Supporting Information

Synthesis of a Series of Rare-Earth-based Multi Anion Chalcogenide Iodides: $RE_3Si_2Se_xS_{8-x}I$ (RE = La, Ce, Pr, and Nd) Flux-Assisted Boron Chalcogen Mixture Method Crystal Growth and Characterization of Magnetic, Optical, and Photoluminescent Properties

Gopabandhu Panigrahi, Habiba B. Kashem, Gregory Morrison, and Hans-Conrad zur Loye*

Department of Chemistry and Biochemistry, University of South Carolina, Columbia, SC, 29208, United States

*E-mail: <u>zurloye@mailbox.sc.edu</u>

	La3Si2Se1.21S6.79I					
Element	La	Si	Se	S	Ι	
Weight%	43.3	7.2	13.2	23.1	13.2	
Atomic%	20.0	16.4	10.7	46.2	6.7	
		Ce ₃ Si ₂ Se _{1.39} S _{6.61} I				
Element	Ce	Si	Se	S	Ι	
Weight%	46.3	6.8	10.2	23.5	13.2	
Atomic%	22.1	14.4	10.6	46.2	6.7	
		Pr ₃ Si ₂ Se _{1.22} S _{6.78} I				
Element	Pr	Si	Se	S	Ι	
Weight%	48.3	6.1	9.8	23.1	12.7	
Atomic%	22.8	14.5	8.2	47.8	6.7	
	Nd3Si2Se1.18S6.82I					
Element	Nd	Si	Se	S	Ι	
Weight%	49.2	6.4	3.6	25.6	15.2	
Atomic%	22.2	14.9	3.1	52.0	7.8	

La ₃ Si ₂ Se _{1.21} S _{6.79} I						
Atom	Wyck.	Site	S.O.F.	x/a	y/b	z/c
Lal	8f	1		0.30268(2)	0.11939(2)	0.31844(2)
La2	4e	2		0	0.09470(2)	1/4
Si1	8f	1		0.16020(4)	0.03745(8)	0.02912(5)
S1	8f	1	0.649(2)	0.06602(2)	0.15741(5)	0.54243(3)
S2	8f	1	0.892(2)	0.14478(3)	0.24478(6)	0.14602(4)
S3	8f	1	0.897(2)	0.21811(3)	0.43077(6)	0.41523(4)
S4	8f	1	0.956(2)	0.34993(3)	0.39900(6)	0.15931(5)
Se1	8f	1	0.351(2)	0.06602(2)	0.15741(5)	0.54243(3)
Se2	8f	1	0.108(2)	0.14478(3)	0.24478(6)	0.14602(4)
Se3	8f	1	0.103(2)	0.21811(3)	0.43077(6)	0.41523(4)
Se4	8f	1	0.044(2)	0.34993(3)	0.39900(6)	0.15931(5)
I1	4e	2		0	0.51393(3)	1/4
			Ce3Si2Se1.39S6.61	I		
Atom	Wyck.	Site	S.O.F.	x/a	y/b	z/c
Cel	8f	1		0.30182(2)	0.12028(2)	0.31787(2)
Ce2	4e	2		0	0.09532(2)	1/4
Si1	8f	1		0.16017(3)	0.03766(6)	0.02881(4)
S1	8f	1	0.6012(18)	0.06558(2)	0.15962(4)	0.54266(3)
S2	8f	1	0.8734(17)	0.14422(2)	0.24640(5)	0.14602(3)
S3	8f	1	0.8785(17)	0.21723(2)	0.43140(5)	0.41537(3)
S4	8f	1	0.9526(17)	0.35016(2)	0.39933(5)	0.16053(4)
Se1	8f	1	0.3988(18)	0.06558(2)	0.15962(4)	0.54266(3)
Se3	8f	1	0.1215(17)	0.21723(2)	0.43140(5)	0.41537(3)
Se2	8f	1	0.1266(17)	0.14422(2)	0.24640(5)	0.14602(3)
Se4	8f	1	0.0474(17)	0.35016(2)	0.39933(5)	0.16053(4)
I1	4e	2		0	0.51382(2)	1/4
Pr ₃ Si ₂ Se _{1.22} S _{6.78} I						
Atom	Wyck.	Site	S.O.F.	x/a	y/b	z/c
Pr1	8f	1		0.30176(2)	0.12067(2)	0.31796(2)
Pr2	4e	2		0	0.09729(2)	1/4
Si1	8f	1		0.16002(2)	0.03757(5)	0.02851(4)
S1	8f	1	0.6471(15)	0.06540(2)	0.16046(3)	0.54230(2)
S2	8f	1	0.8938(15)	0.14413(2)	0.24725(4)	0.14619(3)
S3	8f	1	0.8926(15)	0.21678(2)	0.43113(4)	0.41511(3)
S4	8f	1	0.9557(15)	0.35047(2)	0.39981(4)	0.16192(3)
Se1	8f	1	0.3529(15)	0.06540(2)	0.16046(3)	0.54230(2)
Se2	8f	1	0.1062(15)	0.14413(2)	0.24725(4)	0.14619(3)

Table S2. Fractional atomic coordinates and atomic parameters.

