Single Crystals of EuScCuSe₃: Synthesis, Experimental and DFT Investigations

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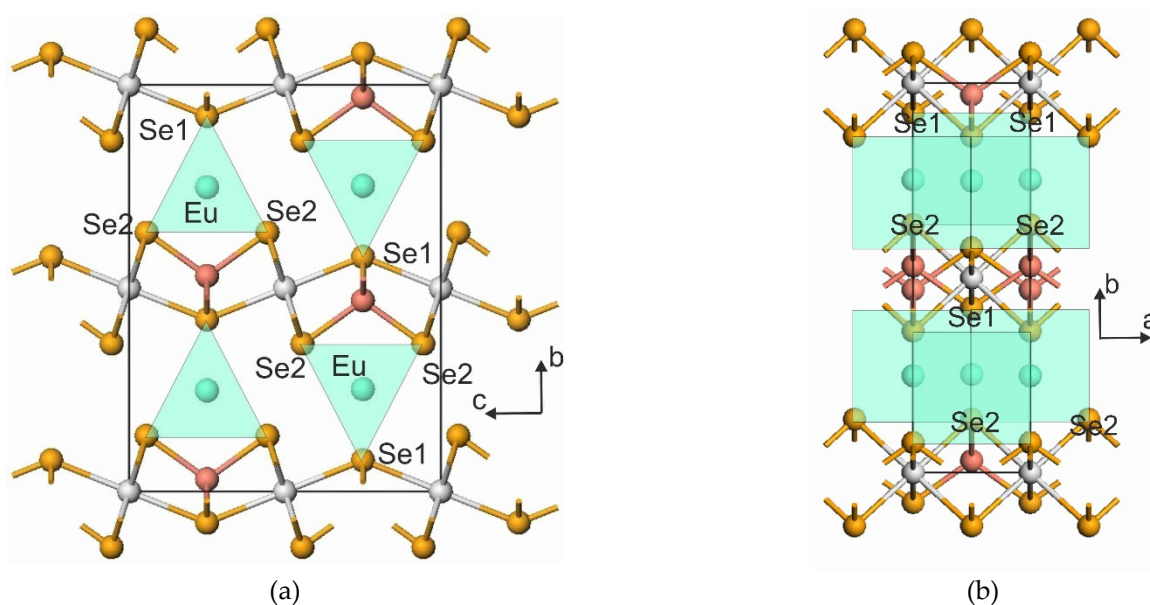
(a)   (b)

