

Pentapotassium europium(III) dilithium decafluoride, $K_5EuLi_2F_{10}$

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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{Eu}-\text{F}) = 0.001$ Å; R factor = 0.021; wR factor = 0.039; data-to-parameter ratio = 49.9.

The title compound, $K_5EuLi_2F_{10}$, belongs to so-called self-activated materials containing lanthanoid ions within the matrix. A common feature of these systems is a large separation between the closest lanthanoid ions, which is one of the crucial factors governing the self-quenching of luminescence. The crystal structure of $K_5EuLi_2F_{10}$ is isotypic with other $K_5RELi_2F_{10}$ compounds ($RE = \text{Nd}, \text{Pr}$). As expected from the lanthanoid contraction, the unit-cell volume for crystal with Eu^{3+} ions is the smallest of the three structures. Accordingly, the corresponding interatomic $RE-RE$ distances are shorter. In the structure, distorted EuF_8 dodecahedra and two different LiF_4 tetrahedra, all with m symmetry, are present, forming sheets parallel to (100). The isolated EuF_8 dodecahedra exhibit a mean $\text{Eu}-\text{F}$ distance of 2.356 Å. The K^+ cations are located within and between the sheets, leading to highly irregular KF_x polyhedra ($x = 8-9$) around the alkali metal cations.

Related literature

The structure of the isotypic Nd analogue was reported by Hong & McCollum (1979); for the structure of the Pr analogue, see: Gagor (2009). For background to bond-valence calculations, see: Brown (1992, 2002); Mattausch *et al.* (1991). Synthetic details were described by Ryba-Romanowski *et al.* (2007).

Experimental

Crystal data

$K_5EuLi_2F_{10}$
 $M_r = 551.35$

Orthorhombic, $Pnma$
 $a = 20.5539$ (6) Å

$b = 7.7356$ (2) Å
 $c = 6.8721$ (2) Å
 $V = 1092.64$ (5) Å³
 $Z = 4$

Mo $K\alpha$ radiation
 $\mu = 7.75$ mm⁻¹
 $T = 295$ K
 $0.35 \times 0.20 \times 0.15$ mm

Data collection

Kuma KM-4 with CCD area-detector diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
 $T_{\min} = 0.146$, $T_{\max} = 0.310$

23852 measured reflections
4895 independent reflections
3564 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.021$
 $wR(F^2) = 0.039$
 $S = 0.83$
4895 reflections

98 parameters
 $\Delta\rho_{\text{max}} = 2.35$ e Å⁻³
 $\Delta\rho_{\text{min}} = -3.02$ e Å⁻³

Table 1

Selected bond lengths (Å).

Eu1—F5	2.2923 (11)	Li1—F6 ⁱⁱⁱ	1.804 (3)
Eu1—F2	2.3236 (11)	Li1—F1 ^{iv}	1.862 (3)
Eu1—F3 ⁱ	2.3262 (7)	Li1—F3 ^v	1.8669 (16)
Eu1—F1	2.3918 (10)	Li2—F7	1.801 (4)
Eu1—F4	2.3954 (7)	Li2—F4 ⁱⁱⁱ	1.817 (2)
Eu1—F8 ⁱⁱ	2.3996 (10)	Li2—F8	1.844 (3)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2006); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2269).

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Comment

Two different LiF_4 tetrahedra together with EuF_8 dodecahedra form sheets expanding perpendicular to [100]. Fig. 1 illustrates the crystal packing of $K_5EuLi_2F_{10}$ as seen down [001]. K1 atoms occupy cavities within the sheets and are surrounded by 9 F^- ions in a mean distance of 2.792 Å. Remaining potassium atoms are located between the sheets, leading to KF_9 and KF_8 polyhedra. The valence sums of K atoms are close to the formal charge of +1, with a slight tendency to over-bonding. The K2 ion in the $K_5EuLi_2F_{10}$ structure is slightly under-bonded ($S = 0.977$ v.u.), whereas the Li position is over-bonded, with a 15.6% higher bond-valence sum than those expected from the formal charge of +1.

Each EuF_8 dodecahedron is surrounded by twelve others with a shortest and longest Eu—Eu distance of 6.6968 (2) and 7.8353 (2) Å, respectively. The mean distance of Eu—Eu is 7.309 Å, with individual distances of 2×6.6968 (2), 2×6.8805 (2), 2×6.8721 (2), 2×7.7356 (2) and 4×7.8353 (2) Å. The bond valence sums of all metal atoms have been calculated from the received structure model on the basis of the bond-valence method (Brown, 1992, 2002; Mattausch *et al.*, 1991): Eu 2.81, K1 1.06, K2 1.00, K3 1.09 and Li 1.16 v.u. The Eu ion is slightly under-bonded. The lower value of Eu valence may be associated with the distorted surrounding of this cation. When such distortions occur, the equal-valence rule is not strictly obeyed (Brown, 1992).