Se3	8f	1	0.1074(15)	0.21678(2)	0.43113(4)	0.41511(3)
Se4	8f	1	0.0443(15)	0.35047(2)	0.39981(4)	0.16192(3)
I1	4e	2		0	0.51425(2)	1/4
]	Nd3Si2Se1.18S6.82	I		
Atom	Wyck.	Site	S.O.F.	x/a	y/b	z/c
Nd2	4e	2		0	0.09814(2)	1/4
Nd1	8f	1		0.30123(2)	0.12100(2)	0.31799(2)
Si1	8f	1		0.15986(3)	0.03811(6)	0.02813(4)
S1	8f	1	0.6453(18)	0.06531(2)	0.16140(4)	0.54172(2)
S2	8f	1	0.9034(17)	0.14394(2)	0.24833(4)	0.14637(3)
S3	8f	1	0.9002(17)	0.21673(2)	0.43147(4)	0.41509(3)
S4	8f	1	0.9624(17)	0.35075(2)	0.39971(5)	0.16293(3)
Se1	8f	1	0.3547(18)	0.06531(2)	0.16140(4)	0.54172(2)
Se3	8f	1	0.0998(17)	0.21673(2)	0.43147(4)	0.41509(3)
Se2	8f	1	0.0966(17)	0.14394(2)	0.24833(4)	0.14637(3)
Se4	8f	1	0.0376(17)	0.35075(2)	0.39971(5)	0.16293(3)
I1	4e	2		0	0.51448(2)	1/4

Table S3. Interatomic distances of Eu₂SiSe_xS_{4-x}.

$La_{3}Si_{2}Se_{1,21}S_{6,79}I$				
Lal	S3 Se3	1x	2.9529(5)	
Lal	S4 Se4	1x	2.9898(6)	
Lal	S3 Se3	1x	3.0161(5)	
Lal	S1 Se1	1x	3.0202(4)	
Lal	S4 Se4	1x	3.0635(6)	
Lal	S3 Se3	1x	3.0855(5)	
Lal	S2 Se2	1x	3.1082(5)	
Lal	S2 Se2	1x	3.1317(5)	
La2	S4 Se4	1x	2.9420(5)	
La2	S4 Se4	1x	2.9427(5)	
La2	S2 Se2	1x	2.9877(5)	
La2	S2 Se2	1x	2.9882(5)	
La2	S1 Se1	1x	3.2842(3)	
La2	S1 Se1	1x	3.2848(3)	
La2	S1 Se1	2x	3.3183(4)	
Si1	S4 Se4	1x	2.1157(8)	
Sil	S2 Se2	1x	2.1244(8)	
Sil	S3 Se3	1x	2.1547(8)	
Sil	S1 Se1	1x	2.1908(7)	
La•••La			4.5034(5)	
[•••]			5.4966(4)	
Ce ₃ Si ₂ Se _{1.39} S _{6.61} I				
Cel	S3 Se3	1x	2.9338(4)	
Cel	S4 Se4	1x	2.9610(5)	