Figure S1. Crystal structure of EuScCuSe₃. Projection onto the *bc* plane (a) and onto the *ab* plane (b). The trigonal prisms [EuSe₆]¹⁰⁻ are colored in turquoise.
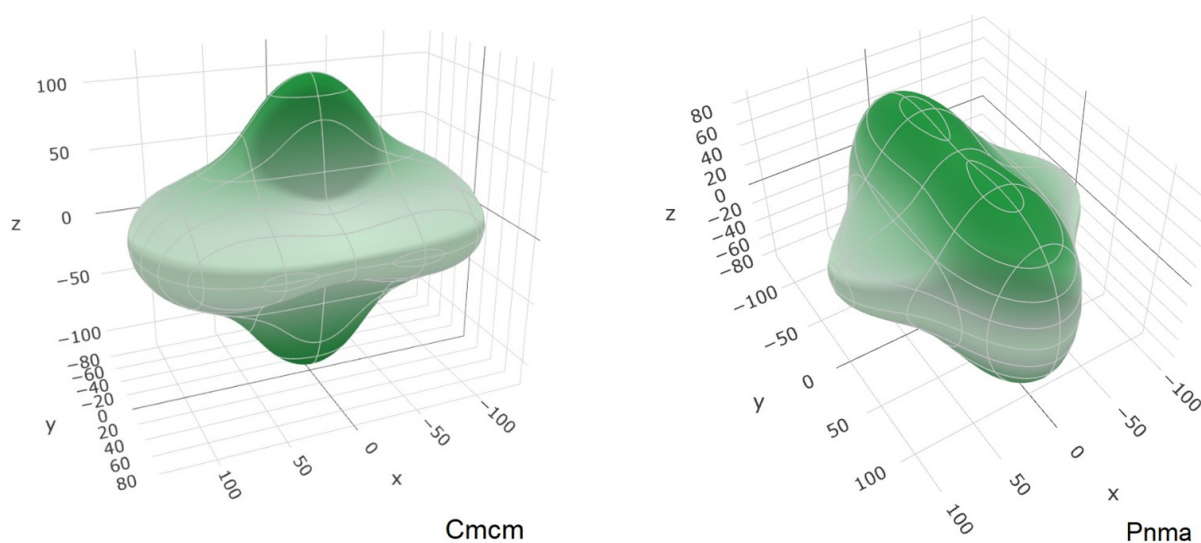
Figure S2. Dependence of the *Young*'s modulus in GPa on the crystallographic directions in EuSc-CuSe₃ for both possible orthorhombic structures.
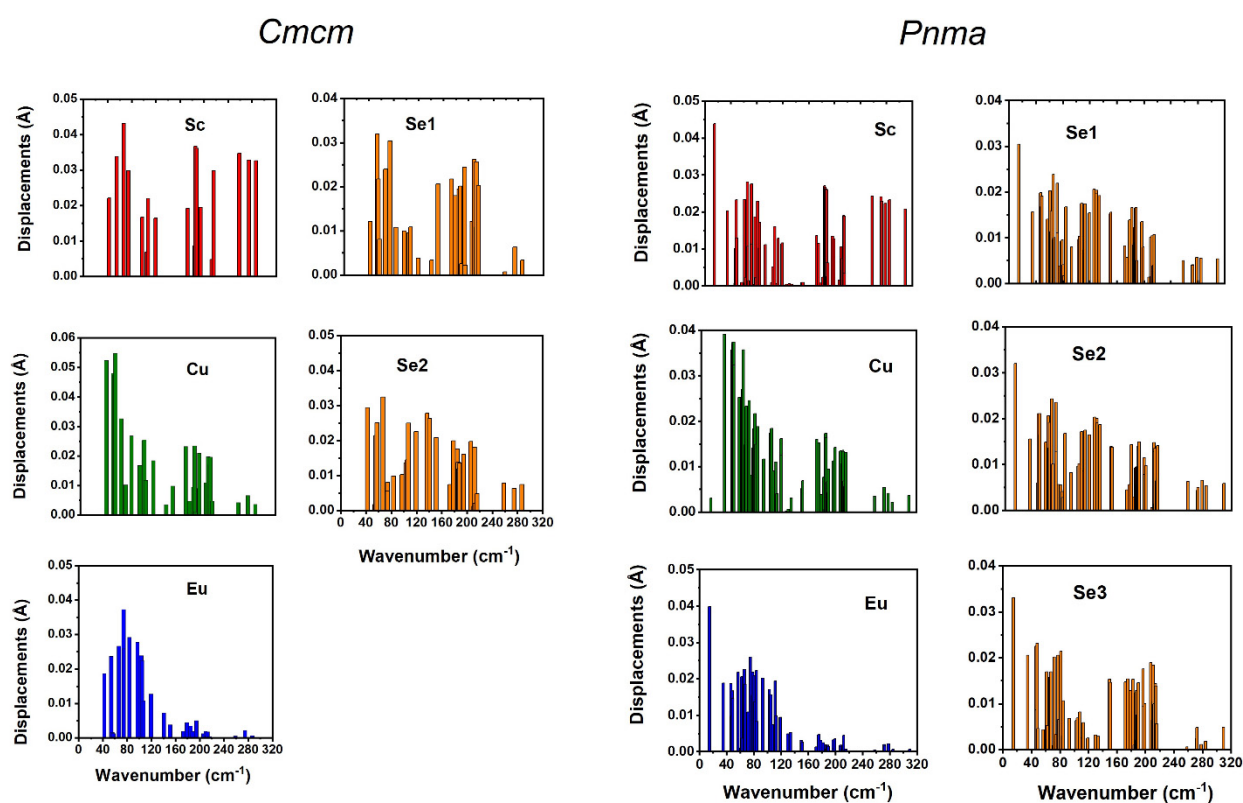