Experimental

Preparation details were taken from Ryba-Romanowski *et al.* (2007). The $K_5EuLi_2F_{10}$ crystal was grown from commercially available KF, EuF_3 and LiF (Aldrich 99.99%, anhydrous) using the Bridgman method. The reagents were heated at 923 K (melting point 813 K) in a graphite crucible under argon atmosphere. The pulling rate was 1mm/h, the temperature gradient 100 %/cm.

Refinement

In the final Fourier map, the highest peak is 0.60 Å from atom Eu1 and the deepest hole is 0.63 Å from the same atom.

Figures

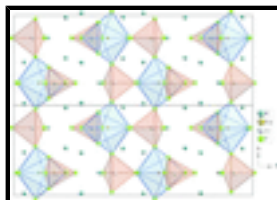


Fig. 1. Crystal packing in $K_5EuLi_2F_{10}$ as seen down the c axis. The thermal ellipsoids have been drawn at the 50% probability level.

Pentapotassium europium(III) dilithium decafluoride

Crystal data

$K_5EuLi_2F_{10}$	$F_{000} = 1016$
$M_r = 551.35$	$D_x = 3.352 \text{ Mg m}^{-3}$
Orthorhombic, $Pnma$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: -P 2ac 2n	Cell parameters from 12717 reflections
$a = 20.5539 (6) \text{ \AA}$	$\theta = 2.8\text{--}47.0^\circ$
$b = 7.7356 (2) \text{ \AA}$	$\mu = 7.75 \text{ mm}^{-1}$
$c = 6.8721 (2) \text{ \AA}$	$T = 295 \text{ K}$
$V = 1092.64 (5) \text{ \AA}^3$	Rectangular prism, colorless
$Z = 4$	$0.35 \times 0.20 \times 0.15 \text{ mm}$

Data collection

Kuma KM-4 with CCD area-detector diffractometer	4895 independent reflections
Radiation source: fine-focus sealed tube	3564 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.034$
Detector resolution: 1024x1024 with blocks 2x2, 33.133pixel/mm pixels mm^{-1}	$\theta_{\text{max}} = 47.2^\circ$
$T = 295 \text{ K}$	$\theta_{\text{min}} = 3.1^\circ$
ω scans	$h = -42 \rightarrow 27$
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	$k = -11 \rightarrow 15$
$T_{\text{min}} = 0.146$, $T_{\text{max}} = 0.310$	$l = -14 \rightarrow 9$
23852 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.02P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.021$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.039$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 0.83$	$\Delta\rho_{\text{max}} = 2.35 \text{ e \AA}^{-3}$
4895 reflections	$\Delta\rho_{\text{min}} = -3.02 \text{ e \AA}^{-3}$
98 parameters	Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0234 (3)

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 $F^2 > \sigma(F^2)$ 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.

