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Rubidium hexafluoridoiridate(IV)

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Key indicators: single-crystal X-ray study; T = 296 K; mean σ(Ir–F) = 0.002 Å; R factor = 0.009; wR factor = 0.024; data-to-parameter ratio = 13.9.

$Rb_2[IrF_6]$ possesses a framework structure constructed from Rb^+ cations and $[IrF_6]^{2-}$ complex anions. The cation is 12-coordinated by F atoms, forming a slightly distorted anticuboctahedron; the anion has the shape of an almost ideal octahedron. Rb, Ir and F atoms are located on special positions of $3m$, $\bar{3}m$ and m symmetry, respectively.

Related literature

The title compound was first characterized by X-ray powder diffraction (Babel, 1967). It is isomorphous with the potassium ($K_2[IrF_6]$; Fitz *et al.*, 2002) and caesium analogues ($Cs_2[IrF_6]$; Smolentsev, Gubanov, Naumov & Danilenko, 2007). The alkaline earth metal hexafluoridoiridates $Ca[IrF_6]\cdot 2H_2O$, $Sr[IrF_6]\cdot 2H_2O$ and $Ba[IrF_6]$ were recently reported (Smolentsev, Gubanov & Danilenko, 2007).

Experimental

Crystal data

$Rb_2[IrF_6]$
M_r = 477.14
Trigonal, $P\bar{3}m1$
a = 5.9718 (2) Å
c = 4.7939 (2) Å
V = 148.06 (1) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 38.91 mm^{-1}
T = 296 (2) K
0.14 × 0.06 × 0.06 mm

Data collection

Bruker–Nonius X8 APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.074, T_{max} = 0.091
(expected range = 0.079–0.097)
1328 measured reflections
181 independent reflections
180 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.009
$wR(F^2)$ = 0.024
S = 1.21
181 reflections
13 parameters
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −1.16 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ir1—F1	1.9328 (19)	Rb1—F1	3.0101 (3)
Rb1—F1^{i}	2.9511 (19)	Rb1—F1^{ii}	3.080 (2)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2004); program(s) used to refine structure: *SHELXTL*; molecular graphics: *BS* (Ozawa & Kang, 2004) and *POV-RAY* (Cason, 2002); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MG2039).

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supplementary materials

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Comment

In $Rb_2[IrF_6]$, the Rb^+ cation is coordinated to twelve F atoms belonging to six anions, forming a slightly distorted anticuboctahedron. Each anion, in the form of a nearly ideal octahedron, interconnects twelve cations (Fig. 1). The Rb–F distances have slightly different values. Anticuboctahedra share all their rectangular faces and two triangular faces with each other, and share three other triangular faces with octahedra, giving rise to the framework structure (Fig. 2).

Experimental

Rb_2CO_3 was reacted with an aqueous solution of $H_2[IrF_6]$ acid. Subsequent slow evaporation at room temperature yielded light-pink crystals in the form of needles or hexagonal plates of the title compound. The precursor, $H_2[IrF_6]$, was prepared as described in Smolentsev, Gubanov & Danilenko, (2007).

Refinement

The maximum peak and deepest hole are located 0.84 Å and 0.81 Å, both from Ir1.

Figures

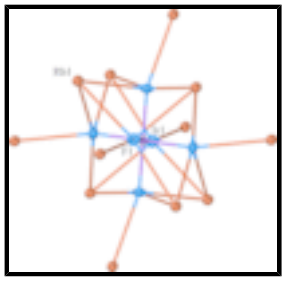

Fig. 1. A fragment of the $Rb_2[IrF_6]$ structure showing the complex anion surrounded by the cations. Displacement ellipsoids are drawn at the 50% probability level.