Cel Silsel 1x $3.0048(4)$ Cel S4[Se4 1x $3.0360(5)$ Cel S2[Se2 1x $3.0657(4)$ Cel S2[Se2 1x $3.0669(4)$ Cel S2[Se2 1x $3.0859(4)$ Cel S2[Se2 1x $3.0109(4)$ Ce2 S4[Se4 1x $2.203(4)$ Ce2 S4[Se4 1x $2.203(4)$ Ce2 S2[Se2 2x $2.9641(4)$ Ce2 S1[Se1 1x $3.3057(3)$ Ce2 S1[Se1 1x $3.3057(3)$ Ce2 S1[Se1 1x $2.1132(6)$ Si1 S2[Se2 1x $2.1132(6)$ Si1 S2[Se3 1x $2.1132(6)$ Si1 S2[Se3 1x $2.1132(6)$ Si1 S2[Se3 1x $2.1956(6)$ Ce1 S3[Se3 1x $2.9338(4)$ Cerece 4.4610(5) Pr1	Cel	S3 Se3	1x	2.9999(4)	
Cel S4[se4 1x 3.0360(5) Cel S3]se3 1x 3.0457(4) Cel S2[se2 1x 3.0657(4) Cel S2[se2 1x 3.0457(4) Cel S2[se2 1x 3.0457(4) Ce2 S4[se4 1x 2.9201(4) Ce2 S4[se4 1x 2.9203(4) Ce2 S1[se1 1x 3.2723(3) Ce2 S1[se1 1x 3.3055(3) Ce2 S1[se1 1x 3.3055(3) Ce2 S1[se1 1x 3.3055(3) Ce2 S1[se1 1x 2.1132(6) Si1 S2[se2 1x 2.1132(6) Si1 S2[se3 1x 2.1132(6) Si1 S1[se1 1x 2.1132(6) Si1 S1[se3 1x 2.1956(6) Ce1 S3[se3 1x 2.9209(4) PrI S3[se3 1x 2.9209(4) PrI S3[Cel	S1 Se1	1x	3.0048(4)	
Cel S3]se3 1x 3.0657(4) Cel S2]se2 1x 3.0869(4) Cel S2]se2 1x 3.109(4) Ce2 S4]se4 1x 2.9201(4) Ce2 S4]se4 1x 2.9203(4) Ce2 S2]se2 2x 2.9641(4) Ce2 S1]se1 1x 3.2723(3) Ce2 S1]se1 1x 3.3057(3) Ce2 S1]se1 1x 3.3057(3) Ce2 S1]se1 1x 2.1305(3) Ce2 S1]se1 1x 2.1305(3) Ce2 S1]se1 1x 2.1324(6) Si1 S3]se3 1x 2.1547(6) Si1 S3]se3 1x 2.9338(4) Ce- 4.4610(5) 1 I 5.4690(4) Pr1 S3]se3 1x 2.9209(4) Pr1 S3]se3 1x 2.9403(4) Pr1 S3]se3 1x	Cel	S4 Se4	1x	3.0360(5)	
Cel S2[8e2 1x $3.0869(4)$ Ce1 S2[8e2 1x $3.1109(4)$ Ce2 S4[8e4 1x $2.9201(4)$ Ce2 S4[8e4 1x $2.9203(4)$ Ce2 S2[8e2 $2x$ $2.9641(4)$ Ce2 S1[8e1 1x $3.2723(3)$ Ce2 S1[8e1 1x $3.3057(3)$ Ce2 S1[8e1 1x $3.3057(3)$ Si1 S4[8e4 1x $2.1132(6)$ Si1 S3[8e3 1x $2.11347(6)$ Si1 S3[8e3 1x $2.1938(4)$ Ce1 S3[8e3 1x $2.9338(4)$ Cerec 4.4610(5) I*** Prisise_1256:rs1 ************************************	Cel	S3 Se3	1x	3.0657(4)	
Cc1 S2[Sc2] 1x 3.1109(4) Cc2 S4[Sc4 1x 2.9201(4) Cc2 S4[Sc4 1x 2.9203(4) Cc2 S2[Sc2] 2x 2.9641(4) Cc2 S1[Sc1 1x 3.2723(3) Cc2 S1[Sc1 1x 3.2726(3) Cc2 S1[Sc1 1x 3.3055(3) Cc2 S1[Sc1 1x 2.132(6) Sil S2[Sc2 1x 2.1132(6) Sil S2[Sc2 1x 2.1132(6) Sil S3[Sc3 1x 2.1956(6) Cc1 S3[Sc3 1x 2.9338(4) Cce+Ce 4.4610(5) I•••1 5.4690(4) Pr1 S3[Sc3 1x 2.9209(4) Pr1 S3[Sc3 1x 2.9403(4) Pr1 S3[Sc3 1x 2.9403(4) Pr1 S3[Sc3 1x 2.9403(4) Pr1 S3[Sc3 1x 2.940	Cel	S2 Se2	1x	3.0869(4)	
Cc2 S4[8e4 1x 2.9203(4) Cc2 S2[Sc2 2x 2.9641(4) Cc2 S2[Sc2 2x 2.9641(4) Cc2 S1[Se1 1x 3.2726(3) Cc2 S1[Se1 1x 3.3055(3) Cc2 S1[Se1 1x 3.3057(3) Si1 S4[Se4 1x 2.1132(6) Si1 S4[Se4 1x 2.1234(6) Si1 S3[Se3 1x 2.1547(6) Si1 S1[Se1 1x 2.1938(4) Cce 4.4610(5) Cet 4.4610(5) Cet 4.4610(5) Itx 2.9209(4) PrI S3[Sc3 1x 2.9209(4) Pr1 S3[Sc3 1x 2.9403(4) Pr1 S3[Sc3 1x 2.9403(4) Pr1 S4[Sc4 1x 2.9403(4) Pr1 S4[Sc4 1x 2.9403(4) Pr1 S3[Sc3	Cel	S2 Se2	1x	3.1109(4)	
Cc2 S4]8c4 1x 2.9203(4) Cc2 S2]8c2 2x 2.9641(4) Cc2 S1]8c1 1x 3.2723(3) Cc2 S1]8c1 1x 3.2726(3) Cc2 S1]8c1 1x 3.3057(3) Cc2 S1]8c1 1x 3.3057(3) Si1 S2]8c2 1x 2.1132(6) Si1 S2]8c3 1x 2.1234(6) Si1 S2]8c3 1x 2.1956(6) Cc1 S3]8c3 1x 2.933(4) CcewCe 4.4610(5) I++1 S3]8c3 1x 2.9209(4) Pr1 S3]8c3 1x 2.9403(4) Pr1 S3]8c3 1x	Ce2	S4 Se4	1x	2.9201(4)	