Figure S3. Displacement of ions at the phonon modes in the crystal structure of EuScCuSe₃ in both possible descriptions (*Cmcm* and *Pnma*).
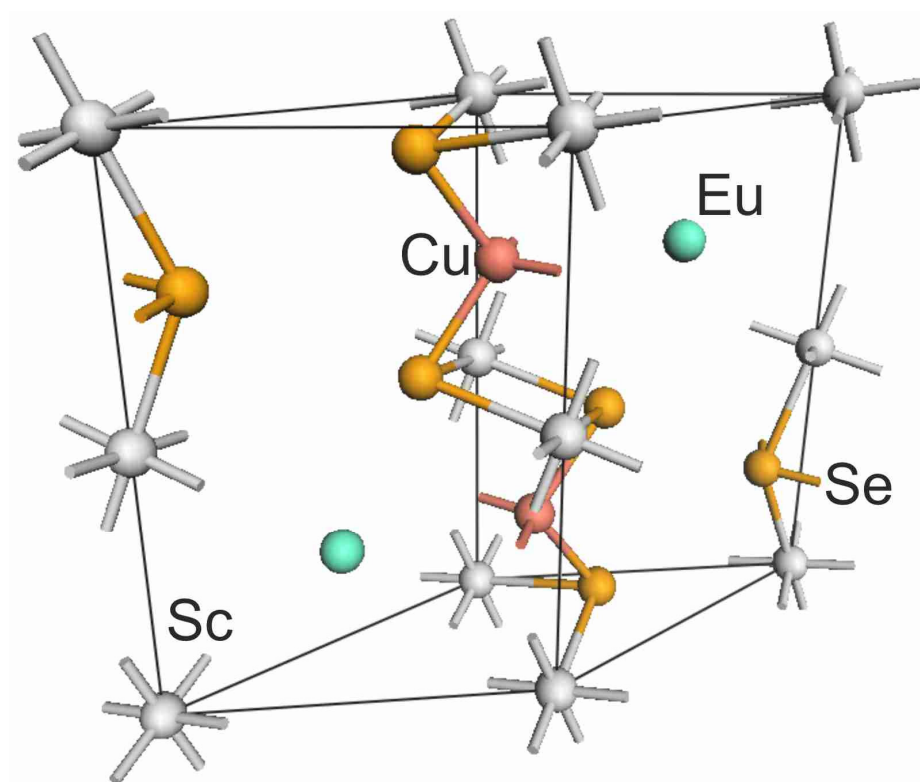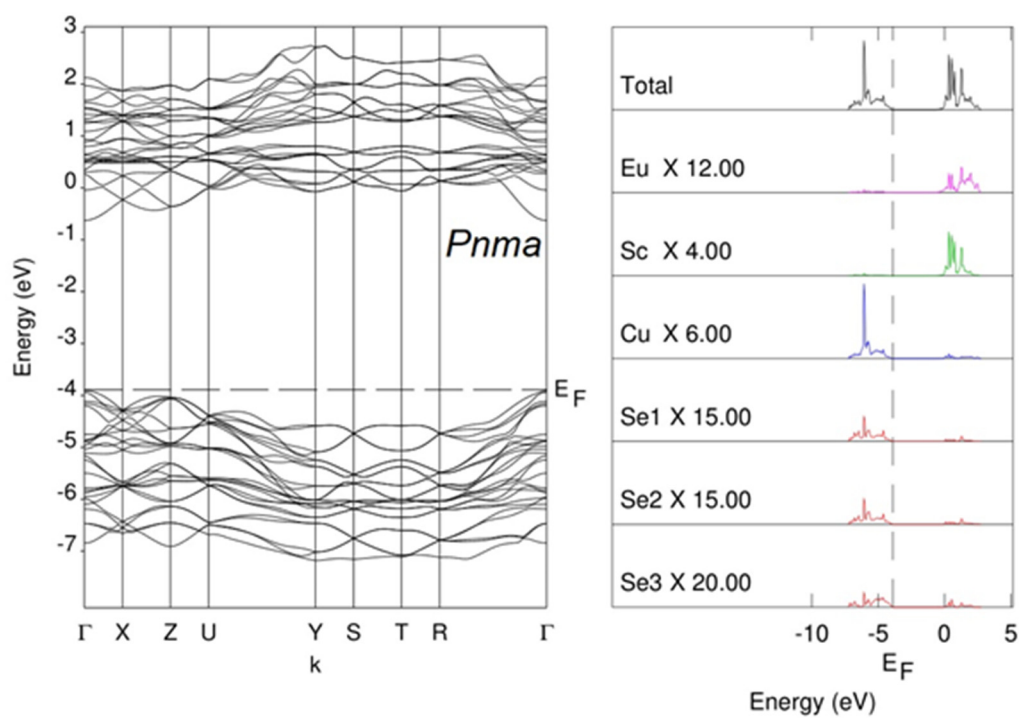
Figure S4. Primitive cell of EuScCuSe₃.