To eliminate the weak reflections measured at high theta angles a 2theta limit was applied during structure refinement. The refinement on the whole data set (2theta = 47°) only slightly improved the standard deviations. Concluding, it was decided to refine the structure using a maximum measured 2theta limit. For completeness calculations the 2theta threshold was set to 28.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
K1	0.457104 (13)	0.97833 (4)	0.25084 (4)	0.01525 (4)
K2	0.282845 (14)	0.02578 (4)	0.42686 (4)	0.01675 (5)
K3	0.36036 (2)	0.2500	0.93720 (6)	0.01762 (7)
Eu1	0.106855 (4)	0.2500	0.236787 (10)	0.00739 (2)
Li1	0.92238 (15)	0.2500	0.9701 (4)	0.0131 (5)
Li2	0.67290 (16)	0.2500	0.8419 (5)	0.0143 (6)
F1	0.00915 (5)	0.2500	0.04773 (15)	0.01369 (18)
F2	0.01991 (5)	0.2500	0.45288 (15)	0.0174 (2)
F3	0.09032 (4)	0.96151 (9)	0.15506 (12)	0.01698 (15)
F4	0.14639 (4)	0.07571 (10)	0.49951 (11)	0.01549 (14)
F5	0.21739 (5)	0.2500	0.19250 (16)	0.0167 (2)
F6	0.37353 (6)	0.2500	0.31189 (16)	0.01580 (19)
F7	0.75888 (5)	0.2500	0.79160 (15)	0.0160 (2)
F8	0.63085 (5)	0.2500	0.60493 (14)	0.01447 (19)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K1	0.01483 (10)	0.01435 (10)	0.01657 (10)	−0.00139 (8)	−0.00065 (9)	−0.00117 (9)
K2	0.01782 (11)	0.01449 (11)	0.01795 (10)	0.00145 (9)	−0.00036 (9)	−0.00152 (9)
K3	0.0292 (2)	0.01074 (15)	0.01291 (14)	0.000	−0.00250 (14)	0.000
Eu1	0.00789 (3)	0.00732 (3)	0.00696 (3)	0.000	−0.00052 (3)	0.000
Li1	0.0131 (13)	0.0150 (14)	0.0112 (12)	0.000	0.0005 (11)	0.000
Li2	0.0160 (15)	0.0147 (14)	0.0121 (12)	0.000	0.0002 (11)	0.000
F1	0.0096 (4)	0.0171 (5)	0.0144 (4)	0.000	−0.0018 (4)	0.000
F2	0.0163 (5)	0.0221 (5)	0.0138 (4)	0.000	0.0025 (4)	0.000
F3	0.0219 (4)	0.0108 (3)	0.0183 (3)	−0.0001 (3)	−0.0047 (3)	−0.0029 (3)
F4	0.0222 (4)	0.0104 (3)	0.0139 (3)	−0.0007 (3)	−0.0029 (3)	−0.0009 (3)
F5	0.0106 (4)	0.0228 (5)	0.0168 (4)	0.000	−0.0014 (4)	0.000

