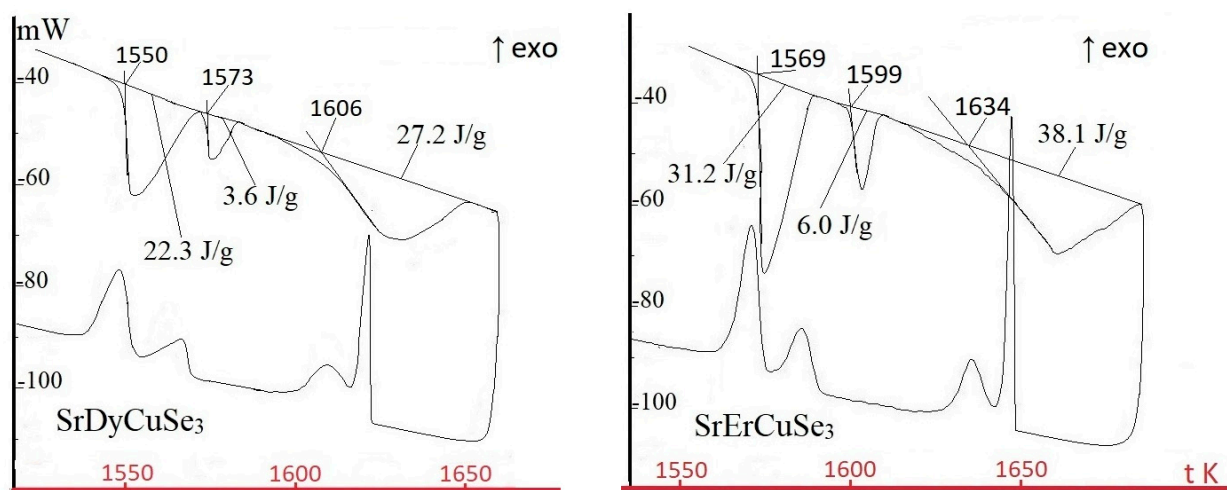


Figure S5. DSC/t dependences of "SETARAM" SETSYS Evolution for samples SrDyCuSe₃, SrErCuSe₃ (the samples were in sealed quartz ampoules).

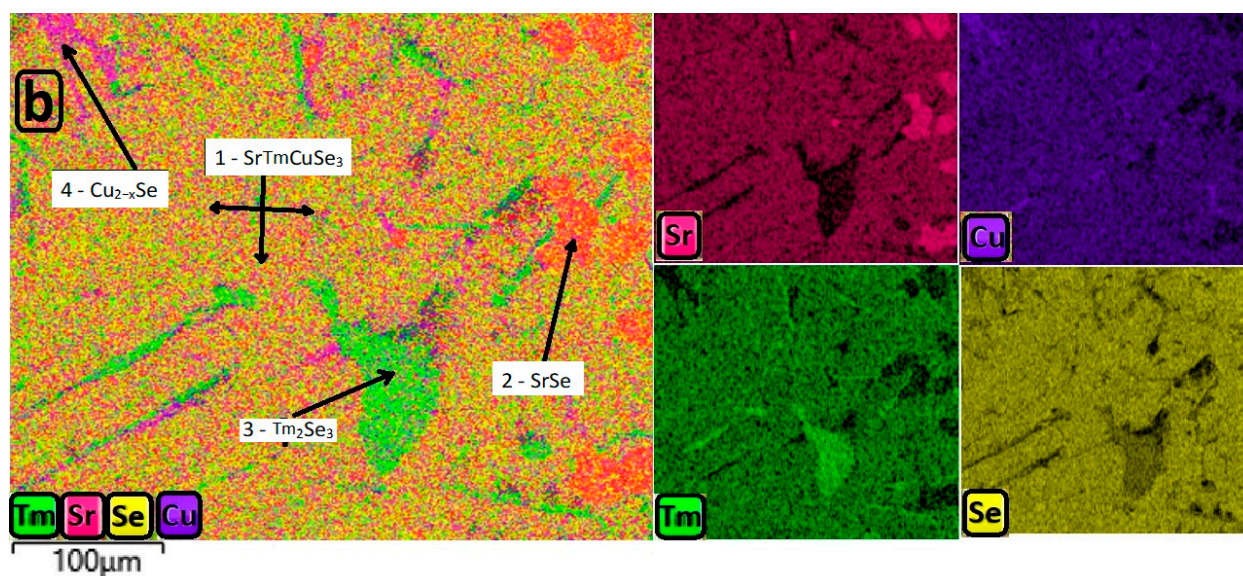


Figure S6. SEM/EDS maps of elemental distribution on the surface SrTmCuSe_3 sample that were cooled after the DSC measurements (1800 K)