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# A polymorph of $K_4Ge_4Se_{10}$

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Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(e–Ge) = 0.001 Å; $R$ factor = 0.041; $wR$ factor = 0.103; data-to-parameter ratio = 29.4.

A new monoclinic polymorph, $\beta$-$K_4Ge_4Se_{10}$ (tetrapotassium decaselenidotetragermanate), that crystallizes in space group $P2_1/c$ has been isolated. The structure contains isolated super-tetrahedral adamantane $[Ge_4Se_{10}]^{4-}$ clusters identical to those in the known $K_4Ge_4Se_{10}$ polymorph ($P2_1/m$), held together in in the crystal structure by ionic interaction with the $K^+$ ions. The adamantane unit, $[Ge_4Se_{10}]^{4-}$, is formed by corner-sharing of four $GeSe_4$ tetrahedra, with average Ge—Se distances of 2.378 and 2.281 Å for $(Ge—Se)_{endo}$ and $(Ge—Se)_{exo}$, respectively. There are four crystallographically distinct $K^+$ ions in $\beta$-$K_4Ge_4Se_{10}$ having coordination numbers of 5, 7 and 8 (× 2), with K—Se distances in the range 2.986 (2)–3.888 (1) Å, while the coordination numbers of the three unique $K^+$ ions in the known $K_4Ge_4Se_{10}$ ($P2_1/m$) vary between 5 and 7. Besides the differences in coordination numbers of $K^+$ ions, the two polymorphs also exhibit a different packing of the adamantane units.

## Related literature

For the first polymorph ($P2_1/m$) of this composition, see: Eisenmann & Hansa (1993); for preparation, see: Wachhold & Kanatzidis (2000); Wachhold *et al.* (2000).

## Experimental

*Crystal data*

| | |
|---|---|
| $K_4Ge_4Se_{10}$ | $b$ = 9.7047 (8) Å |
| $M_r$ = 1236.36 | $c$ = 23.184 (2) Å |
| Monoclinic, $P2_1/c$ | $\beta$ = 94.508 (2)° |
| $a$ = 9.9796 (8) Å | $V$ = 2238.4 (3) Å$^3$ |
| $Z$ = 4 | $T$ = 100 (2) K |
| Mo $K\alpha$ radiation | 0.26 × 0.12 × 0.06 mm |
| $\mu$ = 22.31 mm$^{-1}$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area detector diffractometer | 19344 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | 4823 independent reflections |
| $T_{min}$ = 0.054, $T_{max}$ = 0.262 | 3896 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.069 |

*Refinement*

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.042 | 164 parameters |
| $wR(F^2)$ = 0.103 | $\Delta\rho_{max}$ = 1.72 e Å$^{-3}$ |
| $S$ = 1.04 | $\Delta\rho_{min}$ = −1.47 e Å$^{-3}$ |
| 4823 reflections | |

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Ge1—Se7$^{i}$ | 2.2492 (10) | Ge3—Se9 | 2.1288 (9) |
| Ge1—Se3 | 2.3105 (10) | Ge3—Se5$^{ii}$ | 2.3795 (10) |
| Ge1—Se8$^{ii}$ | 2.3583 (10) | Ge3—Se7 | 2.4092 (10) |
| Ge1—Se2$^{i}$ | 2.4943 (11) | Ge3—Se1 | 2.5131 (10) |
| Ge2—Se5 | 2.2366 (9) | Ge4—Se1 | 2.2335 (9) |
| Ge2—Se4 | 2.2613 (9) | Ge4—Se6$^{ii}$ | 2.3735 (9) |
| Ge2—Se8$^{iii}$ | 2.3769 (10) | Ge4—Se2 | 2.3755 (10) |
| Ge2—Se6 | 2.5384 (10) | Ge4—Se10 | 2.4238 (10) |

Symmetry codes: (i) $x-1, y, z$; (ii) $x, y+1, z$; (iii) $x+1, y, z$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2005); 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: WM2110).

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# supplementary materials

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# A polymorph of $K_4Ge_4Se_{10}$

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## Comment

The structure determination of $K_4Ge_4Se_{10}$ was first carried out by Eisenmann and Hansa (1993). The compound was synthesized by stoichiometric combination of elements in an evacuated graphitized silica ampoule at 1073 K. It crystallizes in space group $P2_1/m$ with cell parameters a = 10.202 (6) Å, b = 11.544 (6) Å, c = 9.806 (6) Å, β = 90.6 (1)°, V = 1154.8 Å$^3$. Wachhold & Kanatzidis (2000) reported the synthesis of $K_4Ge_4Se_{10}$ starting with $K_2Se$, Ge and Se, following the same route by which we have synthesized $K_4Ge_4Se_{10}$ and determined its crystal structure at 100 K, which reveals that the cell pararmeters are different from those reported by Eisenmann and Hansa (1993). The present β-structure crystallizes in the monoclinic system but with a different space group ($P2_1/c$); although there is an obvious metric relationship between the unit cells of the two structures, their symmetries do not allow to transform one structure into another.

Complementary views of the two polymorphs are given in Fig. 1. The structure of β-$K_4Ge_4Se_{10}$ contains isolated adamantane-like $[Ge_4Se_{10}]^{4-}$ units formed by four corner-shared $GeSe_4$ tetrahedra similar to $K_4Ge_4Se_{10}$—$P2_1/m$. However, these units are arranged differently in the two polymorphs. In both the structures, anionic adamantane units are stacked one over the other along the c- and *b* axis for $K_4Ge_4Se_{10}$—$P2_1/m$ and β-$K_4Ge_4Se_{10}$, respectively, held together by $K^+$ cations to form a column. Such columns are placed side by side in a layer like arrangement parallel to the *ac*- and *ab*-plane, for $K_4Ge_4Se_{10}$—$P2_1/m$ and β-$K_4Ge_4Se_{10}$, respectively. In $K_4Ge_4Se_{10}$—$P2_1/m$ the adamantane units are arranged such that $[Ge_4Se_{10}]^{4-}$ super tetrahedra are face up in one layer while they are placed face down in the next layer, which means the Se atoms are arranged in opposite directions in alternate layer. However, in the new polymorph, β-$K_4Ge_4Se_{10}$, the directions of the super tetrahedra (arrangement of Se atoms) alternate in every two layers (Fig. 1). Thus in β-$K_4Ge_4Se_{10}$ the *c* axis is approximately doubled the length of the *b* axis in $K_4Ge_4Se_{10}$—$P2_1/m$. The average Ge—Se distances ($d(\text{Ge—Se})_{endo}$ = 2.378, $d(\text{Ge—Se})_{exo}$ = 2.281 Å; Table 1) and the coordination number of the $K^+$ ions (CN = 5–8) of β-$K_4Ge_4Se_{10}$ are comparable to that of $K_4Ge_4Se_{10}$—$P2_1/m$.

