Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Pentapotassium praseodymium(III) dilithium decafluoride, $K_5PrLi_2F_{10}$

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Received 12 October 2009; accepted 23 October 2009

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(Pr–F) = 0.001 Å; R factor = 0.029; wR factor = 0.045; data-to-parameter ratio = 50.1.

The crystal structure of $K_5PrLi_2F_{10}$ is isotypic with those of other $K_5RELi_2F_{10}$ compounds (*RE* = Eu, Nd). The lanthanoid ions are isolated in $K_5PrLi_2F_{10}$, with a mean separation between the Pr ions of 7.356 Å. It classifies this crystal as a so-called self-activated material containing lanthanoid ions within the matrix. Except for two K^+ and two F^- ions, all atoms are located on sites with *m* symmetry. In the structure, distorted PrF_8 dodecahedra and two different LiF_4 tetrahedra share F atoms, forming sheets parallel to (100). The isolated PrF_8 dodecahedra exhibit a mean Pr—F distance of 2.406 Å. The K^+ cations are located within and between these sheets, leading to highly irregular KF_x polyhedra with coordination numbers of eight and nine for the alkali metal cations.

Related literature

The structures of the isotypic Nd and Eu analogues have been reported by Hong & McCollum (1979) and 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

$K_5PrLi_2F_{10}$
M_r = 540.29
Orthorhombic, *Pnma*
a = 20.6492 (6) Å
b = 7.7903 (3) Å
c = 6.9255 (2) Å
V = 1114.06 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 6.34 mm^{-1}
T = 295 K
0.35 × 0.13 × 0.05 mm

Data collection

Kuma KM-4 with CCD area-detector diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.40, T_{max} = 0.73
24749 measured reflections
4910 independent reflections
3709 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.045
S = 1.02
4910 reflections
98 parameters
$\Delta\rho_{max}$ = 1.17 e Å^{-3}
$\Delta\rho_{min}$ = −2.04 e Å^{-3}

Table 1
Selected bond lengths (Å).

Pr1—F5	2.3426 (12)	Li1—F6^{iii}	1.802 (4)
Pr1—F3^{i}	2.3737 (8)	Li1—F1^{iv}	1.856 (4)
Pr1—F2	2.3751 (12)	Li1—F3^{v}	1.8602 (19)
Pr1—F1	2.4368 (11)	Li2—F7	1.796 (4)
Pr1—F8^{ii}	2.4463 (11)	Li2—F4^{iii}	1.819 (2)
Pr1—F4	2.4488 (8)	Li2—F8	1.843 (4)

Symmetry codes: (i) $x, y-1, z$; (ii) $x-\frac{1}{2}, y, -z+\frac{1}{2}$; (iii) $x+\frac{1}{2}, y, -z+\frac{3}{2}$; (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: WM2268).

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supporting information

Acta Cryst. (2009). E**65**, i81 [https://doi.org/10.1107/S1600536809044043]

Pentapotassium praseodymium(III) dilithium decafluoride, $K_5PrLi_2F_{10}$

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S1. Comment

The title crystal belongs to so-called self-activated materials containing lanthanoid ions within the matrix. An important 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.

In the structure, two different LiF_4 tetrahedra together with distorted PrF_8 dodecahedra form sheets expanding perpendicular to [100]. K1 atoms occupy cavities within the sheets and are surrounded by 9 F^- ions in a mean distance of 2.780 Å. The remaining potassium atoms are located between the sheets within a KF_9 and KF_8 environment. Each PrF_8 dodecahedron is surrounded by twelve others with a minimum and maximum Pr—Pr separation of 6.7656 (2) and 7.8684 (2) Å, and individual distances of: 2× 6.7656 (2), 2× 6.9169 (2), 2× 6.9255 (2), 2× 7.7903 (3) and 4× 7.8684 (2) Å.