Cc2 S2[Sc2 2x 2.9641(4) Cc2 S1[Sc1 1x 3.2723(3) Cc2 S1[Sc1 1x 3.2726(3) Cc2 S1[Sc1 1x 3.3055(3) Cc2 S1[Sc1 1x 3.3055(3) Cc2 S1[Sc1 1x 3.3055(3) Cc2 S1[Sc1 1x 2.1132(6) Si1 S2[Sc2 1x 2.1234(6) Si1 S3[Sc3 1x 2.1597(6) Si1 S3[Sc3 1x 2.9338(4) Cce+**Ce 4.4610(5) I+** PriSisCe_122Se_seI Pr1 S3[Sc3 1x 2.9209(4) Pr1 S4[Sc4 1x 2.9403(4) Pr1 S4[Sc4 1x	Ce2	S4 Se4	1x	2.9203(4)	
Cc2 S1[Se1 1x 3.2723(3) Cc2 S1[Se1 1x 3.2723(3) Cc2 S1[Se1 1x 3.3055(3) Cc2 S1[Se1 1x 3.3057(3) Si1 S4[Se4 1x 2.1132(6) Si1 S2[Se2 1x 2.1134(6) Si1 S3[Se3 1x 2.1534(6) Si1 S1[Se1 1x 2.1547(6) Si1 S1[Se1 1x 2.1547(6) Si1 S1[Se3 1x 2.933(4) Ce•••Ce 4.4610(5) I•••I S3[Se3 1x 2.9209(4) Pr1 S3[Se3 1x 2.9403(4) Pr1 S3[Se3 1x 2.9437(4) Pr1 S3[Se3	Ce2	S2 Se2	2x	2.9641(4)	
Cc2 S1 Se1 1x $3.2726(3)$ Cc2 S1 Se1 1x $3.3057(3)$ Si1 S4 Se4 1x $2.1132(6)$ Si1 S2 Se2 1x $2.1132(6)$ Si1 S2 Se2 1x $2.1132(6)$ Si1 S2 Se2 1x $2.1547(6)$ Si1 S3 Se3 1x $2.1547(6)$ Si1 S3 Se3 1x $2.1956(6)$ Cc1 S3 Se3 1x $2.9338(4)$ Cc+++Ce 4.4610(5) I+1 S3 Se3 1x $2.9209(4)$ Pr1 S3 Se3 1x $2.9209(4)$ Pr1 S3 Se3 1x $2.9430(4)$ Pr1 S3 Se3 1x $2.9430(4)$ Pr1 S3 Se3 1x $3.0470(4)$ Pr1 S3 Se3 1x $3.0470(4)$ Pr1 S3 Se3 1x $3.0470(4)$ Pr1 S2 Se2 1x $3.0932(4)$ Pr2	Ce2	S1 Se1	1x	3.2723(3)	
$\begin{array}{c cccc} Cc2 & S1 Sc1 & 1x & 3.3055(3) \\ \hline Cc2 & S1 Sc1 & 1x & 3.3057(3) \\ \hline Sil & S4 Sc4 & 1x & 2.1132(6) \\ \hline Sil & S2 Sc2 & 1x & 2.1234(6) \\ \hline Sil & S3 Sc3 & 1x & 2.1547(6) \\ \hline Sil & S3 Sc3 & 1x & 2.1547(6) \\ \hline Sil & S3 Sc3 & 1x & 2.1956(6) \\ \hline Ccl & S3 Sc3 & 1x & 2.9338(4) \\ \hline Cc \bullet Cc & & 4.4610(5) \\ \hline I \bullet I & 5.4600(4) \\ \hline \hline I \bullet I & 5.4600(4) \\ \hline \hline I \bullet I & 5.4800(4) \\ \hline \hline I \bullet I & 5.4800(4) \\ \hline I \bullet I & 5.3 Sc3 & 1x & 2.9209(4) \\ \hline Pr1 & S3 Sc3 & 1x & 2.9403(4) \\ Pr1 & S4 Sc4 & 1x & 2.9403(4) \\ Pr1 & S1 Sc1 & 1x & 2.9443(4) \\ Pr1 & S3 Sc3 & 1x & 2.9865(4) \\ Pr1 & S3 Sc3 & 1x & 3.0470(4) \\ Pr1 & S3 Sc3 & 1x & 3.0470(4) \\ Pr1 & S2 Sc2 & 1x & 3.0062(4) \\ Pr1 & S2 Sc2 & 1x & 3.0062(4) \\ Pr2 & S4 Sc4 & 1x & 2.9013(3) \\ Pr2 & S4 Sc4 & 1x & 2.9013(3) \\ Pr2 & S2 Sc2 & 1x & 2.9431(3) \\ Pr2 & S2 Sc2 & 1x & 2.9431(3) \\ Pr2 & S2 Sc2 & 1x & 2.9431(3) \\ Pr2 & S1 Sc1 & 1x & 3.2056(3) \\ Pr2 & S1 Sc1 & 1x & 3.2056(3) \\ Pr2 & S1 Sc1 & 1x & 3.2056(3) \\ Pr2 & S1 Sc1 & 1x & 3.3056(3) \\ Pr2 & S1 Sc1 & 1x & 2.1143(5) \\ Sil & S2 Sc2 & 1x & 2.1512(5) \\ Sil & S3 Sc3 & 1x & 2.1512(5) \\ Sil & S3 Sc3 & 1x & 2.4512(5) \\ \hline \hline \hline \hline \\ \hline $	Ce2	S1 Se1	1x	3.2726(3)	
Cc2 S1 Sel 1x 3,3057(3) Sil S4 Se4 1x 2,1132(6) Sil S2 Se2 1x 2,1234(6) Sil S3 Se3 1x 2,1234(6) Sil S1 Se1 1x 2,134(6) Sil S1 Se1 1x 2,134(6) Cci S3 Se3 1x 2,9338(4) CcerrCe 4,4610(5) I**•1 5,4690(4) Ce**•Ce 4,4610(5) Pr1 S3 Se3 1x 2,9209(4) Pr1 S3 Se3 1x 2,9403(4) Pr1 S3 Se3 1x 2,9403(4) Pr1 S3 Se3 1x 2,9431(4) Pr1 S3 Se3 1x 3,0187(4) Pr1 S3 Se3 1x 3,0470(4) Pr1 S2 Se2 1x 3,0932(4) Pr1 S2 Se2 1x 2,9020(3) Pr2 S4 Se4 1x 2,9020(3)	Ce2	S1 Se1	1x	3.3055(3)	
