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$Cs_3Sm_7Se_{12}$

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ(Sm–Se) = 0.001 Å; disorder in main residue; R factor = 0.035; wR factor = 0.072; data-to-parameter ratio = 29.7.

The title compound, tricaesium heptasamarium(III) dodecaselenide, is setting a new starting point for realization of the channel structure of the $Cs_3M_7Se_{12}$ series, now with M = Sm, Gd–Er. This $Cs_3Y_7Se_{12}$-type arrangement is structurally based on the Z-type sesquiselenides M_2Se_3 adopting the Sc_2S_3 structure. Thus, the structural set-up of $Cs_3Sm_7Se_{12}$ consists of edge- and vertex-connected $[SmSe_6]^{9-}$ octahedra [$d_{\varnothing}(Sm^{3+} - Se^{2-})$ = 2.931 Å], forming a rock-salt-related network $[Sm_7Se_{12}]^{3-}$ with channels along [001] that are apt to take up monovalent cations (here Cs^+) with coordination numbers of 7 + 1 for one and of 6 for the second cation. The latter cation has a trigonal–prismatic coordination and shows half-occupancy, resulting in an impossible short distance [2.394 (4) Å] between symmetrically coupled Cs^+ cations of the same kind. While one Sm atom occupies *Wyckoff* position 2b with site symmetry ..2/m, all other 11 crystallographically different atoms (namely 2 × Cs, 3 × Sm and 6 × Se) are located at *Wyckoff* positions 4g with site symmetry ..m.

Related literature

For prototypic $Cs_3Y_7Se_{12}$ or $Rb_3Yb_7Se_{12}$, see: Folchnandt & Schleid (1996); Kim *et al.* (1996). For other representatives of the $A_3M_7Ch_{12}$ series, see: Folchnandt & Schleid (1997, 1998, 2000); Tougaît *et al.* (2001); Lissner *et al.* (2002). A detailed description of the relation between the crystal structures of the $Cs_3M_7Se_{12}$ series and Z-type Sc_2Ch_3 (Dismukes & White, 1964) is provided by Folchnandt & Schleid (1998).

Experimental

Crystal data

$Cs_3Sm_7Se_{12}$
M_r = 2398.70
Orthorhombic, $Pnnm$
a = 13.0387 (9) Å
b = 26.6742 (19) Å
c = 4.2351 (3) Å
V = 1472.95 (18) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 32.19 mm^{-1}
T = 293 K
0.10 × 0.07 × 0.05 mm

Data collection

Stoe IPDS-I diffractometer
Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 1999)
T_{min} = 0.115, T_{max} = 0.216
15080 measured reflections
2135 independent reflections
1587 reflections with $I > 2\sigma(I)$
R_{int} = 0.065

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.072
S = 0.97
2135 reflections
72 parameters
$\Delta\rho_{max}$ = 2.09 e Å^{-3}
$\Delta\rho_{min}$ = −1.78 e Å^{-3}

Table 1
Selected bond lengths (Å).

Cs1—Se4^i	3.6071 (12)	Cs1—Se1	4.5421 (14)
Cs1—Se4^{ii}	3.6071 (12)	Cs2—Se2^{ii}	3.5286 (16)
Cs1—Se6^{ii}	3.7129 (12)	Cs2—Se2^i	3.5286 (16)
Cs1—Se6^i	3.7129 (12)	Cs2—Se2^v	3.6917 (17)
Cs1—Se3^{iii}	3.7639 (14)	Cs2—Se2^{vi}	3.6917 (17)
Cs1—Se5^i	3.8053 (12)	Cs2—Se5^{iii}	3.719 (2)
Cs1—Se5^{ii}	3.8053 (12)	Cs2—Se6^{iii}	3.924 (2)

Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, z+\frac{1}{2}$; (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, z-\frac{1}{2}$; (iii) $-x+1, -y+1, -z$; (iv) $-x+1, -y, -z$; (v) $x+\frac{1}{2}, -y+\frac{1}{2}, -z-\frac{1}{2}$; (vi) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *DIF4* (Stoe & Cie, 1992); cell refinement: *DIF4*; data reduction: *REDU4* (Stoe & Cie, 1992); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2561).