The bond valence sums of all metal atoms have been calculated from the received structure model using the bond-valence method (Brown, 1992, 2002; Mattausch *et al.*, 1991); Pr 2.86, K1 1.05, K2 0.98, K3 1.06, and Li 1.08 v.u. The Pr ion is slightly under-bonded which may be associated with the distorted surrounding of this cation. When such distortions occur, the equal-valence rule is not obeyed (Brown, 1992). The valences of K atoms are close to the formal charge of +1. The Li position is over-bonded with a 8.3% higher bond-valence sum than those expected from the formal charge of +1.

S2. Experimental

The $K_5PrLi_2F_{10}$ crystal was grown from commercially available KF, PrF_3 and LiF (Aldrich 99.99%, anhydrous) using the Bridgman method in a graphite crucible under argon atmosphere. The reagents were heated at 923 K (melting point 813 K). The pulling rate was 1mm/h, temperature gradient was 100°/cm.

S3. Refinement

In the final Fourier map, the highest peak is 1.22 Å from atom Pr1 and the deepest hole is 0.55 Å from the same atom.

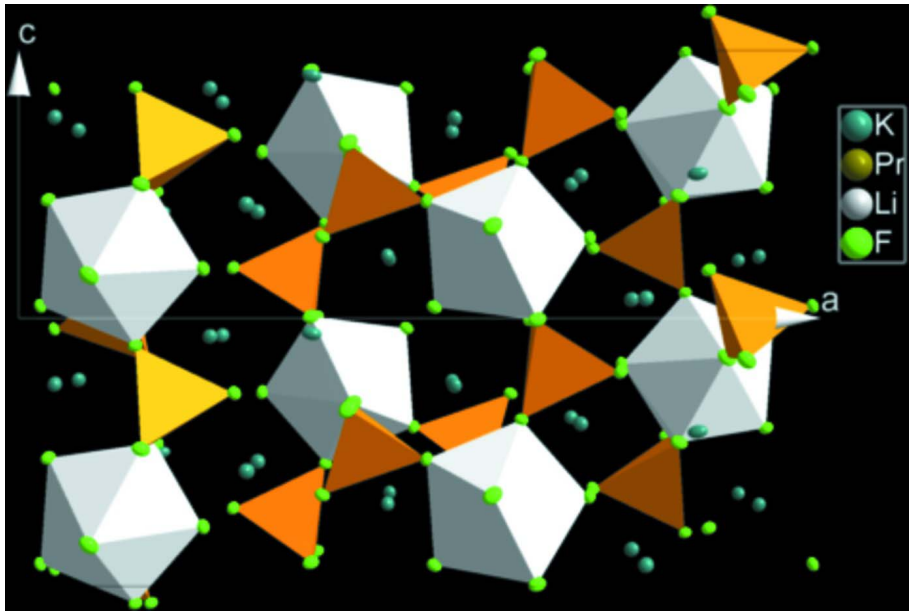

Figure 1

Crystal packing of the $K_5PrLi_2F_{10}$ structure as seen down [010]. Displacement ellipsoids have been drawn at the 50% probability level.

Pentapotassium praseodymium(III) dilithium decafluoride

Crystal data

$K_5PrLi_2F_{10}$
$M_r = 540.29$
Orthorhombic, *Pnma*
Hall symbol: -P 2ac 2n
$a = 20.6492$ (6) Å
$b = 7.7903$ (3) Å
$c = 6.9255$ (2) Å
$V = 1114.06$ (6) Å^3
$Z = 4$
$F(000) = 1000$
$D_x = 3.221$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 11195 reflections
$\theta = 2.6$–$47.0°$
$\mu = 6.34$ mm^{-1}
$T = 295$ K
Rectangular prism, colourless
0.35 × 0.13 × 0.05 mm