Sil S4[Se4 1x 2.1132(6) Sil S2[Se2 1x 2.1234(6) Sil S3[Se3 1x 2.1547(6) Sil S1[Se1 1x 2.1956(6) CcI S3[Se3 1x 2.9338(4) CcI S3[Se3 1x 2.9338(4) CcI S3[Se3 1x 2.9338(4) CcI S3[Se3 1x 2.9209(4) III S3[Se3 1x 2.9209(4) Pr1 S4[Se4 1x 2.9403(4) Pr1 S4[Se4 1x 3.0187(4) Pr1 S4[Se4 1x 3.0187(4) Pr1 S4[Se2 1x 3.0062(4) Pr1 S4[Se4 1x 2.9013(3) Pr2 S4[Se4 1x 2.902(3) Pr2 S4[Se4 1x <td< td=""><td>Ce2</td><td>S1 Se1</td><td>1x</td><td>3.3057(3)</td></td<>	Ce2	S1 Se1	1x	3.3057(3)	
Sil S2[Se2 1x 2.1234(6) Sil S3[Se3 1x 2.1957(6) Sil S1[Se1 1x 2.1956(6) Cel S3[Se3 1x 2.9338(4) Cer*Ce 4.4610(5) 4.4610(5) I** 2.9338(4) 5.4690(4) Pr1 S3[Se3 1x 2.9209(4) Pr1 S4[Se4 1x 2.9403(4) Pr1 S4[Se4 1x 2.9403(4) Pr1 S4[Se4 1x 2.9865(4) Pr1 S3[Se3 1x 2.9865(4) Pr1 S4[Se4 1x 3.0187(4) Pr1 S3[Se3 1x 3.0470(4) Pr1 S2[Se2 1x 3.0032(4) Pr1 S2[Se2 1x 2.9013(3) Pr2 S4[Se4 1x 2.9013(3) Pr2 S2[Se2 1x 2.9437(3) Pr2 S2[Se2 1x 3.20502(2) Pr2 S1[Se1 1x	Sil	S4 Se4	1x	2.1132(6)	
Sil S3Se3 1x 2.1547(6) Sil S1Se3 1x 2.1956(6) Cet S3Se3 1x 2.9338(4) Ce••Ce 4.4610(5) 4.4610(5) I•••I 5.4690(4) 5.4690(4) Pr1 S3[Se3 1x 2.9209(4) Pr1 S4[Se4 1x 2.9403(4) Pr1 S4[Se4 1x 2.9403(4) Pr1 S3[Se3 1x 2.9209(4) Pr1 S4[Se4 1x 2.9403(4) Pr1 S4[Se4 1x 2.9403(4) Pr1 S3[Se3 1x 2.9403(4) Pr1 S3[Se3 1x 3.0470(4) Pr1 S3[Se3 1x 3.0470(4) Pr1 S2[Se2 1x 3.0932(4) Pr1 S2[Se2 1x 2.9013(3) Pr2 S4[Se4 1x 2.9020(3) Pr2 S4[Se4 1x 2.9437(3) Pr2 S2[Se2 1x 3.2505(2) Pr2 S1[Se1 1x 3.2505(2)	Sil	S2 Se2	1x	2.1234(6)	
Sil SI Sel 1x 2.1956(6) Cel S3 Se3 1x 2.9338(4) Ce•••Ce 4.4610(5) 1 I••1 5.4690(4) 5.4690(4) Pr1 S3 Se3 1x 2.9209(4) Pr1 S3 Se3 1x 2.9403(4) Pr1 S4 Se4 1x 2.943(4) Pr1 S3 Se3 1x 2.9843(4) Pr1 S3 Se3 1x 2.9865(4) Pr1 S3 Se3 1x 3.0187(4) Pr1 S4 Se4 1x 3.0187(4) Pr1 S2 Se2 1x 3.0662(4) Pr1 S2 Se2 1x 3.0932(4) Pr2 S4 Se4 1x 2.9013(3) Pr2 S4 Se4 1x 2.9431(3) Pr2 S4 Se4 1x 2.9431(3) Pr2 S2 Se2 1x 2.9431(3) Pr2 S2 Se2 1x 2.9431(3) Pr2 S1 Se1 1x <	Sil	S3 Se3	1x	2.1547(6)	
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Image 5.4690(4) Pri S3 Se3 1x 2.9209(4) Pr1 S4 Se4 1x 2.9403(4) Pr1 S4 Se4 1x 2.9403(4) Pr1 S1 Se1 1x 2.9843(4) Pr1 S3 Se3 1x 2.9865(4) Pr1 S3 Se3 1x 3.0187(4) Pr1 S3 Se3 1x 3.0187(4) Pr1 S3 Se3 1x 3.0187(4) Pr1 S3 Se2 1x 3.0662(4) Pr1 S2 Se2 1x 3.0662(4) Pr1 S2 Se2 1x 3.0662(4) Pr2 S4 Se4 1x 2.9013(3) Pr2 S4 Se4 1x 2.9020(3) Pr2 S2 Se2 1x 2.9437(3) Pr2 S2 Se2 1x 2.9437(3) Pr2 S2 Se2 1x 3.2505(2) Pr2 S1 Se1 1x 3.2505(2) Pr2 S1 Se1 1x 3	Ce•••Ce			4.4610(5)	
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Pr1S4/Se41x2.9403(4)Pr1S1/Se11x2.9843(4)Pr1S3/Se31x2.9865(4)Pr1S3/Se31x3.0187(4)Pr1S3/Se31x3.0470(4)Pr1S2/Se21x3.0662(4)Pr1S2/Se21x3.0932(4)Pr2S4/Se41x2.9013(3)Pr2S4/Se41x2.9020(3)Pr2S2/Se21x2.9437(3)Pr2S2/Se21x2.9437(3)Pr2S2/Se21x3.2502(2)Pr2S1/Se11x3.2505(2)Pr2S1/Se11x3.3056(3)Pr2S1/Se11x3.3056(3)Pr2S1/Se11x2.1143(5)Si1S2/Se21x2.1215(5)Si1S3/Se31x2.1512(5)Si1S3/Se31x2.1512(5)Si1S3/Se21x2.887(3)Nd2S4/Se41x2.887(3)Nd2S4/Se41x2.887(3)Nd2S4/Se41x2.887(3)Nd2S4/Se41x2.9038(3)Nd2S4/Se41x2.9308(3)Nd2S4/Se41x2.9308(3)Nd2S4/Se41x2.9308(3)Nd2S4/Se41x2.9308(3)Nd2S4/Se41x2.9308(3)Nd2S4/Se41x2.9308(3)Nd2S2/Se21x2.9308(3)Nd2S2/Se2	Prl	S3 Se3	lx	2.9209(4)	