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supporting information

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$Cs_3Sm_7Se_{12}$

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S1. Comment

$Cs_3Sm_7Se_{12}$ crystallizes isotypically to the large family of ternary $A_3M_7Ch_{12}$ representatives with a channel-like structure. For *Ch* = S, *A* = K, Rb, *M* = Er, see: Lissner *et al.* (2002); for *Ch* = Se, *A* = Rb, *M* = Dy, Yb, see: Folchnandt & Schleid (2000), Kim *et al.* (1996); for *Ch* = Se, *A* = Cs, *M* = Y, Gd – Er, see: Folchnandt & Schleid (1996, 1997, 1998); for *Ch* = Te, *A* = Cs, *M* = Sm, Gd, Tb, see: Tougaît *et al.* (2001).

In the title compound, $[SmSe_6]^{9-}$ octahedra ($d(Sm^{3+}–Se^{2-})$ = 2.8578 (9)–3.0614 (13) Å) are connected via edges and corners to form a $[Sm_7Se_{12}]^{3-}$ network with triple-channels occupied by Cs^+ cations (Fig. 1). This network represents a defect rock-salt-type structure strongly related to that of the *Z*-type sesquiselenides M_2Se_3 (Dismukes & White, 1964) according to the formula $[\square]_4[M]_8[Se]_{12}$. In tricaesium heptasamarium(III) dodecaselenide three Cs^+ cations replace one Sm^{3+} for charge balance. The triple-channels are arranged in a herringbone pattern and run through the structure parallel to [001]. They are filled with two crystallographically different Cs^+ cations (Fig. 2). While $Cs1^+$ exhibits a coordination number of 7+*1* with an extra secondary contact ($d(Cs1^+–Se^{2-})$ = 3.6071 (12)–3.8053 (12) Å and 4.5421 (14) Å; Fig. 2, *left*), the $Cs2^+$ cations have only six selenide anions as nearest neighbours in the shape of a trigonal prism ($d(Cs2^+–Se^{2-})$ = 3.5286 (16) – 3.924 (2) Å; Fig. 2, *right*). Owing to the very close distances between these $Cs2^+$ cations ($d(Cs2^+\cdots Cs2^+)$ = 2.394 (4) Å) only a half-occupation of this position is possible (Fig. 2, *right* and Fig. 3) and stoichiometrically meaningful.

S2. Experimental

Yellow, transparent, needle-shaped single crystals of $Cs_3Sm_7Se_{12}$ were obtained as the main product of a reaction between 0.10 g Sm, 0.08 g Se and 0.50 g CsCl added as flux and caesium source upon heating at 1073 K for 10 days in a sealed, evacuated fused-silica vessel.

S3. Refinement

In the final difference Fourier map the highest peak is 1.24 Å away from Se2 and the deepest hole is located 0.83 Å away from Sm2.