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F6	0.0150 (5)	0.0197 (5)	0.0127 (4)	0.000	-0.0028 (4)	0.000
F7	0.0129 (5)	0.0203 (5)	0.0147 (4)	0.000	0.0011 (4)	0.000
F8	0.0134 (4)	0.0205 (5)	0.0095 (4)	0.000	-0.0012 (4)	0.000

Geometric parameters (\AA , $^\circ$)

K1—F8 ⁱ	2.7148 (9)	Eu1—F5	2.2923 (11)
K1—F1 ⁱⁱ	2.7344 (7)	Eu1—F2	2.3236 (11)
K1—F2 ⁱⁱⁱ	2.7451 (9)	Eu1—F3 ^{xviii}	2.3262 (7)
K1—F6 ^{iv}	2.7465 (8)	Eu1—F3 ^{xix}	2.3262 (7)
K1—F4 ⁱⁱⁱ	2.7718 (8)	Eu1—F1	2.3918 (10)
K1—F1 ^v	2.7863 (8)	Eu1—F4 ^{xx}	2.3954 (7)
K1—F3 ^{vi}	2.8163 (9)	Eu1—F4	2.3954 (7)
K1—F2 ⁱⁱ	2.8359 (8)	Eu1—F8 ^{xxi}	2.3996 (10)
K1—Li1 ^{vii}	2.933 (2)	Eu1—Li2 ^x	3.198 (3)
K1—F3 ^{viii}	2.9804 (8)	Li1—F6 ^{xvii}	1.804 (3)
K1—Li2 ⁱ	3.266 (3)	Li1—F1 ^{xxii}	1.862 (3)
K1—Li1 ^{ix}	3.395 (3)	Li1—F3 ⁱ	1.8669 (16)
K2—F7 ^x	2.6446 (8)	Li1—F3 ^{xxiii}	1.8669 (16)
K2—F6	2.6658 (10)	Li1—K1 ^{xxiv}	2.933 (2)
K2—F5	2.7225 (9)	Li1—K1 ^{xxv}	2.933 (2)
K2—F7 ^{xi}	2.7460 (7)	Li1—K3 ^{xvii}	3.076 (3)
K2—F8 ^{xi}	2.7831 (7)	Li1—K1 ^{xxvi}	3.395 (3)
K2—F5 ^{xii}	2.8078 (8)	Li1—K1 ^{xxvii}	3.395 (3)
K2—F4	2.8748 (8)	Li1—K2 ^{xvii}	3.426 (3)
K2—Li2 ^{xi}	2.965 (2)	Li1—K2 ^{xxviii}	3.426 (3)
K2—F3 ^v	3.0440 (9)	Li2—F7	1.801 (4)
K2—Li2 ^x	3.262 (3)	Li2—F4 ^{xvii}	1.817 (2)
K2—F4 ^{xiii}	3.3700 (8)	Li2—F4 ^{xxviii}	1.817 (2)
K2—Li1 ^x	3.426 (3)	Li2—F8	1.844 (3)
K3—F4 ^{xii}	2.5594 (8)	Li2—K2 ^{xi}	2.965 (2)
K3—F4 ^{xiv}	2.5594 (8)	Li2—K2 ^{xxix}	2.965 (2)
K3—F6 ^{xv}	2.5891 (11)	Li2—Eu1 ^{xvii}	3.198 (3)
K3—F7 ^x	2.6119 (11)	Li2—K2 ^{xxviii}	3.262 (3)
K3—F3 ^v	2.7320 (8)	Li2—K2 ^{xvii}	3.262 (3)
K3—F3 ^{xvi}	2.7320 (8)	Li2—K1 ⁱ	3.266 (3)
K3—Li1 ^x	3.076 (3)	Li2—K1 ^{xxiii}	3.266 (3)
K3—F2 ^{xvii}	3.3652 (12)		
F8 ⁱ —K1—F1 ⁱⁱ	125.15 (3)	F3 ⁱ —Li1—F3 ^{xxiii}	122.43 (17)
F8 ⁱ —K1—F2 ⁱⁱⁱ	88.19 (3)	F7—Li2—F4 ^{xvii}	114.17 (13)
F1 ⁱⁱ —K1—F2 ⁱⁱⁱ	143.59 (3)	F7—Li2—F4 ^{xxviii}	114.17 (13)
F8 ⁱ —K1—F6 ^{iv}	91.46 (3)	F4 ^{xvii} —Li2—F4 ^{xxviii}	95.80 (16)