Data collection

Kuma KM-4 with CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 1024x1024 with blocks 2x2, 33.133pixel/mm pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
$T_{min} = 0.40$, $T_{max} = 0.73$
24749 measured reflections
4910 independent reflections
3709 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 47.1°$, $\theta_{min} = 3.1°$
$h = -19 \rightarrow 42$
$k = -16 \rightarrow 13$
$l = -13 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.045$
$S = 1.02$
4910 reflections
98 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0151P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.17$ e Å^{-3}
$\Delta\rho_{min} = -2.04$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0319 (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^ > σ(*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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
K1	0.456661 (15)	0.97842 (4)	0.25210 (4)	0.01639 (5)
K2	0.283103 (15)	0.02682 (4)	0.42595 (5)	0.01786 (6)
K3	0.35981 (2)	0.2500	0.94040 (6)	0.01865 (8)
Pr1	0.107262 (4)	0.2500	0.239205 (12)	0.00794 (2)
Li1	0.92241 (16)	0.2500	0.9697 (5)	0.0140 (6)
Li2	0.67429 (16)	0.2500	0.8399 (5)	0.0138 (6)
F1	0.00854 (5)	0.2500	0.04643 (17)	0.0152 (2)
F2	0.01862 (6)	0.2500	0.45774 (17)	0.0189 (2)
F3	0.09014 (4)	0.95753 (10)	0.15779 (13)	0.01896 (17)
F4	0.14806 (4)	0.07426 (10)	0.50594 (12)	0.01643 (16)
F5	0.21956 (6)	0.2500	0.19130 (18)	0.0182 (2)
F6	0.37398 (6)	0.2500	0.31393 (18)	0.0170 (2)
F7	0.75970 (6)	0.2500	0.79114 (17)	0.0171 (2)
F8	0.63138 (6)	0.2500	0.60663 (16)	0.0160 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K1	0.01604 (12)	0.01537 (12)	0.01777 (13)	−0.00135 (9)	−0.00063 (10)	−0.00158 (10)
K2	0.01912 (13)	0.01524 (13)	0.01921 (14)	0.00175 (10)	−0.00062 (11)	−0.00098 (10)
K3	0.0311 (2)	0.01106 (17)	0.01382 (18)	0.000	−0.00294 (15)	0.000
Pr1	0.00890 (4)	0.00760 (4)	0.00733 (4)	0.000	−0.00056 (3)	0.000
Li1	0.0140 (15)	0.0148 (16)	0.0131 (15)	0.000	−0.0021 (12)	0.000
Li2	0.0128 (16)	0.0152 (16)	0.0132 (15)	0.000	0.0005 (12)	0.000
F1	0.0111 (5)	0.0188 (6)	0.0156 (5)	0.000	−0.0023 (4)	0.000
F2	0.0180 (6)	0.0243 (6)	0.0144 (5)	0.000	0.0026 (4)	0.000

F3	0.0249 (4)	0.0109 (4)	0.0211 (4)	0.0000 (3)	−0.0063 (3)	−0.0032 (3)
F4	0.0240 (4)	0.0101 (3)	0.0153 (4)	−0.0001 (3)	−0.0031 (3)	−0.0007 (3)
F5	0.0129 (5)	0.0237 (6)	0.0182 (5)	0.000	−0.0015 (4)	0.000
F6	0.0170 (5)	0.0210 (6)	0.0132 (5)	0.000	−0.0024 (4)	0.000
F7	0.0144 (5)	0.0210 (6)	0.0160 (5)	0.000	0.0017 (4)	0.000
F8	0.0155 (5)	0.0212 (6)	0.0112 (5)	0.000	−0.0015 (4)	0.000

Geometric parameters (Å, º)