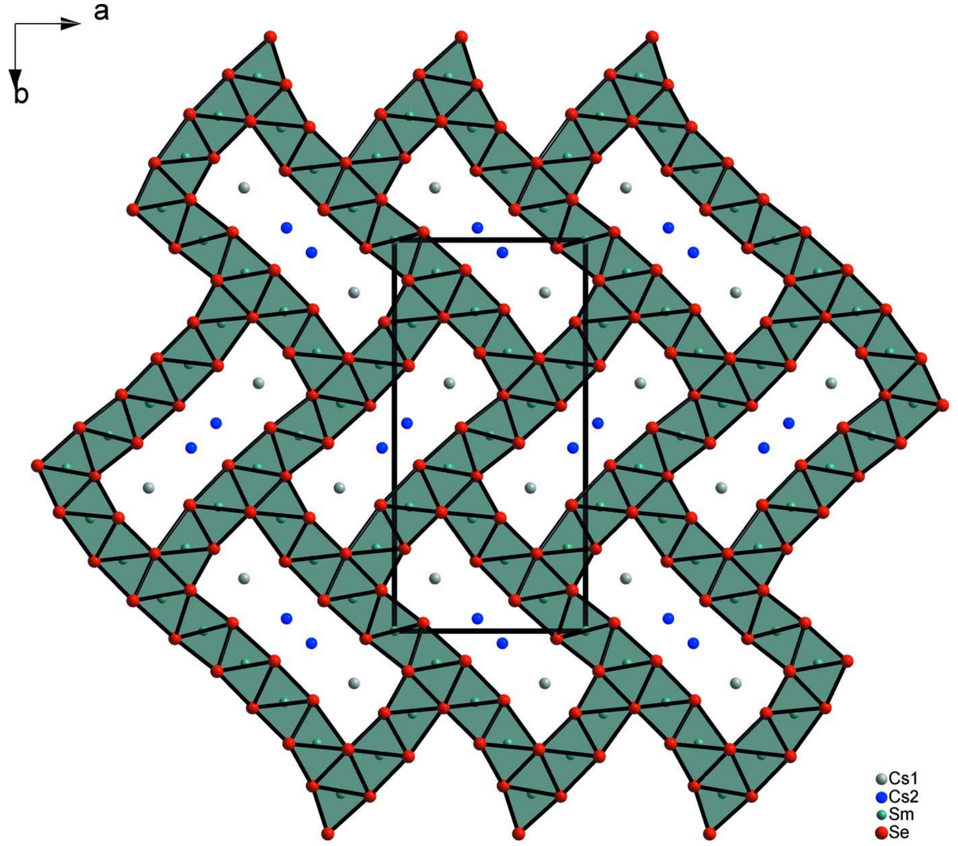

Figure 1

Channel-structure representation of $Cs_3Sm_7Se_{12}$ as octahedral framework with indicated unit cell.

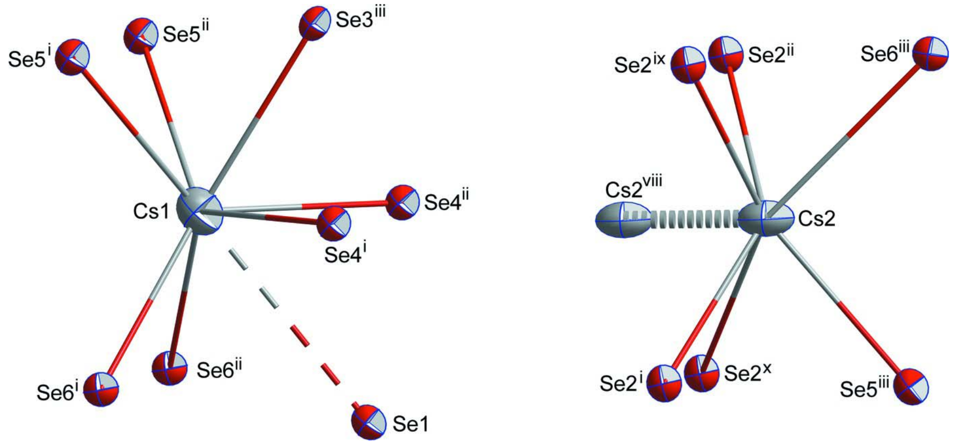

Figure 2

Coordination spheres of the Cs1$^+$ (*left*) and Cs2$^+$ (*right*) cations in $Cs_3Sm_7Se_{12}$. Displacement ellipsoids are drawn at the 90% probability level. Symmetry codes: (i) -*x*+1/2, *y*-1/2, *z*+1/2; (ii) -*x*+1/2, *y*-1/2, *z*-1/2; (iii) -*x*+1, -*y*+1, -*z*; (viii) -*x*+1, -*y*, -*z*; (ix) *x*+1/2, -*y*+1/2, -*z*-1/2; (x) *x*+1/2, -*y*+1/2, -*z*+1/2.