## Experimental

The synthesis of β-$K_4Ge_4Se_{10}$ was carried out according to the reported procedure (Wachhold and Kanatzidis, 2000) but with a longer heating time, 48 hrs compared to 32 hrs. Orange needles of $K_4Ge_4Se_{10}$ were obtained from a solid-state reaction of $K_2Se$, Ge, and Se by mixing stoichiometric amounts (1:2:4) of 471.46 mg $K_2Se$ (prepared following the reported procedure, Wachhold and Kanatzidis, 2000), 435.6 mg Ge (Cerac, 99.999%), and 947.5 mg of Se (Aldrich, 99.5%). The reactants were loaded into a fused-silica tube under $N_2$ atmosphere in a glovebox. The tube was torch-sealed under vacuum and then placed in a furnace. The sample was heated to 1123 K at a rate of 35 K/h, held at 1123 k for 48 h, and then cooled to room temperature at a cooling rate of 35 K/h. The tube was opened under $N_2$, the product was ground and powder X-ray diffraction (PXRD) was carried out. The PXRD did not match with the simulated pattern from the atomic coordinates of known $K_4Ge_4Se_{10}$ ($P2_1/m$) (Eisenmann and Hansa, 1993). This led us to believe that the current product could be a polymorphic modification and subsequent single-crystal X-ray data revealed different cell parameters and structure solution indicated a new polymorph of $K_4Ge_4Se_{10}$ (in $P2_1/c$ space group, β-phase). The experimental PXRD was in good agreement with the simulated pattern of β-$K_4Ge_4Se_{10}$. The finely ground product was air sensitive and decomposed after 20–30 minutes of exposure in air. The single-crystal X-ray data was collected at low temperature (100 K) under a flow of liquid $N_2$ and the crystal did not show any sign of decomposition during the period of data collection. Although β-$K_4Ge_4Se_{10}$ was obtained following the reported synthesis procedure (Wachhold and Kanatzidis, 2000; Wachhold *et al.*, 2000), however, they did not report a detailed crystallographic characterization of their $K_4Ge_4Se_{10}$ and hence it is unclear whether they also obtained the same polymorph as reported here.

### Refinement

The highest peak and the deepest hole in the final Fourier map are 0.96 Å from Ge4 and 2.16 Å from Se10, respectively.

### Figures

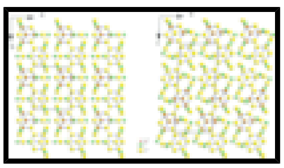

Fig. 1. Ball and stick representation of the packing of adamantane units in the two polymorphs: $K_4Ge_4Se_{10}$—$P2_1/m$ (left), β-$K_4Ge_4Se_{10}$ (right).

### tetrapotassium decaselenidotetragermanate

*Crystal data*

| | |
|---|---|
| $K_4Ge_4Se_{10}$ | $F_{000} = 2176$ |
| $M_r = 1236.36$ | $D_x = 3.669$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo *K*α radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 5478 reflections |
| $a = 9.9796$ (8) Å | θ = 2.3–28.3° |
| $b = 9.7047$ (8) Å | μ = 22.31 mm$^{-1}$ |
| $c = 23.184$ (2) Å | $T = 100$ (2) K |
| β = 94.508 (2)° | Irregular, orange |
| $V = 2238.4$ (3) Å$^3$ | 0.26 × 0.12 × 0.06 mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area detector diffractometer | 4823 independent reflections |
| Radiation source: fine-focus sealed tube | 3896 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.069$ |
| $T = 100(2)$ K | $\theta_{max} = 27.0°$ |
| φ and ω scans | $\theta_{min} = 1.8°$ |
| Absorption correction: multi-scan | $h = -12\rightarrow12$ |

| | |
|---|---|
| (SADABS; Sheldrick, 1996) | |
| $T_{min}$ = 0.054, $T_{max}$ = 0.262 | $k = -12 \rightarrow 12$ |
| 19344 measured reflections | $l = -29 \rightarrow 29$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | $w = 1/[\sigma^2(F_o^2) + (0.0511P)^2 + 6.4498P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)] = 0.042$ | $(\Delta/\sigma)_{max} < 0.001$ |
| $wR(F^2) = 0.103$ | $\Delta\rho_{max}$ = 1.72 e Å$^{-3}$ |
| $S = 1.04$ | $\Delta\rho_{min}$ = −1.47 e Å$^{-3}$ |
| 4823 reflections | Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| 164 parameters | Extinction coefficient: 0.00274 (12) |
| Primary atom site location: structure-invariant direct methods | |