Pr1 S1 Se1 1x 2.9843(4) Pr1 S3 Se3 1x 2.9865(4) Pr1 S4 Se4 1x 3.0187(4) Pr1 S3 Se3 1x 3.0470(4) Pr1 S2 Se2 1x 3.0662(4) Pr1 S2 Se2 1x 3.0062(4) Pr1 S2 Se2 1x 3.0062(4) Pr1 S2 Se2 1x 3.0932(4) Pr2 S4 Se4 1x 2.9013(3) Pr2 S4 Se4 1x 2.9020(3) Pr2 S2 Se2 1x 2.9431(3) Pr2 S2 Se2 1x 2.9437(3) Pr2 S2 Se2 1x 2.9437(3) Pr2 S1 Se1 1x 3.2505(2) Pr2 S1 Se1 1x 3.3056(3) Pr2 S1 Se1 1x 3.3058(3) Si1 S4 Se4 1x 2.1143(5) Si1 S2 Se2 1x 2.1215(5) Si1 S3 Se3 1x 2.1512(5) Si1 S4 Se4 1x <t< td=""><td>Pr1</td><td>S4 Se4</td><td>1x</td><td>2.9403(4)</td></t<>	Pr1	S4 Se4	1x	2.9403(4)	
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Pr1S3 Se31x $3.0470(4)$ Pr1S2 Se21x $3.0662(4)$ Pr1S2 Se21x $3.0932(4)$ Pr2S4 Se41x $2.9013(3)$ Pr2S4 Se41x $2.9020(3)$ Pr2S2 Se21x $2.9431(3)$ Pr2S2 Se21x $2.9437(3)$ Pr2S2 Se21x $2.9437(3)$ Pr2S1 Se11x $3.2502(2)$ Pr2S1 Se11x $3.2505(2)$ Pr2S1 Se11x $3.3056(3)$ Pr2S1 Se11x $3.3056(3)$ Pr2S1 Se11x $3.3058(3)$ Si1S4 Se41x $2.1143(5)$ Si1S2 Se21x $2.1143(5)$ Si1S3 Se31x $2.1512(5)$ Si1S1 Se11x $2.1874(5)$ Pr••Pr $4.4350(5)$ I••I 5.4450 Md2S4 Se41x $2.8867(3)$ Nd2S4 Se41x $2.8874(3)$ Nd2S4 Se41x $2.9308(3)$	Prl	S4 Se4	lx	3.0187(4)	
Pr1 $S2 Se2$ Ix $3.0662(4)$ Pr1 $S2 Se2$ Ix $3.0932(4)$ Pr2 $S4 Se4$ Ix $2.9013(3)$ Pr2 $S4 Se4$ Ix $2.9020(3)$ Pr2 $S2 Se2$ Ix $2.9431(3)$ Pr2 $S2 Se2$ Ix $2.9437(3)$ Pr2 $S1 Se1$ Ix $3.2505(2)$ Pr2 $S1 Se1$ Ix $3.2505(2)$ Pr2 $S1 Se1$ Ix $3.3056(3)$ Pr2 $S1 Se1$ Ix $3.3058(3)$ Si1 $S4 Se4$ Ix $2.1143(5)$ Si1 $S2 Se2$ Ix $2.1512(5)$ Si1 $S3 Se3$ Ix $2.1512(5)$ Si1 $S1 Se1$ Ix $2.4874(5)$ Pr••Pr $4.4350(5)$ I••I 5.4450 Md2 $S4 Se4$ Ix $2.8867(3)$ Nd2 $S4 Se4$ Ix $2.8874(3)$ Nd2 $S4 Se4$ Ix $2.9308(3)$ Nd2 $S2 Se2$ Ix $2.9308(3)$ Nd2 $S2 Se2$ Ix $2.9314(3)$	Prl	S3 Se3	lx 1	3.04/0(4)	
Pr1 $S2 Se2$ Ix $3.0932(4)$ Pr2 $S4 Se4$ Ix $2.9013(3)$ Pr2 $S4 Se4$ Ix $2.9020(3)$ Pr2 $S2 Se2$ Ix $2.9431(3)$ Pr2 $S2 Se2$ Ix $2.9437(3)$ Pr2 $S2 Se2$ Ix $2.9437(3)$ Pr2 $S1 Se1$ Ix $3.2502(2)$ Pr2 $S1 Se1$ Ix $3.2505(2)$ Pr2 $S1 Se1$ Ix $3.3056(3)$ Pr2 $S1 Se1$ Ix $3.3058(3)$ Si1 $S4 Se4$ Ix $2.1143(5)$ Si1 $S2 Se2$ Ix $2.1215(5)$ Si1 $S3 Se3$ Ix $2.1512(5)$ Si1 $S3 Se3$ Ix $2.1512(5)$ Si1 $S1 Se1$ Ix $2.1874(5)$ Pr••Pr $4.4350(5)$ I•••I 5.4450 Md2 $S4 Se4$ Ix $2.8867(3)$ Nd2 $S2 Se2$ Ix $2.9308(3)$ Nd2 $S2 Se2$ Ix $2.9314(3)$	Prl	S2 Se2	1x	3.0662(4)	
Pr2 S4 Se4 1x $2.9013(3)$ Pr2 S4 Se4 1x $2.9020(3)$ Pr2 S2 Se2 1x $2.9431(3)$ Pr2 S2 Se2 1x $2.9437(3)$ Pr2 S2 Se2 1x $2.9437(3)$ Pr2 S1 Se1 1x $3.2502(2)$ Pr2 S1 Se1 1x $3.2505(2)$ Pr2 S1 Se1 1x $3.3056(3)$ Pr2 S1 Se1 1x $3.3056(3)$ Pr2 S1 Se1 1x $3.3058(3)$ Si1 S4 Se4 1x $2.1143(5)$ Si1 S2 Se2 1x $2.1215(5)$ Si1 S2 Se2 1x $2.1215(5)$ Si1 S3 Se3 1x $2.1512(5)$ Si1 S1 Se1 1x $2.1874(5)$ Pr•••Pr $4.4350(5)$ $1•••1$ Nd2 S4 Se4 1x $2.8867(3)$ Nd2 S4 Se4 1x $2.8867(3)$ Nd2 S2 Se2 1x $2.9308(3)$ Nd2 <	Prl	S2 Se2	1	3.0932(4)	