K1—F8^{i}	2.7256 (9)	K3—F5^{xv}	3.3772 (13)
K1—F1^{ii}	2.7514 (8)	Pr1—F5	2.3426 (12)
K1—F2^{iii}	2.7537 (10)	Pr1—F3^{xviii}	2.3737 (8)
K1—F6^{iv}	2.7521 (9)	Pr1—F3^{xix}	2.3737 (8)
K1—F4^{iii}	2.7841 (9)	Pr1—F2	2.3751 (12)
K1—F1^{v}	2.7996 (9)	Pr1—F1	2.4368 (11)
K1—F3^{vi}	2.8307 (10)	Pr1—F8^{xx}	2.4463 (11)
K1—F2^{ii}	2.8679 (9)	Pr1—F4^{xxi}	2.4488 (8)
K1—Li1^{vii}	2.948 (2)	Pr1—F4	2.4488 (8)
K1—F3^{viii}	3.0127 (9)	Pr1—Li2^{x}	3.227 (3)
K1—Li2^{i}	3.299 (3)	Li1—F6^{xvii}	1.802 (4)
K1—Li1^{ix}	3.416 (3)	Li1—F1^{xxii}	1.856 (4)
K2—F7^{x}	2.6636 (9)	Li1—F3^{i}	1.8602 (19)
K2—F6	2.6733 (10)	Li1—F3^{xxiii}	1.8602 (19)
K2—F5	2.7176 (10)	Li1—K1^{xxiv}	2.948 (2)
K2—F7^{xi}	2.7735 (8)	Li1—K1^{xxv}	2.948 (2)
K2—F8^{xi}	2.7964 (8)	Li1—K3^{xvii}	3.120 (3)
K2—F5^{xii}	2.8338 (9)	Li1—K1^{xxvi}	3.416 (3)
K2—F4	2.8669 (9)	Li1—K1^{xxvii}	3.416 (3)
K2—Li2^{xi}	2.969 (2)	Li1—K2^{xvii}	3.438 (3)
K2—F3^{v}	3.0730 (10)	Li1—K2^{xxviii}	3.438 (3)
K2—Li2^{x}	3.271 (3)	Li2—F7	1.796 (4)
K2—F4^{xiii}	3.3319 (9)	Li2—F4^{xvii}	1.819 (2)
K2—Li1^{x}	3.438 (3)	Li2—F4^{xxviii}	1.819 (2)
K3—F4^{xiv}	2.5717 (8)	Li2—F8	1.843 (4)
K3—F4^{xii}	2.5717 (8)	Li2—K2^{xi}	2.969 (2)
K3—F6^{xv}	2.6035 (13)	Li2—K2^{xxix}	2.969 (2)
K3—F7^{x}	2.6161 (12)	Li2—Pr1^{xvii}	3.227 (3)
K3—F3^{v}	2.7409 (9)	Li2—K2^{xxviii}	3.271 (3)
K3—F3^{xvi}	2.7409 (9)	Li2—K2^{xvii}	3.271 (3)
K3—Li1^{x}	3.120 (3)	Li2—K1^{i}	3.299 (3)
K3—F2^{xvii}	3.3544 (13)	Li2—K1^{xxiii}	3.299 (3)
F8^{i}—K1—F1^{ii}	125.43 (3)	F4^{xxi}—Pr1—F4	67.98 (4)
F8^{i}—K1—F2^{iii}	88.14 (3)	F6^{xvii}—Li1—F1^{xxii}	107.07 (18)
F1^{ii}—K1—F2^{iii}	143.14 (3)	F6^{xvii}—Li1—F3^{i}	108.50 (12)
F8^{i}—K1—F6^{iv}	91.85 (3)	F1^{xxii}—Li1—F3^{i}	105.63 (12)
F1^{ii}—K1—F6^{iv}	64.63 (3)	F6^{xvii}—Li1—F3^{xxiii}	108.50 (12)
F2^{iii}—K1—F6^{iv}	136.63 (3)	F1^{xxii}—Li1—F3^{xxiii}	105.63 (12)