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Ge1 | 0.05608 (7) | 0.77088 (7) | 0.37483 (3) | 0.01313 (18) |
| Ge2 | 0.84125 (7) | 0.08752 (7) | 0.37930 (3) | 0.01123 (17) |
| Ge3 | 0.72783 (7) | 0.75584 (7) | 0.30709 (3) | 0.01103 (17) |
| Ge4 | 0.73792 (7) | 0.77065 (7) | 0.47074 (3) | 0.01166 (17) |
| Se1 | 0.61852 (7) | 0.67644 (7) | 0.39529 (3) | 0.01264 (16) |
| Se2 | 0.96086 (7) | 0.68890 (7) | 0.46503 (3) | 0.01607 (18) |
| Se3 | 0.27457 (7) | 0.70088 (7) | 0.36540 (3) | 0.01702 (18) |
| Se4 | 0.83817 (7) | 0.32038 (7) | 0.37588 (3) | 0.01580 (18) |
| Se5 | 0.71983 (7) | 0.00069 (7) | 0.30260 (3) | 0.01306 (17) |
| Se6 | 0.72631 (7) | 0.01489 (7) | 0.46832 (3) | 0.01402 (17) |
| Se7 | 0.95299 (7) | 0.67889 (7) | 0.29407 (3) | 0.01363 (17) |
| Se8 | 0.06604 (7) | 0.01348 (7) | 0.37121 (3) | 0.01835 (18) |
| Se9 | 0.61132 (7) | 0.68152 (7) | 0.23270 (3) | 0.01788 (18) |
| Se10 | 0.62389 (7) | 0.69187 (7) | 0.55318 (3) | 0.01533 (17) |
| K1 | 0.84052 (16) | 0.61928 (16) | 0.65528 (7) | 0.0223 (4) |

| | | | | |
|---|---|---|---|---|
| K2 | 0.43100 (16) | 0.99728 (15) | 0.39359 (7) | 0.0163 (3) |
| K3 | 0.31801 (17) | 0.62238 (16) | 0.50104 (7) | 0.0221 (4) |
| K4 | 0.67980 (19) | 0.35486 (18) | 0.26208 (8) | 0.0288 (4) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ge1 | 0.0119 (4) | 0.0106 (3) | 0.0157 (4) | 0.0012 (3) | −0.0064 (3) | −0.0001 (3) |
| Ge2 | 0.0138 (4) | 0.0092 (3) | 0.0098 (4) | 0.0003 (3) | −0.0052 (3) | 0.0017 (3) |
| Ge3 | 0.0121 (3) | 0.0108 (3) | 0.0090 (4) | 0.0009 (3) | −0.0063 (3) | −0.0009 (3) |
| Ge4 | 0.0156 (4) | 0.0089 (3) | 0.0095 (4) | 0.0005 (3) | −0.0049 (3) | 0.0021 (3) |
| Se1 | 0.0125 (3) | 0.0121 (3) | 0.0126 (4) | −0.0010 (3) | −0.0044 (3) | 0.0010 (3) |
| Se2 | 0.0167 (4) | 0.0141 (3) | 0.0159 (4) | 0.0015 (3) | −0.0083 (3) | 0.0043 (3) |
| Se3 | 0.0112 (3) | 0.0153 (3) | 0.0232 (4) | 0.0008 (3) | −0.0072 (3) | −0.0019 (3) |
| Se4 | 0.0232 (4) | 0.0098 (3) | 0.0133 (4) | −0.0009 (3) | −0.0058 (3) | 0.0013 (3) |
| Se5 | 0.0165 (4) | 0.0111 (3) | 0.0105 (3) | 0.0018 (3) | −0.0065 (3) | 0.0016 (3) |
| Se6 | 0.0233 (4) | 0.0092 (3) | 0.0092 (3) | 0.0015 (3) | −0.0013 (3) | 0.0009 (3) |
| Se7 | 0.0133 (3) | 0.0132 (3) | 0.0136 (4) | 0.0016 (3) | −0.0038 (3) | −0.0020 (3) |
| Se8 | 0.0141 (4) | 0.0122 (3) | 0.0275 (4) | −0.0011 (3) | −0.0063 (3) | 0.0022 (3) |
| Se9 | 0.0203 (4) | 0.0177 (4) | 0.0137 (4) | 0.0009 (3) | −0.0113 (3) | −0.0038 (3) |
| Se10 | 0.0239 (4) | 0.0116 (3) | 0.0101 (3) | −0.0014 (3) | −0.0017 (3) | 0.0020 (3) |
| K1 | 0.0240 (8) | 0.0184 (8) | 0.0233 (9) | −0.0021 (7) | −0.0057 (7) | −0.0017 (7) |
| K2 | 0.0188 (8) | 0.0150 (7) | 0.0143 (8) | −0.0010 (6) | −0.0045 (6) | −0.0027 (6) |
| K3 | 0.0275 (9) | 0.0182 (8) | 0.0196 (8) | 0.0035 (7) | −0.0052 (7) | −0.0052 (7) |
| K4 | 0.0406 (11) | 0.0204 (8) | 0.0220 (9) | −0.0030 (7) | −0.0190 (8) | 0.0049 (7) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Ge1—Se7$^{i}$ | 2.2492 (10) | Se8—K1$^{v}$ | 3.7468 (18) |
| Ge1—Se3 | 2.3105 (10) | Se9—K4 | 3.3027 (19) |
| Ge1—Se8$^{ii}$ | 2.3583 (10) | Se9—K4$^{vi}$ | 3.368 (2) |
| Ge1—Se2$^{i}$ | 2.4943 (11) | Se9—K2$^{x}$ | 3.4284 (17) |
| Ge2—Se5 | 2.2366 (9) | Se9—K1$^{iv}$ | 3.5827 (19) |
| Ge2—Se4 | 2.2613 (9) | Se10—K1 | 3.1574 (17) |
| Ge2—Se8$^{iii}$ | 2.3769 (10) | Se10—K3 | 3.2640 (18) |
| Ge2—Se6 | 2.5384 (10) | Se10—K2$^{xi}$ | 3.3211 (17) |
| Ge3—Se9 | 2.1288 (9) | Se10—K3$^{v}$ | 3.3663 (17) |
| Ge3—Se5$^{ii}$ | 2.3795 (10) | K1—Se3$^{v}$ | 3.3341 (17) |
| Ge3—Se7 | 2.4092 (10) | K1—Se4$^{vii}$ | 3.3929 (19) |
| Ge3—Se1 | 2.5131 (10) | K1—Se9$^{xii}$ | 3.5827 (19) |
| Ge3—K1$^{iv}$ | 3.9678 (19) | K1—Se7$^{vii}$ | 3.6904 (17) |
| Ge4—Se1 | 2.2335 (9) | K1—Se8$^{v}$ | 3.7468 (18) |
| Ge4—Se6$^{ii}$ | 2.3735 (9) | K1—Se7$^{xii}$ | 3.8577 (17) |
| Ge4—Se2 | 2.3755 (10) | K1—Se5$^{xiii}$ | 3.8882 (19) |
| Ge4—Se10 | 2.4238 (10) | K1—Ge3$^{xii}$ | 3.9678 (19) |
| Ge4—K3$^{v}$ | 3.9173 (18) | K1—K3$^{v}$ | 4.499 (2) |