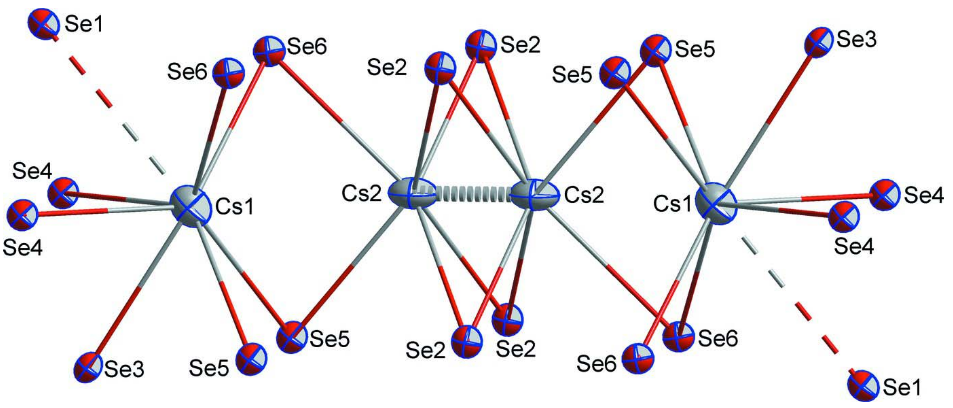

Figure 3

Interplay of the Cs$^+$ cations situated in the triple-channels of the crystal structure of $Cs_3Sm_7Se_{12}$. Displacement ellipsoids are drawn at the 90% probability level.

tricaesium heptasamarium(III) dodecaselenide

Crystal data

$Cs_3Sm_7Se_{12}$
M_r = 2398.70
Orthorhombic, *Pnnm*
Hall symbol: -P 2 2n
a = 13.0387 (9) Å
b = 26.6742 (19) Å
c = 4.2351 (3) Å
V = 1472.95 (18) Å^3
Z = 2
$F(000)$ = 2014
D_x = 5.408 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71069 Å
Cell parameters from 5000 reflections
θ = 2.1–29.3°
μ = 32.19 mm^{-1}
T = 293 K
Needle, yellow
0.10 × 0.07 × 0.05 mm

Data collection

Stoe IPDS-I diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
imaging plate detector system scans
Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 1999)
T_{min} = 0.115, T_{max} = 0.216
15080 measured reflections
2135 independent reflections
1587 reflections with $I > 2\sigma(I)$
R_{int} = 0.065
θ_{max} = 29.0°, θ_{min} = 2.8°
$h = -17 \rightarrow 17$
$k = -36 \rightarrow 36$
$l = -5 \rightarrow 5$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.072
S = 0.97
2135 reflections
72 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0371P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.014
$\Delta\rho_{max}$ = 2.09 e Å^{-3}
$\Delta\rho_{min}$ = −1.78 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00017 (4)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of F^2 > 2sigma(F^2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cs1	0.28796 (6)	0.36600 (3)	0.0000	0.0252 (2)	
Cs2	0.56532 (14)	0.03154 (7)	0.0000	0.0311 (5)	0.50
Sm1	0.0000	0.0000	0.5000	0.0124 (2)	
Sm2	0.21848 (5)	0.08314 (2)	0.0000	0.01316 (15)	
Sm3	0.40590 (4)	0.71214 (2)	0.0000	0.01224 (15)	
Sm4	0.07792 (5)	0.68240 (2)	0.0000	0.01271 (15)	
Se1	0.25592 (8)	0.19644 (4)	0.0000	0.0125 (3)	
Se2	0.12980 (9)	0.57736 (4)	0.0000	0.0142 (3)	
Se3	0.43019 (9)	0.60350 (4)	0.0000	0.0129 (3)	
Se4	0.05307 (8)	0.78890 (4)	0.0000	0.0133 (3)	
Se5	0.15051 (9)	0.98065 (4)	0.0000	0.0142 (3)	
Se6	0.42742 (9)	0.82140 (4)	0.0000	0.0133 (3)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cs1	0.0214 (4)	0.0295 (4)	0.0247 (6)	−0.0002 (3)	0.000	0.000
Cs2	0.0266 (9)	0.0273 (9)	0.0393 (14)	0.0114 (7)	0.000	0.000
Sm1	0.0147 (4)	0.0109 (4)	0.0116 (6)	−0.0030 (3)	0.000	0.000
Sm2	0.0153 (3)	0.0135 (3)	0.0107 (4)	−0.0027 (2)	0.000	0.000
Sm3	0.0137 (3)	0.0117 (3)	0.0113 (4)	−0.0018 (2)	0.000	0.000
Sm4	0.0131 (3)	0.0130 (3)	0.0121 (4)	0.0034 (2)	0.000	0.000
Se1	0.0123 (5)	0.0153 (5)	0.0101 (7)	−0.0004 (4)	0.000	0.000
Se2	0.0147 (6)	0.0142 (5)	0.0137 (8)	0.0007 (4)	0.000	0.000
Se3	0.0154 (5)	0.0096 (5)	0.0138 (7)	0.0007 (4)	0.000	0.000
Se4	0.0144 (5)	0.0128 (5)	0.0126 (8)	0.0000 (4)	0.000	0.000
Se5	0.0155 (5)	0.0129 (5)	0.0141 (8)	−0.0004 (4)	0.000	0.000
Se6	0.0140 (5)	0.0134 (5)	0.0124 (8)	0.0008 (4)	0.000	0.000