Figure S5. Band structure and electronic density of states of EuScCuSe₃ calculated for the dynamically unstable *Pnma* structure.

Table S1. Anisotropic displacement parameters in Å^2 of EuScCuSe$_3$.

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Eu	0.0164(6)	0.0213(7)	0.0320(8)	0	0	0
Sc	0.0137(16)	0.0143(15)	0.0159(17)	0	0	−0.0002(13)
Cu	0.0230(15)	0.0255(16)	0.0241(16)	0	0	0
Se1	0.0152(11)	0.0203(11)	0.0219(12)	0	0	0
Se2	0.0185(8)	0.0190(9)	0.0222(10)	0	0	−0.0016(6)

Table S2. Main bond lengths in Å of EuScCuSe$_3$.

Eu—Se1^{ii}	2×3.0605(19)	Sc—Se1^{i}	2×2.7401(8)	Cu—Se1^{ii}	2×2.449(2)
Eu—Se2^{ii}	4×3.1711(14)	Sc—Se2^{i}	4×2.7579(10)	Cu—Se2	2×2.428(2)
<Eu—Se>	3.1342	<Sc—Se>	2.7520	<Cu—Se>	2.4385

Symmetry codes EuScCuSe$_3$: (i) −0.5+x, −0.5+y, z; (ii) −0.5+x, 0.5+y, z; (iii) 0.5+x, −0.5+y, z; (iv) −0.5+x, 0.5−y, −z; (v) −x, −y, −0.5+z; (vi) 0.5+x, 0.5+y, z; (vii) −0.5−x, 0.5+y, 0.5−z; (viii) 0.5−x, 0.5+y, 0.5−z; (ix) −x, y, 0.5−z.

Table S3. Geometric parameters for EuScCuSe$_3$.

Atoms 1,2,3	Angle 1,2,3 /°	Atoms 1,2,3	Angle 1,2,3 /°
Se2^{iii}—Sc—Se2^{i}	92.62(4)	Se1—Eu—Se2^{ix}	86.80(3)
Se2^{iv}—Sc—Se2^{i}	87.38(4)	Se1—Eu—Se2	139.79(3)
Se1^{v}—Sc—Se2^{iv}	93.05(5)	Se1—Eu—Se1	81.32(6)
Se1^{v}—Sc—Se2^{iii}	86.95(5)	Se2—Cu—Se2^{ix}	108.68(12)
Se2^{ix}—Eu—Se2	76.92(5)	Se1^{ii}—Cu—Se2	109.79(3)
Se2^{ix}—Eu—Se2^{ix}	77.93(4)	Se1^{ii}—Cu—Se1^{vi}	109.01(14)
Se2^{ix}—Eu—Se2	124.38(6)		