| | | | |
|---|---|---|---|
| Se1—K2 | 3.6314 (16) | K1—K2$^{xi}$ | 4.689 (2) |
| Se1—K3$^{v}$ | 3.7879 (18) | K1—K4$^{vii}$ | 5.021 (2) |
| Se2—Ge1$^{iii}$ | 2.4943 (11) | K2—Se6$^{ii}$ | 3.3035 (16) |
| Se2—K3$^{iii}$ | 3.6537 (18) | K2—Se10$^{xi}$ | 3.3211 (17) |
| Se3—K3 | 3.2317 (18) | K2—Se9$^{vi}$ | 3.4284 (17) |
| Se3—K2 | 3.3133 (16) | K2—Se8$^{ii}$ | 3.6418 (17) |
| Se3—K1$^{v}$ | 3.3341 (17) | K2—Se6$^{v}$ | 3.6768 (18) |
| Se3—K4$^{vi}$ | 3.374 (2) | K2—Se5$^{ii}$ | 3.7034 (18) |
| Se4—K4 | 2.9859 (17) | K2—K4$^{vi}$ | 3.941 (2) |
| Se4—K1$^{vii}$ | 3.3929 (19) | K2—K3 | 4.600 (2) |
| Se4—K3$^{v}$ | 3.4028 (19) | K2—K1$^{xi}$ | 4.689 (2) |
| Se5—Ge3$^{viii}$ | 2.3795 (10) | K2—K3$^{xi}$ | 4.990 (2) |
| Se5—K4 | 3.5773 (18) | K3—Se10$^{v}$ | 3.3663 (17) |
| Se5—K2$^{viii}$ | 3.7034 (18) | K3—Se4$^{v}$ | 3.4028 (19) |
| Se5—K1$^{ix}$ | 3.8882 (19) | K3—Se6$^{v}$ | 3.6252 (17) |
| Se6—Ge4$^{viii}$ | 2.3735 (9) | K3—Se2$^{i}$ | 3.6537 (18) |
| Se6—K2$^{viii}$ | 3.3035 (16) | K3—Se1$^{v}$ | 3.7879 (18) |
| Se6—K3$^{v}$ | 3.6252 (17) | K3—Ge4$^{v}$ | 3.9173 (18) |
| Se6—K2$^{v}$ | 3.6768 (18) | K3—K3$^{v}$ | 4.344 (3) |
| Se7—Ge1$^{iii}$ | 2.2492 (10) | K3—K1$^{v}$ | 4.499 (2) |
| Se7—K1$^{vii}$ | 3.6904 (17) | K3—K2$^{xi}$ | 4.990 (2) |
| Se7—K1$^{iv}$ | 3.8577 (17) | K4—Se9$^{x}$ | 3.368 (2) |
| Se8—Ge1$^{viii}$ | 2.3583 (10) | K4—Se3$^{x}$ | 3.374 (2) |
| Se8—Ge2$^{i}$ | 2.3769 (10) | K4—K2$^{x}$ | 3.941 (2) |
| Se8—K2$^{viii}$ | 3.6418 (17) | K4—K1$^{vii}$ | 5.021 (2) |
| Se7$^{i}$—Ge1—Se3 | 100.24 (4) | Se10—K1—K4$^{vii}$ | 148.33 (6) |
| Se7$^{i}$—Ge1—Se8$^{ii}$ | 112.61 (4) | Se3$^{v}$—K1—K4$^{vii}$ | 114.13 (4) |
| Se3—Ge1—Se8$^{ii}$ | 104.32 (4) | Se4$^{vii}$—K1—K4$^{vii}$ | 35.31 (3) |
| Se7$^{i}$—Ge1—Se2$^{i}$ | 113.08 (4) | Se9$^{xii}$—K1—K4$^{vii}$ | 114.14 (4) |
| Se3—Ge1—Se2$^{i}$ | 114.21 (4) | Se7$^{vii}$—K1—K4$^{vii}$ | 54.97 (3) |
| Se8$^{ii}$—Ge1—Se2$^{i}$ | 111.60 (4) | Se8$^{v}$—K1—K4$^{vii}$ | 76.87 (3) |
| Se5—Ge2—Se4 | 110.10 (4) | Se7$^{xii}$—K1—K4$^{vii}$ | 56.64 (3) |
| Se5—Ge2—Se8$^{iii}$ | 106.21 (4) | Se5$^{xiii}$—K1—K4$^{vii}$ | 91.81 (4) |
| Se4—Ge2—Se8$^{iii}$ | 108.04 (4) | Ge3$^{xii}$—K1—K4$^{vii}$ | 88.53 (4) |
| Se5—Ge2—Se6 | 106.89 (4) | K3$^{v}$—K1—K4$^{vii}$ | 126.72 (5) |
| Se4—Ge2—Se6 | 107.47 (4) | K2$^{xi}$—K1—K4$^{vii}$ | 124.61 (4) |
| Se8$^{iii}$—Ge2—Se6 | 118.02 (4) | Se6$^{ii}$—K2—Se3 | 122.37 (5) |
| Se9—Ge3—Se5$^{ii}$ | 106.77 (4) | Se6$^{ii}$—K2—Se10$^{xi}$ | 85.67 (4) |
| Se9—Ge3—Se7 | 104.41 (4) | Se3—K2—Se10$^{xi}$ | 140.62 (6) |
| Se5$^{ii}$—Ge3—Se7 | 109.42 (4) | Se6$^{ii}$—K2—Se9$^{vi}$ | 117.77 (5) |