F8^{i}—K1—F4^{iii}	66.76 (3)	F3^{i}—Li1—F3^{xxiii}	120.71 (19)
F1^{ii}—K1—F4^{iii}	136.58 (3)	F7—Li2—F4^{xvii}	113.76 (13)
F2^{iii}—K1—F4^{iii}	66.13 (3)	F7—Li2—F4^{xxviii}	113.76 (13)
F6^{iv}—K1—F4^{iii}	74.14 (3)	F4^{xvii}—Li2—F4^{xxviii}	97.67 (17)
F8^{i}—K1—F1^{v}	59.66 (3)	F7—Li2—F8	107.90 (19)
F1^{ii}—K1—F1^{v}	91.123 (11)	F4^{xvii}—Li2—F8	111.81 (14)
F2^{iii}—K1—F1^{v}	94.63 (3)	F4^{xxviii}—Li2—F8	111.81 (14)
F6^{iv}—K1—F1^{v}	122.31 (3)	Li1^{xxx}—F1—Pr1	163.42 (12)
F4^{iii}—K1—F1^{v}	123.47 (3)	Li1^{xxx}—F1—K1^{xxxi}	76.83 (7)
F8^{i}—K1—F3^{vi}	122.20 (3)	Pr1—F1—K1^{xxxi}	92.75 (3)
F1^{ii}—K1—F3^{vi}	63.47 (3)	Li1^{xxx}—F1—K1^{xxxii}	76.83 (7)
F2^{iii}—K1—F3^{vi}	86.88 (3)	Pr1—F1—K1^{xxxii}	92.75 (3)
F6^{iv}—K1—F3^{vi}	127.87 (3)	K1^{xxxi}—F1—K1^{xxxii}	100.52 (4)
F4^{iii}—K1—F3^{vi}	151.98 (3)	Li1^{xxx}—F1—K1^{iii}	92.14 (9)
F1^{v}—K1—F3^{vi}	63.45 (3)	Pr1—F1—K1^{iii}	100.61 (3)
F8^{i}—K1—F2^{ii}	163.96 (3)	K1^{xxxi}—F1—K1^{iii}	88.877 (11)
F1^{ii}—K1—F2^{ii}	61.06 (3)	K1^{xxxii}—F1—K1^{iii}	163.31 (4)
F2^{iii}—K1—F2^{ii}	91.081 (12)	Li1^{xxx}—F1—K1^{xxxiii}	92.14 (9)
F6^{iv}—K1—F2^{ii}	77.79 (3)	Pr1—F1—K1^{xxxiii}	100.61 (3)
F4^{iii}—K1—F2^{ii}	98.33 (3)	K1^{xxxi}—F1—K1^{xxxiii}	163.31 (4)
F1^{v}—K1—F2^{ii}	136.33 (3)	K1^{xxxii}—F1—K1^{xxxiii}	88.877 (11)
F3^{vi}—K1—F2^{ii}	73.73 (3)	K1^{iii}—F1—K1^{xxxiii}	78.93 (3)
F8^{i}—K1—F3^{viii}	63.86 (3)	Pr1—F2—K1^{xvi}	109.20 (4)