Table S4. Wavenumbers in cm^{-1} and types of the phonon modes at the Γ-point for EuScCuSe$_3$ in the *Cmcm* structure. The intensity of the Raman modes was calculated for λ = 532 nm and T = 298 K.

wavenumber, cm^{-1} type	IR active/inactive	IR intensity, a.u.	Raman active/inactive	Raman intensity, relative units	participating ions
42.3B_{1u}	A	35.28	I		Eu, Sc^S, Cu^S, Se1, Se2^S
53.7B_{1g}	I	0	A	1000	Eu^S, Cu^S, Se1^S,
55.4B_{2u}	A	18.31	I		Sc^S, Cu^S, Se1^S, Se2^S
57.3B_{2g}	I	0	A	87.60	Cu^S, Se1^W, Se2^S
66.7A_{g}	I	0	A	169.13	Eu^S, Cu^S, Se1^S, Se2
66.9A_{u}	I	0	I		Sc^S, Se2^S
74.0B_{2g}	I	0	A	31.80	Eu^S, Cu^W, Se2^W
74.3B_{1u}	A	34.48	I		Eu^S, Sc^S, Cu, Se1^S, Se2^W
83.8B_{1g}	I	0	A	83.90	Eu^S, Cu^S, Se1, Se2^W
97.2B_{2u}	A	44.2	I		Eu^S, Sc, Cu, Se1, Se2
103.3A_{g}	I	0	A	122.47	Eu^S, Cu^S, Se1^W, Se2
104.6B_{3u}	A	190.65	I		Eu^S, Sc^W, Cu^S, Se1^W, Se2
107.1B_{1u}	A	87.97	I		Eu, Sc^S, Cu, Se1, Se2^S
119.5B_{3u}	A	109.68	I		Eu, Sc, Cu, Se2^S
136.8B_{3g}	I	0	A	37.97	Se2^S
140.7B_{1g}	I	0	A	2.21	Eu^W, Se2^S
151.0B_{2g}	I	0	A	1.78	Cu^W, Se1^S, Se2^S

wavenumber, cm^{-1}	type	IR active/inactive	IR intensity, a.u.	Raman active/inactive	Raman intensity, relative units	participating ions
172.7B_{3u}	A		12.99I			Sc, Cu^S, Se1^S, Se2^W
178.8A_{g}	I		0A		116.72	Se1, Se2
184.9B_{3u}	A		1.44I			Sc^W, Cu^W, Se1, Se2
185.7A_{u}	I		0I			Sc^S, Se2
187.1A_{g}	I		0A		28.63	Cu^S, Se1^S, Se2
188.3B_{2u}	A		1143.54I			Sc^S, Se2
194.3B_{2g}	I		0A		37.61	Eu^W, Cu^W, Se1^S, Se2
194.8B_{1u}	A		474.57I			Sc, Cu^S, Se2
205.9A_{g}	I		0A		215.74	Cu, Se1, Se2
209.5B_{1g}	I		0A		9.34	Cu, Se1^S
212.1B_{2g}	I		0A		18.56	Cu, Se1, Se2
212.8B_{2u}	A		129.89I			Cu, Se1^S
216.2B_{1u}	A		601.66I			Sc^S, Se1^S
258.7B_{1u}	A		67.47I			Sc^S, Se2^W
274.6B_{3u}	A		390.67I			Sc^S, Cu^W, Se1^W, Se2^W
286.7B_{3u}	A		36.18I			Sc^S, Se2^W

Note: Superscripts "S" and "W" in the last column denote strong and weak ion displacements in this mode, respectively. If the displacement is more or equal 0.02 Å, it is denoted as "S"; if the displacement is 0.005–0.01 Å, it is denoted as "W"; if the displacement is <0.005 Å, the ion is omitted from consideration.