Geometric parameters (Å, º)

Cs1—Se4$^{\text{i}}$	3.6071 (12)	Sm1—Se5$^{\text{xi}}$	2.9328 (8)
Cs1—Se4$^{\text{ii}}$	3.6071 (12)	Sm1—Se5$^{\text{xii}}$	2.9328 (8)
Cs1—Se6$^{\text{ii}}$	3.7129 (12)	Sm1—Se5$^{\text{xiii}}$	2.9328 (8)
Cs1—Se6$^{\text{i}}$	3.7129 (12)	Sm2—Se5$^{\text{xiii}}$	2.8738 (13)
Cs1—Se3$^{\text{iii}}$	3.7639 (14)	Sm2—Se2$^{\text{i}}$	2.9020 (10)

Cs1—Se5$^{\mathrm{i}}$	3.8053 (12)	Sm2—Se2$^{\mathrm{ii}}$	2.9020 (10)
Cs1—Se5$^{\mathrm{ii}}$	3.8053 (12)	Sm2—Se3$^{\mathrm{ii}}$	2.9217 (9)
Cs1—Se1	4.5421 (14)	Sm2—Se3$^{\mathrm{i}}$	2.9217 (9)
Cs1—Cs1$^{\mathrm{iv}}$	4.2351 (3)	Sm2—Se1	3.0614 (13)
Cs1—Cs1$^{\mathrm{v}}$	4.2351 (3)	Sm3—Se4$^{\mathrm{xiv}}$	2.8578 (9)
Cs2—Cs2$^{\mathrm{vi}}$	2.394 (4)	Sm3—Se4$^{\mathrm{xv}}$	2.8578 (9)
Cs2—Se2$^{\mathrm{ii}}$	3.5286 (16)	Sm3—Se3	2.9152 (13)
Cs2—Se2$^{\mathrm{i}}$	3.5286 (16)	Sm3—Se6	2.9279 (13)
Cs2—Se2$^{\mathrm{vii}}$	3.6917 (17)	Sm3—Se1$^{\mathrm{xvi}}$	3.0185 (9)
Cs2—Se2$^{\mathrm{viii}}$	3.6917 (17)	Sm3—Se1$^{\mathrm{xvii}}$	3.0185 (9)
Cs2—Se5$^{\mathrm{iii}}$	3.719 (2)	Sm4—Se4	2.8591 (13)
Cs2—Se6$^{\mathrm{iii}}$	3.924 (2)	Sm4—Se2	2.8823 (13)
Cs2—Sm2$^{\mathrm{vi}}$	4.1597 (18)	Sm4—Se6$^{\mathrm{xviii}}$	2.8888 (9)
Sm1—Se3$^{\mathrm{i}}$	2.9070 (11)	Sm4—Se6$^{\mathrm{xix}}$	2.8888 (9)
Sm1—Se3$^{\mathrm{ix}}$	2.9070 (11)	Sm4—Se1$^{\mathrm{xvii}}$	3.0526 (9)
Sm1—Se5$^{\mathrm{x}}$	2.9328 (8)	Sm4—Se1$^{\mathrm{xvi}}$	3.0526 (9)