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| Se9—Ge3—Se1 | 108.11 (4) | Se3—K2—Se9$^{vi}$ | 105.06 (4) |
| Se5$^{ii}$—Ge3—Se1 | 109.06 (4) | Se10$^{xi}$—K2—Se9$^{vi}$ | 80.26 (4) |
| Se7—Ge3—Se1 | 118.41 (3) | Se6$^{ii}$—K2—Se1 | 66.48 (3) |
| Se9—Ge3—K1$^{iv}$ | 63.87 (4) | Se3—K2—Se1 | 59.48 (3) |
| Se5$^{ii}$—Ge3—K1$^{iv}$ | 70.55 (3) | Se10$^{xi}$—K2—Se1 | 151.02 (5) |
| Se7—Ge3—K1$^{iv}$ | 69.59 (3) | Se9$^{vi}$—K2—Se1 | 119.03 (5) |
| Se1—Ge3—K1$^{iv}$ | 170.69 (4) | Se6$^{ii}$—K2—Se8$^{ii}$ | 155.99 (5) |
| Se1—Ge4—Se6$^{ii}$ | 111.61 (4) | Se3—K2—Se8$^{ii}$ | 63.83 (3) |
| Se1—Ge4—Se2 | 105.31 (4) | Se10$^{xi}$—K2—Se8$^{ii}$ | 79.71 (4) |
| Se6$^{ii}$—Ge4—Se2 | 112.11 (4) | Se9$^{vi}$—K2—Se8$^{ii}$ | 78.53 (3) |
| Se1—Ge4—Se10 | 103.52 (4) | Se1—K2—Se8$^{ii}$ | 123.18 (4) |
| Se6$^{ii}$—Ge4—Se10 | 107.97 (4) | Se6$^{ii}$—K2—Se6$^{v}$ | 88.25 (4) |
| Se2—Ge4—Se10 | 116.00 (4) | Se3—K2—Se6$^{v}$ | 85.24 (4) |
| Se1—Ge4—K3$^{v}$ | 70.00 (3) | Se10$^{xi}$—K2—Se6$^{v}$ | 67.14 (3) |
| Se6$^{ii}$—Ge4—K3$^{v}$ | 165.69 (4) | Se9$^{vi}$—K2—Se6$^{v}$ | 136.72 (5) |
| Se2—Ge4—K3$^{v}$ | 80.24 (3) | Se1—K2—Se6$^{v}$ | 102.59 (4) |
| Se10—Ge4—K3$^{v}$ | 58.62 (3) | Se8$^{ii}$—K2—Se6$^{v}$ | 68.58 (3) |
| Ge4—Se1—Ge3 | 105.83 (4) | Se6$^{ii}$—K2—Se5$^{ii}$ | 66.18 (3) |
| Ge4—Se1—K2 | 84.27 (3) | Se3—K2—Se5$^{ii}$ | 105.73 (4) |
| Ge3—Se1—K2 | 89.12 (3) | Se10$^{xi}$—K2—Se5$^{ii}$ | 111.23 (4) |
| Ge4—Se1—K3$^{v}$ | 76.36 (3) | Se9$^{vi}$—K2—Se5$^{ii}$ | 63.77 (3) |
| Ge3—Se1—K3$^{v}$ | 133.58 (4) | Se1—K2—Se5$^{ii}$ | 65.82 (3) |
| K2—Se1—K3$^{v}$ | 136.35 (4) | Se8$^{ii}$—K2—Se5$^{ii}$ | 137.13 (5) |
| Ge4—Se2—Ge1$^{iii}$ | 111.12 (3) | Se6$^{v}$—K2—Se5$^{ii}$ | 154.29 (5) |
| Ge4—Se2—K3$^{iii}$ | 161.33 (4) | Se6$^{ii}$—K2—K4$^{vi}$ | 132.29 (6) |
| Ge1$^{iii}$—Se2—K3$^{iii}$ | 79.56 (4) | Se3—K2—K4$^{vi}$ | 54.62 (4) |
| Ge1—Se3—K3 | 91.87 (4) | Se10$^{xi}$—K2—K4$^{vi}$ | 128.04 (5) |
| Ge1—Se3—K2 | 99.19 (4) | Se9$^{vi}$—K2—K4$^{vi}$ | 52.69 (4) |
| K3—Se3—K2 | 89.29 (4) | Se1—K2—K4$^{vi}$ | 79.42 (4) |
| Ge1—Se3—K1$^{v}$ | 88.32 (4) | Se8$^{ii}$—K2—K4$^{vi}$ | 71.29 (4) |
| K3—Se3—K1$^{v}$ | 86.48 (4) | Se6$^{v}$—K2—K4$^{vi}$ | 132.68 (5) |
| K2—Se3—K1$^{v}$ | 171.51 (4) | Se5$^{ii}$—K2—K4$^{vi}$ | 69.90 (4) |
| Ge1—Se3—K4$^{vi}$ | 98.40 (4) | Se6$^{ii}$—K2—K3 | 90.20 (4) |
| K3—Se3—K4$^{vi}$ | 160.00 (5) | Se3—K2—K3 | 44.63 (3) |
| K2—Se3—K4$^{vi}$ | 72.21 (4) | Se10$^{xi}$—K2—K3 | 117.56 (5) |
| K1$^{v}$—Se3—K4$^{vi}$ | 110.82 (5) | Se9$^{vi}$—K2—K3 | 148.88 (5) |
| Ge2—Se4—K4 | 98.50 (4) | Se1—K2—K3 | 57.59 (3) |
| Ge2—Se4—K1$^{vii}$ | 99.76 (4) | Se8$^{ii}$—K2—K3 | 80.00 (4) |
| K4—Se4—K1$^{vii}$ | 103.65 (5) | Se6$^{v}$—K2—K3 | 50.46 (3) |
| Ge2—Se4—K3$^{v}$ | 98.03 (4) | Se5$^{ii}$—K2—K3 | 123.40 (4) |
| K4—Se4—K3$^{v}$ | 118.50 (5) | K4$^{vi}$—K2—K3 | 98.95 (5) |