F1 ⁱⁱ —K1—F6 ^{iv}	65.12 (3)	F7—Li2—F8	106.88 (17)
F2 ⁱⁱⁱ —K1—F6 ^{iv}	135.55 (3)	F4 ^{xvii} —Li2—F8	112.90 (13)
F8 ⁱ —K1—F4 ⁱⁱⁱ	67.56 (3)	F4 ^{xxviii} —Li2—F8	112.90 (13)
F1 ⁱⁱ —K1—F4 ⁱⁱⁱ	137.02 (3)	F7—Li2—K2 ^{xi}	65.12 (8)
F2 ⁱⁱⁱ —K1—F4 ⁱⁱⁱ	64.55 (3)	F4 ^{xvii} —Li2—K2 ^{xi}	86.08 (4)
F6 ^{iv} —K1—F4 ⁱⁱⁱ	74.37 (3)	F4 ^{xxviii} —Li2—K2 ^{xi}	178.10 (12)
F8 ⁱ —K1—F1 ^v	59.07 (3)	F8—Li2—K2 ^{xi}	66.01 (8)
F1 ⁱⁱ —K1—F1 ^v	91.096 (10)	F7—Li2—K2 ^{xxix}	65.12 (8)
F2 ⁱⁱⁱ —K1—F1 ^v	95.48 (2)	F4 ^{xvii} —Li2—K2 ^{xxix}	178.10 (12)
F6 ^{iv} —K1—F1 ^v	121.93 (3)	F4 ^{xxviii} —Li2—K2 ^{xxix}	86.08 (4)
F4 ⁱⁱⁱ —K1—F1 ^v	123.48 (2)	F8—Li2—K2 ^{xxix}	66.01 (8)
F8 ⁱ —K1—F3 ^{vi}	122.24 (3)	K2 ^{xi} —Li2—K2 ^{xxix}	92.03 (9)
F1 ⁱⁱ —K1—F3 ^{vi}	62.54 (2)	Li1 ^{xxx} —F1—Eu1	163.75 (11)
F2 ⁱⁱⁱ —K1—F3 ^{vi}	88.52 (3)	Li1 ^{xxx} —F1—K1 ^{xxxi}	76.71 (6)
F6 ^{iv} —K1—F3 ^{vi}	127.47 (3)	Eu1—F1—K1 ^{xxxi}	93.07 (3)
F4 ⁱⁱⁱ —K1—F3 ^{vi}	151.91 (2)	Li1 ^{xxx} —F1—K1 ^{xxxii}	76.71 (6)
F1 ^v —K1—F3 ^{vi}	63.93 (3)	Eu1—F1—K1 ^{xxxii}	93.07 (3)
F8 ⁱ —K1—F2 ⁱⁱ	164.89 (3)	K1 ^{xxxi} —F1—K1 ^{xxxii}	100.45 (3)
F1 ⁱⁱ —K1—F2 ⁱⁱ	60.15 (3)	Li1 ^{xxx} —F1—K1 ⁱⁱⁱ	91.64 (8)
F2 ⁱⁱⁱ —K1—F2 ⁱⁱ	91.732 (11)	Eu1—F1—K1 ⁱⁱⁱ	100.88 (3)
F6 ^{iv} —K1—F2 ⁱⁱ	78.06 (3)	K1 ^{xxxi} —F1—K1 ⁱⁱⁱ	88.904 (10)
F4 ⁱⁱⁱ —K1—F2 ⁱⁱ	98.83 (3)	K1 ^{xxxii} —F1—K1 ⁱⁱⁱ	162.80 (4)
F1 ^v —K1—F2 ⁱⁱ	135.88 (3)	Li1 ^{xxx} —F1—K1 ^{xxxiii}	91.64 (8)
F3 ^{vi} —K1—F2 ⁱⁱ	72.85 (3)	Eu1—F1—K1 ^{xxxiii}	100.88 (3)
F8 ⁱ —K1—F3 ^{viii}	62.84 (2)	K1 ^{xxxi} —F1—K1 ^{xxxiii}	162.80 (4)
F1 ⁱⁱ —K1—F3 ^{viii}	62.36 (3)	K1 ^{xxxii} —F1—K1 ^{xxxiii}	88.904 (10)
F2 ⁱⁱⁱ —K1—F3 ^{viii}	148.43 (2)	K1 ⁱⁱⁱ —F1—K1 ^{xxxiii}	78.68 (3)
F6 ^{iv} —K1—F3 ^{viii}	62.20 (3)	Eu1—F2—K1 ^{xvi}	110.14 (3)
F4 ⁱⁱⁱ —K1—F3 ^{viii}	110.69 (2)	Eu1—F2—K1 ^v	110.14 (3)
F1 ^v —K1—F3 ^{viii}	59.86 (2)	K1 ^{xvi} —F2—K1 ^v	80.09 (3)
F3 ^{vi} —K1—F3 ^{viii}	96.38 (2)	Eu1—F2—K1 ^{xxxi}	91.98 (3)
F2 ⁱⁱ —K1—F3 ^{viii}	119.55 (2)	K1 ^{xvi} —F2—K1 ^{xxxi}	157.42 (4)
Li1 ^{vii} —K1—F3 ^{viii}	36.79 (4)	K1 ^v —F2—K1 ^{xxxi}	88.268 (11)
F8 ⁱ —K1—Li2 ⁱ	34.37 (6)	Eu1—F2—K1 ^{xxxii}	91.98 (3)
F7 ^x —K2—F6	85.43 (3)	K1 ^{xvi} —F2—K1 ^{xxxii}	88.268 (11)
F7 ^x —K2—F5	85.58 (3)	K1 ^v —F2—K1 ^{xxxii}	157.42 (4)
F6—K2—F5	75.86 (3)	K1 ^{xxxi} —F2—K1 ^{xxxii}	95.64 (3)
F7 ^x —K2—F7 ^{xi}	148.354 (19)	Eu1—F2—K3 ^x	153.25 (4)
F6—K2—F7 ^{xi}	124.18 (3)	K1 ^{xvi} —F2—K3 ^x	90.02 (3)
F5—K2—F7 ^{xi}	90.98 (2)	K1 ^v —F2—K3 ^x	90.02 (3)
F7 ^x —K2—F8 ^{xi}	132.75 (3)	K1 ^{xxxi} —F2—K3 ^x	70.57 (2)