Se4$^{\mathrm{i}}$—Cs1—Se4$^{\mathrm{ii}}$	71.90 (3)	Se2$^{\mathrm{ii}}$—Sm2—Se1	86.77 (3)
Se4$^{\mathrm{i}}$—Cs1—Se6$^{\mathrm{ii}}$	125.93 (3)	Se3$^{\mathrm{ii}}$—Sm2—Se1	85.54 (3)
Se4$^{\mathrm{ii}}$—Cs1—Se6$^{\mathrm{ii}}$	85.24 (2)	Se3$^{\mathrm{i}}$—Sm2—Se1	85.54 (3)
Se4$^{\mathrm{i}}$—Cs1—Se6$^{\mathrm{i}}$	85.24 (2)	Se4$^{\mathrm{xiv}}$—Sm3—Se4$^{\mathrm{xv}}$	95.63 (4)
Se4$^{\mathrm{ii}}$—Cs1—Se6$^{\mathrm{i}}$	125.93 (3)	Se4$^{\mathrm{xiv}}$—Sm3—Se3	85.26 (3)
Se6$^{\mathrm{ii}}$—Cs1—Se6$^{\mathrm{i}}$	69.55 (3)	Se4$^{\mathrm{xv}}$—Sm3—Se3	85.26 (3)
Se4$^{\mathrm{i}}$—Cs1—Se3$^{\mathrm{iii}}$	64.04 (3)	Se4$^{\mathrm{xiv}}$—Sm3—Se6	86.87 (3)
Se4$^{\mathrm{ii}}$—Cs1—Se3$^{\mathrm{iii}}$	64.04 (3)	Se4$^{\mathrm{xv}}$—Sm3—Se6	86.87 (3)
Se6$^{\mathrm{ii}}$—Cs1—Se3$^{\mathrm{iii}}$	143.874 (16)	Se3—Sm3—Se6	168.27 (4)
Se6$^{\mathrm{i}}$—Cs1—Se3$^{\mathrm{iii}}$	143.874 (16)	Se4$^{\mathrm{xiv}}$—Sm3—Se1$^{\mathrm{xvi}}$	171.05 (4)
Se4$^{\mathrm{i}}$—Cs1—Se5$^{\mathrm{i}}$	90.60 (2)	Se4$^{\mathrm{xv}}$—Sm3—Se1$^{\mathrm{xvi}}$	87.03 (2)
Se4$^{\mathrm{ii}}$—Cs1—Se5$^{\mathrm{i}}$	131.59 (3)	Se3—Sm3—Se1$^{\mathrm{xvi}}$	86.44 (3)
Se6$^{\mathrm{ii}}$—Cs1—Se5$^{\mathrm{i}}$	137.25 (3)	Se6—Sm3—Se1$^{\mathrm{xvi}}$	101.84 (3)
Se6$^{\mathrm{i}}$—Cs1—Se5$^{\mathrm{i}}$	95.72 (2)	Se4$^{\mathrm{xiv}}$—Sm3—Se1$^{\mathrm{xvii}}$	87.03 (2)
Se3$^{\mathrm{iii}}$—Cs1—Se5$^{\mathrm{i}}$	67.69 (3)	Se4$^{\mathrm{xv}}$—Sm3—Se1$^{\mathrm{xvii}}$	171.05 (4)
Se4$^{\mathrm{i}}$—Cs1—Se5$^{\mathrm{ii}}$	131.59 (3)	Se3—Sm3—Se1$^{\mathrm{xvii}}$	86.44 (3)
Se4$^{\mathrm{ii}}$—Cs1—Se5$^{\mathrm{ii}}$	90.60 (2)	Se6—Sm3—Se1$^{\mathrm{xvii}}$	101.84 (3)
Se6$^{\mathrm{ii}}$—Cs1—Se5$^{\mathrm{ii}}$	95.72 (2)	Se1$^{\mathrm{xvi}}$—Sm3—Se1$^{\mathrm{xvii}}$	89.10 (3)
Se6$^{\mathrm{i}}$—Cs1—Se5$^{\mathrm{ii}}$	137.25 (3)	Se4—Sm4—Se2	172.93 (4)
Se3$^{\mathrm{iii}}$—Cs1—Se5$^{\mathrm{ii}}$	67.69 (3)	Se4—Sm4—Se6$^{\mathrm{xviii}}$	87.59 (3)
Se5$^{\mathrm{i}}$—Cs1—Se5$^{\mathrm{ii}}$	67.63 (2)	Se2—Sm4—Se6$^{\mathrm{xviii}}$	97.20 (3)
Se2$^{\mathrm{ii}}$—Cs2—Se2$^{\mathrm{vii}}$	95.31 (3)	Se4—Sm4—Se6$^{\mathrm{xix}}$	87.59 (3)
Se2$^{\mathrm{i}}$—Cs2—Se2$^{\mathrm{vii}}$	141.35 (6)	Se2—Sm4—Se6$^{\mathrm{xix}}$	97.20 (3)
Se2$^{\mathrm{ii}}$—Cs2—Se2$^{\mathrm{viii}}$	141.35 (6)	Se6$^{\mathrm{xviii}}$—Sm4—Se6$^{\mathrm{xix}}$	94.28 (4)
Se2$^{\mathrm{i}}$—Cs2—Se2$^{\mathrm{viii}}$	95.31 (3)	Se4—Sm4—Se1$^{\mathrm{xvii}}$	87.63 (3)
Se2$^{\mathrm{vii}}$—Cs2—Se2$^{\mathrm{viii}}$	70.00 (4)	Se2—Sm4—Se1$^{\mathrm{xvii}}$	87.29 (3)
Se2$^{\mathrm{ii}}$—Cs2—Se5$^{\mathrm{iii}}$	138.46 (3)	Se6$^{\mathrm{xviii}}$—Sm4—Se1$^{\mathrm{xvii}}$	174.23 (4)
Se2$^{\mathrm{i}}$—Cs2—Se5$^{\mathrm{iii}}$	138.46 (3)	Se6$^{\mathrm{xix}}$—Sm4—Se1$^{\mathrm{xvii}}$	88.74 (2)
Se2$^{\mathrm{vii}}$—Cs2—Se5$^{\mathrm{iii}}$	72.81 (4)	Se4—Sm4—Se1$^{\mathrm{xvi}}$	87.63 (3)
Se2$^{\mathrm{viii}}$—Cs2—Se5$^{\mathrm{iii}}$	72.81 (4)	Se2—Sm4—Se1$^{\mathrm{xvi}}$	87.29 (3)
Se2$^{\mathrm{ii}}$—Cs2—Se6$^{\mathrm{iii}}$	70.80 (4)	Se6$^{\mathrm{xviii}}$—Sm4—Se1$^{\mathrm{xvi}}$	88.74 (2)