Table S5. Wavenumbers in cm^{-1} and types of the phonon modes at the Γ-point for EuScCuSe₃ in the *Pnma* structure. The intensity of the Raman modes was calculated for λ = 532 nm and T = 298 K.

wavenumber, cm^{-1}	type	IR		Raman		participating ions
		active/inactive	intensity, a.u.	active/inactive	intensity, relative units	
14.7A_{g}	I		0A		25.23	Eu^S, Sc^S, Se1^S, Se2^S, Se3^S
34.9B_{1g}	I		0A		0.06	Eu, Sc^S, Cu^S, Se1, Se2, Se3^S
46.5A_{u}	I		0I			Eu, Cu^S, Se1^W, Se2^W, Se3^S
47.0A_{g}	I		0A		7.28	Eu^W, Sc, Cu^S, Se1, Se2^S, Se3^W
48.3B_{2u}	A		17.08I			Sc^S, Cu^S, Se1, Se2, Se3
48.6B_{3g}	I		0A		1000	Eu, Cu^S, Se3^S
48.9B_{3u}	A		88.54I			Eu, Sc, Cu^S, Se1, Se2^S
57.0B_{1u}	A		0.15I			Eu^S, Cu^S, Se1, Se2
61.1B_{1g}	I		0A		0.68	Sc^S, Cu, Se1^S, Se2^S, Se3
61.7B_{1u}	A		0.62I			Eu^S, Cu^S, Se1, Se2
62.8B_{2g}	I		0A		73.15	Cu^S, Se1, Se2, Se3^W
65.7A_{u}	I		0I			Sc^S, Se1^S, Se2^S
66.1B_{2g}	I		0A		0.79	Eu^S, Sc, Cu, Se1^W, Se2^W, Se3
66.9A_{g}	I		0A		133.36	Eu, Cu^S, Se1^W, Se2, Se3
71.7B_{3g}	I		0A		7.99	Sc^S, Se1^S, Se2^S
71.9B_{3u}	A		8.53I			Eu, Sc, Cu^S, Se1, Se2, Se3^S
75.2B_{2g}	I		0A		17.23	Eu^S, Cu^W, Se2^W
77.6B_{3u}	A		39.59I			Eu, Sc, Cu, Se1^W, Se2^W, Se3^S
78.7B_{3g}	I		0A		57.51	Eu^S, Cu, Se1^W, Se2^W, Se3^W
80.3A_{u}	I		0I			Eu^S, Cu^S, Se3^W
81.4A_{g}	I		0A		2.8	Eu, Sc^S, Cu, Se3^S
84.0B_{1g}	I		0A		1.02	Eu^S, Sc, Cu, Se1^W
84.4B_{2g}	I		0A		0.41	Eu^W, Sc, Cu, Se1, Se2, Se3
93.2B_{2u}	A		119.44I			Eu^S, Sc, Cu, Se1^W, Se2^W, Se3^W
103.2A_{g}	I		0A		94.69	Eu, Cu, Se1^W, Se2^W, Se3^W