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| K1$^{vii}$—Se4—K3$^{v}$ | 130.79 (4) | Se6$^{ii}$—K2—K1$^{xi}$ | 124.08 (4) |
| Ge2—Se5—Ge3$^{viii}$ | 109.10 (3) | Se3—K2—K1$^{xi}$ | 112.76 (4) |
| Ge2—Se5—K4 | 83.63 (4) | Se10$^{xi}$—K2—K1$^{xi}$ | 42.26 (3) |
| Ge3$^{viii}$—Se5—K4 | 166.82 (4) | Se9$^{vi}$—K2—K1$^{xi}$ | 49.44 (3) |
| Ge2—Se5—K2$^{viii}$ | 87.00 (4) | Se1—K2—K1$^{xi}$ | 166.05 (5) |
| Ge3$^{viii}$—Se5—K2$^{viii}$ | 89.49 (3) | Se8$^{ii}$—K2—K1$^{xi}$ | 51.60 (3) |
| K4—Se5—K2$^{viii}$ | 94.72 (4) | Se6$^{v}$—K2—K1$^{xi}$ | 87.58 (4) |
| Ge2—Se5—K1$^{ix}$ | 128.71 (4) | Se5$^{ii}$—K2—K1$^{xi}$ | 108.43 (4) |
| Ge3$^{viii}$—Se5—K1$^{ix}$ | 74.21 (3) | K4$^{vi}$—K2—K1$^{xi}$ | 86.66 (4) |
| K4—Se5—K1$^{ix}$ | 95.33 (4) | K3—K2—K1$^{xi}$ | 126.65 (5) |
| K2$^{viii}$—Se5—K1$^{ix}$ | 143.75 (4) | Se6$^{ii}$—K2—K3$^{xi}$ | 46.55 (3) |
| Ge4$^{viii}$—Se6—Ge2 | 105.79 (3) | Se3—K2—K3$^{xi}$ | 161.67 (5) |
| Ge4$^{viii}$—Se6—K2$^{viii}$ | 90.04 (4) | Se10$^{xi}$—K2—K3$^{xi}$ | 40.30 (3) |
| Ge2—Se6—K2$^{viii}$ | 91.69 (4) | Se9$^{vi}$—K2—K3$^{xi}$ | 93.19 (4) |
| Ge4$^{viii}$—Se6—K3$^{v}$ | 166.30 (4) | Se1—K2—K3$^{xi}$ | 112.99 (4) |
| Ge2—Se6—K3$^{v}$ | 87.68 (4) | Se8$^{ii}$—K2—K3$^{xi}$ | 119.72 (4) |
| K2$^{viii}$—Se6—K3$^{v}$ | 92.03 (4) | Se6$^{v}$—K2—K3$^{xi}$ | 80.20 (4) |
| Ge4$^{viii}$—Se6—K2$^{v}$ | 88.32 (3) | Se5$^{ii}$—K2—K3$^{xi}$ | 83.63 (4) |
| Ge2—Se6—K2$^{v}$ | 165.46 (4) | K4$^{vi}$—K2—K3$^{xi}$ | 143.28 (5) |
| K2$^{viii}$—Se6—K2$^{v}$ | 91.75 (4) | K3—K2—K3$^{xi}$ | 117.06 (4) |
| K3$^{v}$—Se6—K2$^{v}$ | 78.09 (4) | K1$^{xi}$—K2—K3$^{xi}$ | 77.86 (3) |
| Ge1$^{iii}$—Se7—Ge3 | 98.20 (4) | Se3—K3—Se10 | 111.20 (6) |
| Ge1$^{iii}$—Se7—K1$^{vii}$ | 80.73 (4) | Se3—K3—Se10$^{v}$ | 82.19 (4) |
| Ge3—Se7—K1$^{vii}$ | 134.92 (4) | Se10—K3—Se10$^{v}$ | 98.16 (5) |
| Ge1$^{iii}$—Se7—K1$^{iv}$ | 125.24 (4) | Se3—K3—Se4$^{v}$ | 137.92 (6) |
| Ge3—Se7—K1$^{iv}$ | 74.58 (3) | Se10—K3—Se4$^{v}$ | 97.61 (4) |
| K1$^{vii}$—Se7—K1$^{iv}$ | 141.46 (3) | Se10$^{v}$—K3—Se4$^{v}$ | 124.39 (5) |
| Ge1$^{viii}$—Se8—Ge2$^{i}$ | 104.85 (4) | Se3—K3—Se6$^{v}$ | 87.29 (4) |
| Ge1$^{viii}$—Se8—K2$^{viii}$ | 89.79 (3) | Se10—K3—Se6$^{v}$ | 81.47 (4) |
| Ge2$^{i}$—Se8—K2$^{viii}$ | 160.28 (4) | Se10$^{v}$—K3—Se6$^{v}$ | 168.57 (6) |
| Ge1$^{viii}$—Se8—K1$^{v}$ | 165.28 (5) | Se4$^{v}$—K3—Se6$^{v}$ | 66.81 (3) |
| Ge2$^{i}$—Se8—K1$^{v}$ | 88.51 (4) | Se3—K3—Se2$^{i}$ | 71.47 (4) |
| K2$^{viii}$—Se8—K1$^{v}$ | 78.78 (4) | Se10—K3—Se2$^{i}$ | 156.24 (5) |
| Ge3—Se9—K4 | 93.85 (4) | Se10$^{v}$—K3—Se2$^{i}$ | 105.56 (4) |
| Ge3—Se9—K4$^{vi}$ | 102.68 (4) | Se4$^{v}$—K3—Se2$^{i}$ | 70.12 (4) |
| K4—Se9—K4$^{vi}$ | 129.58 (4) | Se6$^{v}$—K3—Se2$^{i}$ | 75.01 (3) |
| Ge3—Se9—K2$^{x}$ | 153.05 (4) | Se3—K3—Se1$^{v}$ | 143.22 (5) |
| K4—Se9—K2$^{x}$ | 71.65 (4) | Se10—K3—Se1$^{v}$ | 79.53 (4) |
| K4$^{vi}$—Se9—K2$^{x}$ | 104.03 (4) | Se10$^{v}$—K3—Se1$^{v}$ | 61.20 (3) |
| Ge3—Se9—K1$^{iv}$ | 83.89 (4) | Se4$^{v}$—K3—Se1$^{v}$ | 69.98 (4) |
| K4—Se9—K1$^{iv}$ | 119.43 (5) | Se6$^{v}$—K3—Se1$^{v}$ | 129.49 (5) |