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F6—K2—F8 ^{xi}	91.71 (2)	K1 ^{xxxii} —F2—K3 ^x	70.57 (2)
F5—K2—F8 ^{xi}	139.19 (3)	Li1 ⁱ —F3—Eu1 ^{iv}	166.53 (9)
F7 ^{xi} —K2—F8 ^{xi}	63.94 (3)	Li1 ⁱ —F3—K3 ⁱⁱⁱ	81.61 (9)
F7 ^x —K2—F5 ^{xii}	91.28 (2)	Eu1 ^{iv} —F3—K3 ⁱⁱⁱ	110.42 (3)
F6—K2—F5 ^{xii}	133.49 (3)	Li1 ⁱ —F3—K1 ^{xxi}	90.59 (10)
F5—K2—F5 ^{xii}	150.205 (12)	Eu1 ^{iv} —F3—K1 ^{xxi}	92.43 (3)
F7 ^{xi} —K2—F5 ^{xii}	76.39 (3)	K3 ⁱⁱⁱ —F3—K1 ^{xxi}	103.03 (3)
F8 ^{xi} —K2—F5 ^{xii}	57.98 (3)	Li1 ⁱ —F3—K1 ^{xxxiv}	70.22 (9)
F7 ^x —K2—F4	66.62 (3)	Eu1 ^{iv} —F3—K1 ^{xxxiv}	97.07 (3)
F6—K2—F4	130.25 (2)	K3 ⁱⁱⁱ —F3—K1 ^{xxxiv}	151.20 (3)
F5—K2—F4	62.29 (3)	K1 ^{xxi} —F3—K1 ^{xxxiv}	83.62 (2)
F7 ^{xi} —K2—F4	83.95 (3)	Li1 ⁱ —F3—K2 ⁱⁱⁱ	84.87 (10)
F8 ^{xi} —K2—F4	137.60 (2)	Eu1 ^{iv} —F3—K2 ⁱⁱⁱ	88.18 (3)
F5 ^{xii} —K2—F4	89.28 (3)	K3 ⁱⁱⁱ —F3—K2 ⁱⁱⁱ	93.85 (3)
F7 ^x —K2—F3 ^v	76.20 (3)	K1 ^{xxi} —F3—K2 ⁱⁱⁱ	161.70 (3)
F6—K2—F3 ^v	62.15 (3)	K1 ^{xxxiv} —F3—K2 ⁱⁱⁱ	78.16 (2)
F5—K2—F3 ^v	135.02 (2)	Li2 ^x —F4—Eu1	97.82 (8)
F7 ^{xi} —K2—F3 ^v	125.05 (3)	Li2 ^x —F4—K3 ^{xiii}	147.88 (8)
F8 ^{xi} —K2—F3 ^v	61.27 (2)	Eu1—F4—K3 ^{xiii}	114.18 (3)
F5 ^{xii} —K2—F3 ^v	72.01 (3)	Li2 ^x —F4—K1 ^v	88.18 (11)
F4—K2—F3 ^v	137.88 (2)	Eu1—F4—K1 ^v	107.11 (3)
Li2 ^{xi} —K2—F3 ^v	94.67 (7)	K3 ^{xiii} —F4—K1 ^v	85.08 (2)
F7 ^x —K2—F4 ^{xiii}	150.54 (2)	Li2 ^x —F4—K2	84.91 (11)
F6—K2—F4 ^{xiii}	65.89 (2)	Eu1—F4—K2	106.00 (3)
F5—K2—F4 ^{xiii}	81.15 (3)	K3 ^{xiii} —F4—K2	83.77 (2)
F7 ^{xi} —K2—F4 ^{xiii}	58.49 (3)	K1 ^v —F4—K2	146.79 (3)
F8 ^{xi} —K2—F4 ^{xiii}	58.53 (2)	Li2 ^x —F4—K2 ^{xii}	61.37 (8)
F5 ^{xii} —K2—F4 ^{xiii}	112.98 (2)	Eu1—F4—K2 ^{xii}	159.13 (3)
F4—K2—F4 ^{xiii}	127.14 (2)	K3 ^{xiii} —F4—K2 ^{xii}	86.55 (2)
Li2 ^{xi} —K2—F4 ^{xiii}	32.54 (5)	K1 ^v —F4—K2 ^{xii}	75.704 (19)
F3 ^v —K2—F4 ^{xiii}	94.98 (2)	K2—F4—K2 ^{xii}	72.480 (17)
Li2 ^x —K2—F4 ^{xiii}	147.93 (5)	Eu1—F5—K2 ^{xx}	114.28 (3)
F4 ^{xii} —K3—F4 ^{xiv}	159.74 (4)	Eu1—F5—K2	114.28 (3)
F4 ^{xii} —K3—F6 ^{xv}	80.751 (19)	K2 ^{xx} —F5—K2	79.15 (3)
F4 ^{xiv} —K3—F6 ^{xv}	80.751 (19)	Eu1—F5—K2 ^{xiii}	94.85 (3)
F4 ^{xii} —K3—F7 ^x	93.29 (2)	K2 ^{xx} —F5—K2 ^{xiii}	150.40 (4)
F4 ^{xiv} —K3—F7 ^x	93.29 (2)	K2—F5—K2 ^{xiii}	84.342 (11)
F6 ^{xv} —K3—F7 ^x	133.01 (4)	Eu1—F5—K2 ^{xxxv}	94.85 (3)
F4 ^{xii} —K3—F3 ^v	63.21 (2)	K2 ^{xx} —F5—K2 ^{xxxv}	84.342 (11)
F4 ^{xiv} —K3—F3 ^v	136.75 (3)	K2—F5—K2 ^{xxxv}	150.40 (4)
F6 ^{xv} —K3—F3 ^v	131.84 (3)	K2 ^{xiii} —F5—K2 ^{xxxv}	98.89 (4)