Se2^{i}—Cs2—Se6^{iii}	70.80 (4)
Se2^{vii}—Cs2—Se6^{iii}	141.36 (3)
Se2^{viii}—Cs2—Se6^{iii}	141.36 (3)
Se5^{iii}—Cs2—Se6^{iii}	93.63 (5)
Se3^{i}—Sm1—Se3^{ix}	180.000 (14)
Se3^{i}—Sm1—Se5^{x}	92.43 (3)
Se3^{ix}—Sm1—Se5^{x}	87.57 (3)
Se3^{i}—Sm1—Se5^{xi}	87.57 (3)
Se3^{ix}—Sm1—Se5^{xi}	92.43 (3)
Se5^{x}—Sm1—Se5^{xi}	180.00 (4)
Se3^{i}—Sm1—Se5^{xii}	92.43 (3)
Se3^{ix}—Sm1—Se5^{xii}	87.57 (3)
Se5^{x}—Sm1—Se5^{xii}	92.44 (3)
Se5^{xi}—Sm1—Se5^{xii}	87.56 (3)
Se3^{i}—Sm1—Se5^{xiii}	87.57 (3)
Se3^{ix}—Sm1—Se5^{xiii}	92.43 (3)
Se5^{x}—Sm1—Se5^{xiii}	87.56 (3)
Se5^{xi}—Sm1—Se5^{xiii}	92.44 (3)
Se5^{xii}—Sm1—Se5^{xiii}	180.0
Se5^{xiii}—Sm2—Se2^{i}	99.19 (3)
Se5^{xiii}—Sm2—Se2^{ii}	99.19 (3)
Se2^{i}—Sm2—Se2^{ii}	93.72 (4)
Se5^{xiii}—Sm2—Se3^{ii}	88.41 (3)
Se2^{i}—Sm2—Se3^{ii}	172.31 (4)
Se2^{ii}—Sm2—Se3^{ii}	86.18 (2)
Se5^{xiii}—Sm2—Se3^{i}	88.41 (3)
Se2^{i}—Sm2—Se3^{i}	86.18 (2)
Se2^{ii}—Sm2—Se3^{i}	172.31 (4)
Se3^{ii}—Sm2—Se3^{i}	92.90 (4)
Se5^{xiii}—Sm2—Se1	171.21 (4)
Se2^{i}—Sm2—Se1	86.77 (3)
Se6^{xix}—Sm4—Se1^{xvi}	174.23 (4)
Se1^{xvii}—Sm4—Se1^{xvi}	87.85 (3)
Sm3^{ii}—Se1—Sm3^{i}	89.10 (3)
Sm3^{ii}—Se1—Sm4^{i}	178.80 (4)
Sm3^{i}—Se1—Sm4^{i}	91.519 (12)
Sm3^{ii}—Se1—Sm4^{ii}	91.519 (12)
Sm3^{i}—Se1—Sm4^{ii}	178.80 (4)
Sm4^{i}—Se1—Sm4^{ii}	87.85 (3)
Sm3^{ii}—Se1—Sm2	91.46 (3)
Sm3^{i}—Se1—Sm2	91.46 (3)
Sm4^{i}—Se1—Sm2	89.55 (3)
Sm4^{ii}—Se1—Sm2	89.55 (3)
Sm4—Se2—Sm2^{xvii}	96.22 (3)
Sm4—Se2—Sm2^{xvi}	96.22 (3)
Sm2^{xvii}—Se2—Sm2^{xvi}	93.72 (4)
Sm1^{viii}—Se3—Sm3	167.99 (5)
Sm1^{viii}—Se3—Sm2^{xvi}	91.79 (3)
Sm3—Se3—Sm2^{xvi}	96.47 (3)
Sm1^{viii}—Se3—Sm2^{xvii}	91.79 (3)
Sm3—Se3—Sm2^{xvii}	96.47 (3)
Sm2^{xvi}—Se3—Sm2^{xvii}	92.90 (4)
Sm3^{xviii}—Se4—Sm3^{xix}	95.63 (4)
Sm3^{xviii}—Se4—Sm4	93.81 (3)
Sm3^{xix}—Se4—Sm4	93.81 (3)
Sm2^{xx}—Se5—Sm1^{xxi}	92.23 (3)
Sm2^{xx}—Se5—Sm1^{xx}	92.23 (3)
Sm1^{xxi}—Se5—Sm1^{xx}	92.44 (3)
Sm4^{xiv}—Se6—Sm4^{xv}	94.28 (4)
Sm4^{xiv}—Se6—Sm3	91.72 (3)
Sm4^{xv}—Se6—Sm3	91.72 (3)