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| K4$^{vi}$—Se9—K1$^{iv}$ | 109.57 (5) | Se2$^{i}$—K3—Se1$^{v}$ | 113.06 (5) |
| K2$^{x}$—Se9—K1$^{iv}$ | 83.93 (4) | Se3—K3—Ge4$^{v}$ | 112.46 (5) |
| Ge4—Se10—K1 | 108.99 (5) | Se10—K3—Ge4$^{v}$ | 106.30 (4) |
| Ge4—Se10—K3 | 104.87 (4) | Se10$^{v}$—K3—Ge4$^{v}$ | 37.93 (2) |
| K1—Se10—K3 | 142.83 (5) | Se4$^{v}$—K3—Ge4$^{v}$ | 86.46 (4) |
| Ge4—Se10—K2$^{xi}$ | 96.19 (4) | Se6$^{v}$—K3—Ge4$^{v}$ | 153.08 (6) |
| K1—Se10—K2$^{xi}$ | 92.71 (4) | Se2$^{i}$—K3—Ge4$^{v}$ | 93.50 (4) |
| K3—Se10—K2$^{xi}$ | 98.54 (4) | Se1$^{v}$—K3—Ge4$^{v}$ | 33.65 (2) |
| Ge4—Se10—K3$^{v}$ | 83.45 (4) | Se3—K3—K3$^{v}$ | 99.58 (6) |
| K1—Se10—K3$^{v}$ | 87.13 (4) | Se10—K3—K3$^{v}$ | 50.10 (4) |
| K3—Se10—K3$^{v}$ | 81.84 (5) | Se10$^{v}$—K3—K3$^{v}$ | 48.06 (3) |
| K2$^{xi}$—Se10—K3$^{v}$ | 179.54 (5) | Se4$^{v}$—K3—K3$^{v}$ | 122.49 (6) |
| Se10—K1—Se3$^{v}$ | 83.82 (4) | Se6$^{v}$—K3—K3$^{v}$ | 130.41 (6) |
| Se10—K1—Se4$^{vii}$ | 113.87 (5) | Se2$^{i}$—K3—K3$^{v}$ | 153.60 (7) |
| Se3$^{v}$—K1—Se4$^{vii}$ | 116.80 (5) | Se1$^{v}$—K3—K3$^{v}$ | 59.34 (4) |
| Se10—K1—Se9$^{xii}$ | 80.14 (4) | Ge4$^{v}$—K3—K3$^{v}$ | 66.40 (4) |
| Se3$^{v}$—K1—Se9$^{xii}$ | 110.40 (5) | Se3—K3—K1$^{v}$ | 47.71 (3) |
| Se4$^{vii}$—K1—Se9$^{xii}$ | 131.67 (5) | Se10—K3—K1$^{v}$ | 131.72 (5) |
| Se10—K1—Se7$^{vii}$ | 138.23 (5) | Se10$^{v}$—K3—K1$^{v}$ | 44.51 (3) |
| Se3$^{v}$—K1—Se7$^{vii}$ | 59.50 (3) | Se4$^{v}$—K3—K1$^{v}$ | 127.26 (5) |
| Se4$^{vii}$—K1—Se7$^{vii}$ | 71.92 (4) | Se6$^{v}$—K3—K1$^{v}$ | 128.57 (5) |
| Se9$^{xii}$—K1—Se7$^{vii}$ | 128.77 (5) | Se2$^{i}$—K3—K1$^{v}$ | 68.47 (4) |
| Se10—K1—Se8$^{v}$ | 80.18 (4) | Se1$^{v}$—K3—K1$^{v}$ | 98.21 (4) |
| Se3$^{v}$—K1—Se8$^{v}$ | 161.84 (6) | Ge4$^{v}$—K3—K1$^{v}$ | 65.24 (3) |
| Se4$^{vii}$—K1—Se8$^{v}$ | 63.21 (3) | K3$^{v}$—K3—K1$^{v}$ | 86.98 (5) |
| Se9$^{xii}$—K1—Se8$^{v}$ | 75.27 (4) | Se3—K3—K2 | 46.08 (3) |
| Se7$^{vii}$—K1—Se8$^{v}$ | 131.15 (5) | Se10—K3—K2 | 77.01 (4) |
| Se10—K1—Se7$^{xii}$ | 130.48 (5) | Se10$^{v}$—K3—K2 | 117.23 (5) |
| Se3$^{v}$—K1—Se7$^{xii}$ | 131.87 (5) | Se4$^{v}$—K3—K2 | 118.23 (5) |
| Se4$^{vii}$—K1—Se7$^{xii}$ | 82.65 (4) | Se6$^{v}$—K3—K2 | 51.46 (3) |
| Se9$^{xii}$—K1—Se7$^{xii}$ | 57.56 (3) | Se2$^{i}$—K3—K2 | 90.73 (4) |
| Se7$^{vii}$—K1—Se7$^{xii}$ | 90.81 (4) | Se1$^{v}$—K3—K2 | 155.97 (5) |
| Se8$^{v}$—K1—Se7$^{xii}$ | 66.04 (3) | Ge4$^{v}$—K3—K2 | 154.80 (5) |
| Se10—K1—Se5$^{xiii}$ | 118.96 (5) | K3$^{v}$—K3—K2 | 100.70 (6) |
| Se3$^{v}$—K1—Se5$^{xiii}$ | 73.76 (4) | K1$^{v}$—K3—K2 | 93.54 (4) |
| Se4$^{vii}$—K1—Se5$^{xiii}$ | 127.01 (5) | Se3—K3—K2$^{xi}$ | 109.01 (5) |
| Se9$^{xii}$—K1—Se5$^{xiii}$ | 57.82 (3) | Se10—K3—K2$^{xi}$ | 41.16 (3) |
| Se7$^{vii}$—K1—Se5$^{xiii}$ | 71.91 (3) | Se10$^{v}$—K3—K2$^{xi}$ | 139.32 (5) |
| Se8$^{v}$—K1—Se5$^{xiii}$ | 121.81 (5) | Se4$^{v}$—K3—K2$^{xi}$ | 73.39 (4) |
| Se7$^{xii}$—K1—Se5$^{xiii}$ | 60.61 (3) | Se6$^{v}$—K3—K2$^{xi}$ | 41.42 (3) |
| Se10—K1—Ge3$^{xii}$ | 111.83 (5) | Se2$^{i}$—K3—K2$^{xi}$ | 115.10 (4) |