F7 ^x —K3—F3 ^v	82.48 (3)	Li1 ^x —F6—K3 ^{xxxvi}	152.17 (12)
F4 ^{xii} —K3—F3 ^{xvi}	136.75 (3)	Li1 ^x —F6—K2 ^{xx}	98.23 (8)
F4 ^{xiv} —K3—F3 ^{xvi}	63.21 (2)	K3 ^{xxxvi} —F6—K2 ^{xx}	102.81 (3)
F6 ^{xv} —K3—F3 ^{xvi}	131.84 (3)	Li1 ^x —F6—K2	98.23 (8)
F7 ^x —K3—F3 ^{xvi}	82.48 (3)	K3 ^{xxxvi} —F6—K2	102.81 (3)
F3 ^v —K3—F3 ^{xvi}	73.58 (3)	K2 ^{xx} —F6—K2	81.18 (4)
F4 ^{xii} —K3—F2 ^{xvii}	90.874 (19)	Li1 ^x —F6—K1 ^{xviii}	77.21 (7)
F4 ^{xiv} —K3—F2 ^{xvii}	90.874 (19)	K3 ^{xxxvi} —F6—K1 ^{xviii}	85.04 (3)
F6 ^{xv} —K3—F2 ^{xvii}	71.03 (3)	K2 ^{xx} —F6—K1 ^{xviii}	168.64 (4)
F7 ^x —K3—F2 ^{xvii}	155.96 (3)	K2—F6—K1 ^{xviii}	89.126 (9)
F3 ^v —K3—F2 ^{xvii}	78.33 (3)	Li1 ^x —F6—K1 ^{xix}	77.21 (7)
F3 ^{xvi} —K3—F2 ^{xvii}	78.33 (3)	K3 ^{xxxvi} —F6—K1 ^{xix}	85.04 (3)
Li1 ^x —K3—F2 ^{xvii}	78.49 (6)	K2 ^{xx} —F6—K1 ^{xix}	89.126 (9)
F5—Eu1—F2	147.91 (4)	K2—F6—K1 ^{xix}	168.64 (4)
F5—Eu1—F3 ^{xviii}	96.48 (2)	K1 ^{xviii} —F6—K1 ^{xix}	99.84 (4)
F2—Eu1—F3 ^{xviii}	92.40 (2)	Li2—F7—K3 ^{xvii}	154.06 (11)
F5—Eu1—F3 ^{xix}	96.48 (2)	Li2—F7—K2 ^{xxviii}	92.42 (8)
F2—Eu1—F3 ^{xix}	92.40 (2)	K3 ^{xvii} —F7—K2 ^{xxviii}	106.96 (3)
F3 ^{xviii} —Eu1—F3 ^{xix}	147.22 (4)	Li2—F7—K2 ^{xvii}	92.42 (8)
F5—Eu1—F1	139.47 (4)	K3 ^{xvii} —F7—K2 ^{xvii}	106.96 (3)
F2—Eu1—F1	72.63 (4)	K2 ^{xxviii} —F7—K2 ^{xvii}	81.97 (3)
F3 ^{xviii} —Eu1—F1	75.29 (2)	Li2—F7—K2 ^{xi}	78.37 (7)
F3 ^{xix} —Eu1—F1	75.30 (2)	K3 ^{xvii} —F7—K2 ^{xi}	85.43 (3)
F5—Eu1—F4 ^{xx}	76.34 (3)	K2 ^{xxviii} —F7—K2 ^{xi}	165.38 (4)
F2—Eu1—F4 ^{xx}	77.25 (3)	K2 ^{xvii} —F7—K2 ^{xi}	87.055 (6)
F3 ^{xviii} —Eu1—F4 ^{xx}	140.49 (3)	Li2—F7—K2 ^{xxix}	78.37 (7)
F3 ^{xix} —Eu1—F4 ^{xx}	72.04 (3)	K3 ^{xvii} —F7—K2 ^{xxix}	85.43 (3)
F1—Eu1—F4 ^{xx}	133.97 (2)	K2 ^{xxviii} —F7—K2 ^{xxix}	87.055 (6)
F5—Eu1—F4	76.34 (3)	K2 ^{xvii} —F7—K2 ^{xxix}	165.38 (4)
F2—Eu1—F4	77.25 (3)	K2 ^{xi} —F7—K2 ^{xxix}	101.95 (4)
F3 ^{xviii} —Eu1—F4	72.04 (3)	Li2—F8—Eu1 ^{vi}	163.91 (12)
F3 ^{xix} —Eu1—F4	140.49 (3)	Li2—F8—K1 ⁱ	89.41 (9)
F1—Eu1—F4	133.97 (2)	Eu1 ^{vi} —F8—K1 ⁱ	102.73 (3)
F4 ^{xx} —Eu1—F4	68.51 (4)	Li2—F8—K1 ^{xxiii}	89.41 (9)
F5—Eu1—F8 ^{xxi}	70.51 (4)	Eu1 ^{vi} —F8—K1 ^{xxiii}	102.73 (3)
F2—Eu1—F8 ^{xxi}	141.59 (4)	K1 ⁱ —F8—K1 ^{xxiii}	81.17 (3)
F3 ^{xviii} —Eu1—F8 ^{xxi}	78.10 (2)	Li2—F8—K2 ^{xxix}	76.74 (7)
F3 ^{xix} —Eu1—F8 ^{xxi}	78.10 (2)	Eu1 ^{vi} —F8—K2 ^{xxix}	93.11 (3)
F1—Eu1—F8 ^{xxi}	68.96 (4)	K1 ⁱ —F8—K2 ^{xxix}	162.14 (4)
F4 ^{xx} —Eu1—F8 ^{xxi}	131.91 (2)	K1 ^{xxiii} —F8—K2 ^{xxix}	87.386 (10)
F4—Eu1—F8 ^{xxi}	131.91 (2)	Li2—F8—K2 ^{xi}	76.74 (7)