F1^{ii}—K1—F3^{viii}	61.62 (3)	Pr1—F2—K1^{v}	109.20 (4)
F2^{iii}—K1—F3^{viii}	148.97 (3)	K1^{xvi}—F2—K1^{v}	80.51 (3)
F6^{iv}—K1—F3^{viii}	61.87 (3)	Pr1—F2—K1^{xxxi}	91.20 (3)
F4^{iii}—K1—F3^{viii}	110.26 (3)	K1^{xvi}—F2—K1^{xxxi}	159.16 (5)
F1^{v}—K1—F3^{viii}	60.57 (3)	K1^{v}—F2—K1^{xxxi}	88.919 (12)
F3^{vi}—K1—F3^{viii}	96.68 (2)	Pr1—F2—K1^{xxxii}	91.20 (3)
F2^{ii}—K1—F3^{viii}	119.57 (3)	K1^{xvi}—F2—K1^{xxxii}	88.919 (12)
Li1^{vii}—K1—F3^{viii}	36.35 (5)	K1^{v}—F2—K1^{xxxii}	159.16 (5)
F7^{x}—K2—F6	85.20 (3)	K1^{xxxi}—F2—K1^{xxxii}	95.07 (4)
F7^{x}—K2—F5	86.26 (3)	Pr1—F2—K3^{x}	152.55 (5)
F6—K2—F5	75.48 (3)	K1^{xvi}—F2—K3^{x}	91.46 (3)
F7^{x}—K2—F7^{xi}	148.04 (2)	K1^{v}—F2—K3^{x}	91.46 (3)
F6—K2—F7^{xi}	124.90 (3)	K1^{xxxi}—F2—K3^{x}	70.76 (3)
F5—K2—F7^{xi}	91.11 (3)	K1^{xxxii}—F2—K3^{x}	70.76 (3)
F7^{x}—K2—F8^{xi}	132.63 (3)	Li1^{i}—F3—Pr1^{iv}	165.41 (10)
F6—K2—F8^{xi}	92.00 (3)	Li1^{i}—F3—K3^{iii}	83.04 (9)
F5—K2—F8^{xi}	138.59 (3)	Pr1^{iv}—F3—K3^{iii}	109.90 (3)
F7^{xi}—K2—F8^{xi}	63.76 (3)	Li1^{i}—F3—K1^{xx}	91.08 (11)
F7^{x}—K2—F5^{xii}	90.93 (3)	Pr1^{iv}—F3—K1^{xx}	92.15 (3)
F6—K2—F5^{xii}	134.17 (3)	K3^{iii}—F3—K1^{xx}	104.10 (3)
F5—K2—F5^{xii}	149.912 (14)	Li1^{i}—F3—K1^{xxxiv}	69.92 (9)
F7^{xi}—K2—F5^{xii}	75.74 (3)	Pr1^{iv}—F3—K1^{xxxiv}	96.33 (3)
F8^{xi}—K2—F5^{xii}	58.52 (3)	K3^{iii}—F3—K1^{xxxiv}	152.20 (3)
F7^{x}—K2—F4	66.25 (3)	K1^{xx}—F3—K1^{xxxiv}	83.32 (2)
F6—K2—F4	130.92 (3)	Li1^{i}—F3—K2^{iii}	84.56 (11)