Symmetry codes: (i) −*x*+1/2, *y*−1/2, *z*+1/2; (ii) −*x*+1/2, *y*−1/2, *z*−1/2; (iii) −*x*+1, −*y*+1, −*z*; (iv) *x*, *y*, *z*−1; (v) *x*, *y*, *z*+1; (vi) −*x*+1, −*y*, −*z*; (vii) *x*+1/2, −*y*+1/2, −*z*−1/2; (viii) *x*+1/2, −*y*+1/2, −*z*+1/2; (ix) *x*−1/2, −*y*+1/2, −*z*+1/2; (x) −*x*, −*y*+1, −*z*; (xi) *x*, *y*−1, *z*+1; (xii) −*x*, −*y*+1, −*z*+1; (xiii) *x*, *y*−1, *z*; (xiv) *x*+1/2, −*y*+3/2, −*z*+1/2; (xv) *x*+1/2, −*y*+3/2, −*z*−1/2; (xvi) −*x*+1/2, *y*+1/2, *z*−1/2; (xvii) −*x*+1/2, *y*+1/2, *z*+1/2; (xviii) *x*−1/2, −*y*+3/2, −*z*−1/2; (xix) *x*−1/2, −*y*+3/2, −*z*+1/2; (xx) *x*, *y*+1, *z*; (xxi) *x*, *y*+1, *z*−1.