$104.9B_{1u}$	A	370.45I		Eu, Sc^{W}, Cu, $Se1$, $Se2$, $Se3^{W}$
$107.6B_{3u}$	A	191.32I		Eu^{W}, Sc, Cu^{W}, $Se1$, $Se2$, $Se3^{W}$
$111.4B_{3u}$	A	0.05I		Eu, Cu, $Se1^{W}$, $Se2^{W}$
$112.7A_{g}$	I	0A	1.01	Eu^{W}, Sc, $Se1$, $Se2$, $Se3^{W}$
$119.1B_{2g}$	I	0A	0.45	Eu^{W}, Sc, Cu, $Se1$, $Se2$
$119.3B_{1u}$	A	229.2I		Eu^{W}, Sc, Cu, $Se1$, $Se2$
$126.1B_{2u}$	A	0.65I		$Se1^{S}$, $Se2^{S}$
$129.9B_{1g}$	I	0A	33.52	$Se1^{S}$, $Se2^{S}$
$130.0A_{u}$	I	0I		$Se1$, $Se2$
$134.1B_{3g}$	I	0A	1.16	Eu^{W}, $Se1$, $Se2$
$149.9B_{1u}$	A	0.16I		Cu^{W}, $Se1$, $Se2$, $Se3$
$151.2B_{2g}$	I	0A	1.66	Cu^{W}, $Se1$, $Se2$, $Se3$
$172.0B_{1u}$	A	22.03I		Sc, Cu, $Se1^{W}$, $Se3$
$175.4B_{2g}$	I	0A	0.89	Sc, Cu, $Se1^{W}$, $Se2^{W}$, $Se3$
$178.8A_{g}$	I	0A	94.17	$Se1$, $Se2$, $Se3$
$182.2B_{1u}$	A	4.02I		Cu^{W}, $Se1$, $Se3$
$184.6A_{u}$	I	0I		Sc^{S}, $Se1^{W}$, $Se2^{W}$
$185.7B_{3g}$	I	0A	0.25	Sc^{S}, $Se1^{W}$, $Se2^{W}$
$185.7B_{3u}$	A	261.78I		Sc^{W}, Cu, $Se1$, $Se3$
$186.3A_{g}$	I	0A	19.72	Sc^{W}, Cu, $Se1$, $Se2^{W}$, $Se3$
$187.1B_{2u}$	A	2231.26I		Sc^{S}, $Se1^{W}$, $Se2^{W}$
$187.8B_{1g}$	I	0A	0.1	Sc^{S}, $Se1^{W}$, $Se2^{W}$
$187.8B_{2g}$	I	0A	4.39	Sc^{W}, Cu^{W}, $Se1$, $Se2^{W}$, $Se3$
$188.7B_{3u}$	A	32.53I		$Se1$, $Se2$, $Se3^{W}$
$189.7B_{1u}$	A	0.32I		Sc^{W}, Cu^{W}, $Se1^{W}$, $Se2$, $Se3$
$196.7B_{2g}$	I	0A	17.99	Cu^{W}, $Se1^{W}$, $Se2$, $Se3$
$196.9A_{g}$	I	0A	50.86	Sc, Cu, $Se1$, $Se2^{W}$, $Se3^{W}$
$199.2B_{3u}$	A	776.9I		Sc, Cu, $Se1^{W}$, $Se2^{W}$, $Se3^{W}$
$207.6A_{u}$	I	0I		Cu, $Se3$
$207.6B_{3g}$	I	0A	5.99	Cu, $Se3$
$210.2A_{g}$	I	0A	106.79	Sc, Cu, $Se1^{W}$, $Se2$, $Se3^{W}$
$210.5B_{1u}$	A	0.36I		Cu, $Se1$, $Se2$, $Se3$
$211.0B_{2u}$	A	299.08I		Cu, $Se3$
$211.2B_{1g}$	I	0A	0.57	Cu, $Se3$
$212.1B_{3u}$	A	235.06I		Sc^{W}, Cu^{W}, $Se1$, $Se2$, $Se3^{W}$
$214.0B_{3u}$	A	837.3I		Sc, Cu^{W}, $Se2^{W}$, $Se3$
$215.0A_{g}$	I	0A	20.41	Sc, Cu^{W}, $Se2^{W}$, $Se3$
$215.4B_{2g}$	I	0A	17.73	Cu, $Se1$, $Se2$, $Se3^{W}$
$258.2B_{3u}$	A	129.34I		Sc^{S}, $Se2^{W}$,
$272.1B_{2g}$	I	0A	0.62	Sc^{S}
$272.6B_{1u}$	A	714.67I		Sc^{S}, Cu^{W}, $Se2^{W}$
$278.5A_{g}$	I	0A	2.9	Sc^{S}, $Se1^{W}$, $Se2^{W}$
$284.5B_{1u}$	A	140.62I		Sc^{S}, $Se1^{W}$, $Se2^{W}$
$309.3B_{2g}$	I	0A	0.05	Sc^{S}, $Se1^{W}$, $Se2^{W}$

Note: Superscripts "S" and "W" in the last column denote strong and weak ion displacements in this mode, respectively. If the displacement is more or equal 0.02 Å, it is denoted as "S"; if the displacement is 0.005–0.01 Å, it is denoted as "W"; if the displacement is <0.005 Å, the ion is omitted from consideration.