supplementary materials

F6 ^{xvii} —Li1—F1 ^{xxii}	107.19 (16)	Eu1 ^{vi} —F8—K2 ^{xi}	93.11 (3)
F6 ^{xvii} —Li1—F3 ⁱ	107.75 (11)	K1 ⁱ —F8—K2 ^{xi}	87.386 (10)
F1 ^{xxii} —Li1—F3 ⁱ	105.42 (11)	K1 ^{xxiii} —F8—K2 ^{xi}	162.14 (4)
F6 ^{xvii} —Li1—F3 ^{xxiii}	107.75 (11)	K2 ^{xxix} —F8—K2 ^{xi}	100.09 (4)
F1 ^{xxii} —Li1—F3 ^{xxiii}	105.42 (11)		

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x+1/2, y+1, -z+1/2$; (iii) $-x+1/2, -y+1, z-1/2$; (iv) $x, y+1, z$; (v) $-x+1/2, -y+1, z+1/2$; (vi) $x+1/2, y, -z+1/2$; (vii) $x-1/2, y+1, -z+3/2$; (viii) $-x+1/2, -y+2, z+1/2$; (ix) $-x+3/2, -y+1, z-1/2$; (x) $x-1/2, y, -z+3/2$; (xi) $-x+1, -y, -z+1$; (xii) $-x+1/2, -y, z+1/2$; (xiii) $-x+1/2, -y, z-1/2$; (xiv) $-x+1/2, y+1/2, z+1/2$; (xv) $x, y, z+1$; (xvi) $-x+1/2, y-1/2, z+1/2$; (xvii) $x+1/2, y, -z+3/2$; (xviii) $x, y-1, z$; (xix) $x, -y+3/2, z$; (xx) $x, -y+1/2, z$; (xxi) $x-1/2, y, -z+1/2$; (xxii) $x+1, y, z+1$; (xxiii) $-x+1, y-1/2, -z+1$; (xxiv) $x+1/2, -y+3/2, -z+3/2$; (xxv) $x+1/2, y-1, -z+3/2$; (xxvi) $-x+3/2, -y+1, z+1/2$; (xxvii) $-x+3/2, y-1/2, z+1/2$; (xxviii) $x+1/2, -y+1/2, -z+3/2$; (xxix) $-x+1, y+1/2, -z+1$; (xxx) $x-1, y, z-1$; (xxxi) $x-1/2, y-1, -z+1/2$; (xxxii) $x-1/2, -y+3/2, -z+1/2$; (xxxiii) $-x+1/2, y-1/2, z-1/2$; (xxxiv) $-x+1/2, -y+2, z-1/2$; (xxxv) $-x+1/2, y+1/2, z-1/2$; (xxxvi) $x, y, z-1$.

Fig. 1