Pr2S4 Se41x2.9020(3)Pr2S2 Se21x2.9431(3)Pr2S2 Se21x2.9437(3)Pr2S1 Se11x3.2502(2)Pr2S1 Se11x3.2505(2)Pr2S1 Se11x3.3056(3)Pr2S1 Se11x3.3058(3)Si1S4 Se41x2.1143(5)Si1S2 Se21x2.1215(5)Si1S3 Se31x2.1512(5)Si1S1 Se11x2.1874(5)Pr••Pr4.4350(5)I••I5.4450Nd ₃ Si ₂ Se _{1.18} S _{6.82} INd2S4 Se41x2.8867(3)Nd2S4 Se41x2.9308(3)Nd2S2 Se21x2.9308(3)Nd2S2 Se21x2.9308(3)Nd2S2 Se21x2.9314(3)	Pr2	S4 Se4	1X 1	2.9013(3)	
Pr2S2 [Se21x2.9431(3)Pr2S2 [Se21x2.9437(3)Pr2S1 [Se11x3.2502(2)Pr2S1 [Se11x3.2505(2)Pr2S1 [Se11x3.3056(3)Pr2S1 [Se11x3.3058(3)Si1S4 [Se41x2.1143(5)Si1S2 [Se21x2.1215(5)Si1S3 [Se31x2.1512(5)Si1S1 [Se11x2.1874(5)Pr••Pr4.4350(5)1I••I5.4450Nd3Si2Se1.18S6.82INd2S4 [Se41x2.8867(3)Nd2S4 [Se41x2.8874(3)Nd2S2 [Se21x2.9308(3)Nd2S2 [Se21x2.9308(3)Nd2S2 [Se21x2.9314(3)	Pr2	54 Se4	1X 1	2.9020(3)	
Pr2 S2 Se2 1x $2.9437(3)$ Pr2 S1 Se1 1x $3.2502(2)$ Pr2 S1 Se1 1x $3.2505(2)$ Pr2 S1 Se1 1x $3.3056(3)$ Pr2 S1 Se1 1x $3.3056(3)$ Pr2 S1 Se1 1x $3.3058(3)$ Si1 S4 Se4 1x $2.1143(5)$ Si1 S2 Se2 1x $2.1215(5)$ Si1 S2 Se2 1x $2.1512(5)$ Si1 S3 Se3 1x $2.1512(5)$ Si1 S1 Se1 1x $2.1874(5)$ Pr•••Pr 4.4350(5) 1 I••I 5.4450 1 Nd ₃ Si ₂ Se _{1.18} S _{6.82} I Nd2 S4 Se4 1x $2.8867(3)$ Nd2 S4 Se4 1x $2.9308(3)$ Nd2 S2 Se2 1x $2.9308(3)$ Nd2 S2 Se2 1x $2.9314(3)$	Pr2	52 5e2 52 5-2	1X 1	2.9431(3)	
P12 S1/Se1 1x $3.2302(2)$ Pr2 S1/Se1 1x $3.2505(2)$ Pr2 S1/Se1 1x $3.3056(3)$ Pr2 S1/Se1 1x $3.3058(3)$ Si1 S4/Se4 1x $2.1143(5)$ Si1 S2/Se2 1x $2.1215(5)$ Si1 S3/Se3 1x $2.1215(5)$ Si1 S3/Se3 1x $2.1512(5)$ Si1 S1/Se1 1x $2.1874(5)$ Pr•••Pr 4.4350(5) 1 I•••I 5.4450 1 Nd2 S4/Se4 1x $2.8867(3)$ Nd2 S4/Se4 1x $2.8867(3)$ Nd2 S4/Se4 1x $2.9308(3)$ Nd2 S2/Se2 1x $2.9314(3)$	Pr2	S2 Se2	1X 1v	2.9437(3)	
P12 $S1 Se1$ $1x$ $3.2303(2)$ $Pr2$ $S1 Se1$ $1x$ $3.3056(3)$ $Pr2$ $S1 Se1$ $1x$ $3.3058(3)$ $Si1$ $S4 Se4$ $1x$ $2.1143(5)$ $Si1$ $S2 Se2$ $1x$ $2.1215(5)$ $Si1$ $S2 Se2$ $1x$ $2.1215(5)$ $Si1$ $S3 Se3$ $1x$ $2.1512(5)$ $Si1$ $S1 Se1$ $1x$ $2.1874(5)$ $Pr••Pr$ $4.4350(5)$ $1•••I$ $I•••I$ 5.4450 Nd ₃ Si ₂ Se _{1.18} S _{6.82} INd2 $S4 Se4$ $1x$ $2.8867(3)$ $Nd2$ $S2 Se2$ $1x$ $2.9308(3)$ Nd2 $S2 Se2$ $1x$ $2.9308(3)$ $Nd2$ $S2 Se2$ $1x$ $2.9314(3)$	Pr2		1X 1	3.2302(2)	
$P12$ $S1 Se1$ $1x$ $3.3050(3)$ $Pr2$ $S1 Se1$ $1x$ $3.3058(3)$ $Si1$ $S4 Se4$ $1x$ $2.1143(5)$ $Si1$ $S2 Se2$ $1x$ $2.1215(5)$ $Si1$ $S3 Se3$ $1x$ $2.1512(5)$ $Si1$ $S3 Se3$ $1x$ $2.1512(5)$ $Si1$ $S1 Se1$ $1x$ $2.1874(5)$ $Pr•••Pr$ $4.4350(5)$ $4.4350(5)$ $I•••I$ $S.4450$ $Nd_3Si_2Se_{1.18}S_{6.82}I$ Nd2 $S4 Se4$ $1x$ $2.8867(3)$ Nd2 $S4 Se4$ $1x$ $2.8874(3)$ Nd2 $S2 Se2$ $1x$ $2.9308(3)$ Nd2 $S2 Se2$ $1x$ $2.9314(3)$	Pr2		1X 1v	3.2303(2)	
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Nd2 S4 Se4 1x 2.8867(3) Nd2 S4 Se4 1x 2.8874(3) Nd2 S2 Se2 1x 2.9308(3) Nd2 S2 Se2 1x 2.9314(3)	NdzSizSex inScarI				
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Nd2 S2 Se2 1x 2.9308(3) Nd2 S2 Se2 1x 2.9314(3)	Nd2	S4 Se4	1x	2.8874(3)	
Nd2 S2 Se2 1x 2.9314(3)	Nd2	S2 Se2	1x	2.9308(3)	
	Nd2	S2 Se2	1x	2.9314(3)	
Nd2 S1 Se1 1x 3.2311(2)	Nd2	S1 Se1	1x	3.2311(2)	