F5—K2—F4	64.12 (3)	Pr1^{iv}—F3—K2^{iii}	87.66 (3)
F7^{xi}—K2—F4	83.97 (3)	K3^{iii}—F3—K2^{iii}	94.32 (3)
F8^{xi}—K2—F4	136.82 (3)	K1^{xx}—F3—K2^{iii}	160.43 (4)
F5^{xii}—K2—F4	87.36 (3)	K1^{xxxiv}—F3—K2^{iii}	77.26 (2)
F7^{x}—K2—F3^{v}	75.18 (3)	Li2^{x}—F4—Pr1	97.15 (9)
F6—K2—F3^{v}	61.83 (3)	Li2^{x}—F4—K3^{xiii}	149.53 (9)
F5—K2—F3^{v}	134.29 (3)	Pr1—F4—K3^{xiii}	113.22 (3)
F7^{xi}—K2—F3^{v}	125.84 (3)	Li2^{x}—F4—K1^{v}	89.01 (11)
F8^{xi}—K2—F3^{v}	62.28 (3)	Pr1—F4—K1^{v}	106.09 (3)
F5^{xii}—K2—F3^{v}	73.02 (3)	K3^{xiii}—F4—K1^{v}	85.08 (3)
F4—K2—F3^{v}	136.25 (3)	Li2^{x}—F4—K2	85.46 (11)
Li2^{xi}—K2—F3^{v}	95.76 (7)	Pr1—F4—K2	105.13 (3)
F7^{x}—K2—F4^{xiii}	150.90 (3)	K3^{xiii}—F4—K2	84.30 (3)
F6—K2—F4^{xiii}	66.48 (3)	K1^{v}—F4—K2	148.74 (3)
F5—K2—F4^{xiii}	80.51 (3)	Li2^{x}—F4—K2^{xii}	62.51 (9)
F7^{xi}—K2—F4^{xiii}	58.60 (3)	Pr1—F4—K2^{xii}	159.63 (3)
F8^{xi}—K2—F4^{xiii}	58.53 (3)	K3^{xiii}—F4—K2^{xii}	87.07 (3)
F5^{xii}—K2—F4^{xiii}	113.24 (3)	K1^{v}—F4—K2^{xii}	76.23 (2)
F4—K2—F4^{xiii}	127.88 (3)	K2—F4—K2^{xii}	73.936 (19)
Li2^{xi}—K2—F4^{xiii}	32.91 (5)	Pr1—F5—K2^{xxi}	113.16 (4)
F3^{v}—K2—F4^{xiii}	95.86 (2)	Pr1—F5—K2	113.16 (4)
Li2^{x}—K2—F4^{xiii}	148.36 (6)	K2^{xxi}—F5—K2	79.55 (4)
F4^{xiv}—K3—F4^{xii}	158.39 (4)	Pr1—F5—K2^{xiii}	94.16 (3)
F4^{xiv}—K3—F6^{xv}	80.31 (2)	K2^{xxi}—F5—K2^{xiii}	152.13 (5)
F4^{xii}—K3—F6^{xv}	80.31 (2)	K2—F5—K2^{xiii}	84.854 (11)
F4^{xiv}—K3—F7^{x}	93.34 (2)	Pr1—F5—K2^{xxxv}	94.16 (3)
F4^{xii}—K3—F7^{x}	93.34 (2)	K2^{xxi}—F5—K2^{xxxv}	84.854 (11)
F6^{xv}—K3—F7^{x}	134.26 (4)	K2—F5—K2^{xxxv}	152.13 (5)
F4^{xiv}—K3—F3^{v}	136.82 (3)	K2^{xiii}—F5—K2^{xxxv}	99.10 (4)
F4^{xii}—K3—F3^{v}	64.56 (3)	Pr1—F5—K3^{xxxvi}	157.18 (5)
F6^{xv}—K3—F3^{v}	131.85 (3)	K2^{xxi}—F5—K3^{xxxvi}	83.90 (3)
F7^{x}—K3—F3^{v}	81.97 (3)	K2—F5—K3^{xxxvi}	83.90 (3)
F4^{xiv}—K3—F3^{xvi}	64.56 (3)	K2^{xiii}—F5—K3^{xxxvi}	71.52 (3)
F4^{xii}—K3—F3^{xvi}	136.82 (3)	K2^{xxxv}—F5—K3^{xxxvi}	71.52 (3)
F6^{xv}—K3—F3^{xvi}	131.85 (3)	Li1^{x}—F6—K3^{xxxvi}	152.74 (12)
F7^{x}—K3—F3^{xvi}	81.97 (3)	Li1^{x}—F6—K2	98.53 (9)
F3^{v}—K3—F3^{xvi}	72.29 (4)	K3^{xxxvi}—F6—K2	102.09 (4)
F4^{xiv}—K3—F2^{xvii}	91.41 (2)	Li1^{x}—F6—K2^{xxi}	98.53 (9)
F4^{xii}—K3—F2^{xvii}	91.41 (2)	K3^{xxxvi}—F6—K2^{xxi}	102.09 (4)
F6^{xv}—K3—F2^{xvii}	71.40 (4)	K2—F6—K2^{xxi}	81.14 (4)
F7^{x}—K3—F2^{xvii}	154.34 (4)	Li1^{x}—F6—K1^{xix}	77.59 (7)
F3^{v}—K3—F2^{xvii}	77.38 (3)	K3^{xxxvi}—F6—K1^{xix}	85.13 (3)
F3^{xvi}—K3—F2^{xvii}	77.38 (3)	K2—F6—K1^{xix}	168.70 (4)
Li1^{x}—K3—F2^{xvii}	77.66 (7)	K2^{xxi}—F6—K1^{xix}	88.891 (10)
F4^{xiv}—K3—F5^{xv}	81.66 (2)	Li1^{x}—F6—K1^{xviii}	77.59 (7)
F4^{xii}—K3—F5^{xv}	81.66 (2)	K3^{xxxvi}—F6—K1^{xviii}	85.13 (3)
F6^{xv}—K3—F5^{xv}	65.49 (4)	K2—F6—K1^{xviii}	88.892 (10)
F7^{x}—K3—F5^{xv}	68.77 (3)	K2^{xxi}—F6—K1^{xviii}	168.70 (4)