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| $Se3^{v}$—K1—$Ge3^{xii}$ | 107.08 (5) | $Se1^{v}$—K3—$K2^{xi}$ | 101.72 (4) |
| $Se4^{vii}$—K1—$Ge3^{xii}$ | 118.34 (4) | $Ge4^{v}$—K3—$K2^{xi}$ | 135.32 (4) |
| $Se9^{xii}$—K1—$Ge3^{xii}$ | 32.24 (2) | $K3^{v}$—K3—$K2^{xi}$ | 91.26 (5) |
| $Se7^{vii}$—K1—$Ge3^{xii}$ | 98.47 (4) | $K1^{v}$—K3—$K2^{xi}$ | 155.67 (5) |
| $Se8^{v}$—K1—$Ge3^{xii}$ | 86.93 (4) | K2—K3—$K2^{xi}$ | 62.94 (4) |
| $Se7^{xii}$—K1—$Ge3^{xii}$ | 35.83 (2) | Se4—K4—Se9 | 112.11 (5) |
| $Se5^{xiii}$—K1—$Ge3^{xii}$ | 35.24 (2) | Se4—K4—$Se9^{x}$ | 108.09 (6) |
| Se10—K1—$K3^{v}$ | 48.36 (3) | Se9—K4—$Se9^{x}$ | 108.77 (5) |
| $Se3^{v}$—K1—$K3^{v}$ | 45.81 (3) | Se4—K4—$Se3^{x}$ | 128.74 (6) |
| $Se4^{vii}$—K1—$K3^{v}$ | 101.35 (5) | Se9—K4—$Se3^{x}$ | 106.52 (5) |
| $Se9^{xii}$—K1—$K3^{v}$ | 119.14 (5) | $Se9^{x}$—K4—$Se3^{x}$ | 89.23 (4) |
| $Se7^{vii}$—K1—$K3^{v}$ | 89.99 (4) | Se4—K4—Se5 | 67.66 (4) |
| $Se8^{v}$—K1—$K3^{v}$ | 116.11 (5) | Se9—K4—Se5 | 173.44 (7) |
| $Se7^{xii}$—K1—$K3^{v}$ | 175.97 (5) | $Se9^{x}$—K4—Se5 | 65.76 (4) |
| $Se5^{xiii}$—K1—$K3^{v}$ | 115.98 (5) | $Se3^{x}$—K4—Se5 | 77.56 (4) |
| $Ge3^{xii}$—K1—$K3^{v}$ | 140.14 (5) | Se4—K4—$K2^{x}$ | 159.96 (7) |
| Se10—K1—$K2^{xi}$ | 45.02 (3) | Se9—K4—$K2^{x}$ | 55.66 (4) |
| $Se3^{v}$—K1—$K2^{xi}$ | 121.25 (5) | $Se9^{x}$—K4—$K2^{x}$ | 91.57 (4) |
| $Se4^{vii}$—K1—$K2^{xi}$ | 110.45 (5) | $Se3^{x}$—K4—$K2^{x}$ | 53.18 (4) |
| $Se9^{xii}$—K1—$K2^{xi}$ | 46.64 (3) | Se5—K4—$K2^{x}$ | 126.51 (5) |
| $Se7^{vii}$—K1—$K2^{xi}$ | 175.36 (5) | Se4—K4—$K1^{vii}$ | 41.05 (3) |
| $Se8^{v}$—K1—$K2^{xi}$ | 49.62 (3) | Se9—K4—$K1^{vii}$ | 101.91 (4) |
| $Se7^{xii}$—K1—$K2^{xi}$ | 85.61 (4) | $Se9^{x}$—K4—$K1^{vii}$ | 144.16 (5) |
| $Se5^{xiii}$—K1—$K2^{xi}$ | 103.70 (4) | $Se3^{x}$—K4—$K1^{vii}$ | 99.56 (5) |
| $Ge3^{xii}$—K1—$K2^{xi}$ | 76.90 (4) | Se5—K4—$K1^{vii}$ | 82.21 (4) |
| $K3^{v}$—K1—$K2^{xi}$ | 93.39 (4) | $K2^{x}$—K4—$K1^{vii}$ | 121.49 (5) |

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

Fig. 1