Nd2	S1 Se1	1x	3.2314(2)
Nd2	S1 Se1	1x	3.3041(3)
Nd2	S1 Se1	1x	3.3043(3)
Nd1	S3 Se3	1x	2.9087(4)
Nd1	S4 Se4	1x	2.9225(4)
Nd1	S1 Se1	1x	2.9739(4)
Nd1	S3 Se3	1x	2.9744(4)
Nd1	S4 Se4	1x	3.0045(4)
Nd1	S3 Se3	1x	3.0294(4)
Nd1	S2 Se2	1x	3.0467(4)
Nd1	S2 Se2	1x	3.0776(4)
Si1	S4 Se4	1x	2.1115(5)
Si1	S2 Se2	1x	2.1187(6)
Si1	S3 Se3	1x	2.1467(6)
Si1	S1 Se1	1x	2.1857(6)
Nd•••Nd			4.4065(5)
[•••]			5.4067(4)



Figure S1. The PXRD pattern of polycrystalline La₃Si₂Se_{1.21}S_{6.79}I compound (simulated pattern (black) experimental pattern (red) and Bragg position (blue)).



Figure S2. The PXRD pattern of polycrystalline Ce₃Si₂Se_{1.39}S_{6.61}I compound (simulated pattern (black) experimental pattern (red) and Bragg position (blue)).



Figure S3. The pxrd pattern of polycrystalline Pr₃Si₂Se_{1.22}S_{6.78}I compound (simulated pattern (black) experimental pattern (red) and Bragg position (blue)) (* unidentified peaks).



Figure. S4 TGA plot of polycrystalline Ce₃Si₂Se_{1.39}S_{6.61}I under N₂ atmosphere.



Figure S5. The PXRD pattern of polycrystalline Ce₃Si₂Se_{1.39}S_{6.61}I compound after TGA experiment (experimental pattern (black) simulated pattern (red) and Bragg position (blue)).



Figure S6. Scintillation of Ce₃Si₂Se_{1.39}S_{6.61}I under exposer of X-ray



Figure S7. Molar and inverse molar magnetic susceptibility vs Temperature (ZFC) plots for (a) Ce₃Si₂Se_{1.39}S_{6.61}I and (b) Nd₃Si₂Se_{1.18}S_{6.82}I.