F3^{v}—K3—F5^{xv}	133.69 (2)	K1^{xix}—F6—K1^{xviii}	100.48 (4)
F3^{xvi}—K3—F5^{xv}	133.69 (2)	Li2—F7—K3^{xvii}	153.04 (13)
Li1^{x}—K3—F5^{xv}	145.44 (7)	Li2—F7—K2^{xxviii}	92.28 (9)
F2^{xvii}—K3—F5^{xv}	136.89 (3)	K3^{xvii}—F7—K2^{xxviii}	107.91 (4)
F5—Pr1—F3^{xviii}	96.53 (2)	Li2—F7—K2^{xvii}	92.28 (9)
F5—Pr1—F3^{xix}	96.53 (2)	K3^{xvii}—F7—K2^{xvii}	107.91 (4)
F3^{xviii}—Pr1—F3^{xix}	147.44 (4)	K2^{xxviii}—F7—K2^{xvii}	81.49 (4)
F5—Pr1—F2	148.56 (4)	Li2—F7—K2^{xi}	77.81 (7)
F3^{xviii}—Pr1—F2	92.10 (2)	K3^{xvii}—F7—K2^{xi}	85.39 (3)
F3^{xix}—Pr1—F2	92.10 (2)	K2^{xxviii}—F7—K2^{xi}	164.59 (4)
F5—Pr1—F1	138.64 (4)	K2^{xvii}—F7—K2^{xi}	87.078 (7)
F3^{xviii}—Pr1—F1	75.24 (2)	Li2—F7—K2^{xxix}	77.81 (7)
F3^{xix}—Pr1—F1	75.24 (2)	K3^{xvii}—F7—K2^{xxix}	85.39 (3)
F2—Pr1—F1	72.81 (4)	K2^{xxviii}—F7—K2^{xxix}	87.078 (7)
F5—Pr1—F8^{xx}	70.11 (4)	K2^{xvii}—F7—K2^{xxix}	164.59 (4)
F3^{xviii}—Pr1—F8^{xx}	78.33 (2)	K2^{xi}—F7—K2^{xxix}	102.07 (4)
F3^{xix}—Pr1—F8^{xx}	78.33 (2)	Li2—F8—Pr1^{vi}	163.01 (13)
F2—Pr1—F8^{xx}	141.33 (4)	Li2—F8—K1^{i}	90.34 (9)
F1—Pr1—F8^{xx}	68.53 (4)	Pr1^{vi}—F8—K1^{i}	102.45 (3)
F5—Pr1—F4^{xxi}	76.48 (3)	Li2—F8—K1^{xxiii}	90.34 (9)
F3^{xviii}—Pr1—F4^{xxi}	140.09 (3)	Pr1^{vi}—F8—K1^{xxiii}	102.45 (3)
F3^{xix}—Pr1—F4^{xxi}	72.17 (3)	K1^{i}—F8—K1^{xxiii}	81.52 (3)
F2—Pr1—F4^{xxi}	77.55 (3)	Li2—F8—K2^{xxix}	76.53 (7)
F1—Pr1—F4^{xxi}	134.52 (3)	Pr1^{vi}—F8—K2^{xxix}	92.84 (3)
F8^{xx}—Pr1—F4^{xxi}	131.95 (3)	K1^{i}—F8—K2^{xxix}	162.49 (4)
F5—Pr1—F4	76.48 (3)	K1^{xxiii}—F8—K2^{xxix}	86.943 (11)
F3^{xviii}—Pr1—F4	72.17 (3)	Li2—F8—K2^{xi}	76.53 (7)
F3^{xix}—Pr1—F4	140.09 (3)	Pr1^{vi}—F8—K2^{xi}	92.84 (3)
F2—Pr1—F4	77.55 (3)	K1^{i}—F8—K2^{xi}	86.943 (11)
F1—Pr1—F4	134.52 (3)	K1^{xxiii}—F8—K2^{xi}	162.49 (4)
F8^{xx}—Pr1—F4	131.95 (3)	K2^{xxix}—F8—K2^{xi}	100.92 (4)

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*−1/2, *y*, −*z*+1/2; (xxi) *x*, −*y*+1/2, *z*; (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.