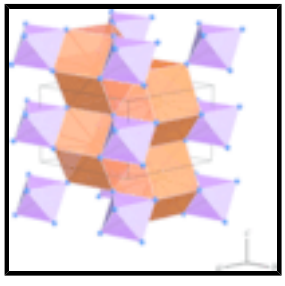

Fig. 2. Packing diagram for $Rb_2[IrF_6]$, viewed in perspective, with Rb-centered anticuboctahedra (orange) and Ir-centered octahedra (purple).

Rubidium hexafluoridoiridate(IV)

Crystal data

$Rb_2[IrF_6]$
$M_r = 477.14$
Trigonal, $P\bar{3}m1$
Hall symbol: -P 3 2"
$a = 5.9718$ (2) Å
$b = 5.9718$ (2) Å
$c = 4.7939$ (2) Å
$\alpha = 90°$
$\beta = 90°$
$\gamma = 120°$
$V = 148.057$ (9) Å^3
$Z = 1$
$F_{000} = 205$
$D_x = 5.351$ Mg m^{-3}
Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 1219 reflections
$\theta = 3.9–29.7°$
$\mu = 38.91$ mm^{-1}
$T = 296$ (2) K
Needle, light-pink
0.14 × 0.06 × 0.06 mm

Data collection

Bruker–Nonius X8 APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
Detector resolution: 25 pixels mm^{-1}
$T = 296(2)$ K
φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2004)
$T_{min} = 0.074$, $T_{max} = 0.091$
1328 measured reflections
181 independent reflections
180 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 29.9°$
$\theta_{min} = 3.9°$
$h = -8\rightarrow8$
$k = -8\rightarrow8$
$l = -6\rightarrow3$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.009$
$wR(F^2) = 0.024$
$S = 1.21$
181 reflections
13 parameters
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0105P)^2 + 0.2201P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.60$ e Å^{-3}
$\Delta\rho_{min} = -1.16$ e Å^{-3}
Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.029 (2)

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 $F^2 > 2\text{sigma}(F^2)$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ir1	0.0000	0.0000	0.5000	0.01235 (12)
Rb1	0.6667	0.3333	0.20338 (12)	0.01942 (13)
F1	0.15652 (18)	0.3130 (4)	0.2798 (4)	0.0224 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ir1	0.01143 (13)	0.01143 (13)	0.01420 (16)	0.00571 (7)	0.000	0.000
Rb1	0.01815 (17)	0.01815 (17)	0.0219 (2)	0.00908 (8)	0.000	0.000
F1	0.0230 (7)	0.0175 (9)	0.0249 (8)	0.0088 (4)	0.0032 (4)	0.0065 (7)

Geometric parameters (Å, °)

Ir1—F1^{i}	1.9328 (19)	Rb1—F1^{xi}	3.0101 (3)
Ir1—F1^{ii}	1.9328 (19)	Rb1—F1^{iii}	3.0101 (3)
Ir1—F1^{iii}	1.9328 (19)	Rb1—F1^{xii}	3.0101 (3)
Ir1—F1^{iv}	1.9328 (19)	Rb1—F1	3.0101 (3)
Ir1—F1	1.9328 (19)	Rb1—F1^{xiii}	3.080 (2)
Ir1—F1^{v}	1.9328 (19)	Rb1—F1^{xiv}	3.080 (2)
Rb1—F1^{vi}	2.9511 (19)	Rb1—F1^{ii}	3.080 (2)
Rb1—F1^{vii}	2.9511 (19)	F1—Rb1^{xv}	2.9511 (19)
Rb1—F1^{viii}	2.9511 (19)	F1—Rb1^{xvi}	3.0101 (3)
Rb1—F1^{ix}	3.0101 (3)	F1—Rb1^{xvii}	3.080 (2)
Rb1—F1^{x}	3.0101 (3)		
F1^{i}—Ir1—F1^{ii}	180.00 (10)	F1^{ix}—Rb1—F1	165.46 (7)
F1^{i}—Ir1—F1^{iii}	93.01 (8)	F1^{x}—Rb1—F1	118.542 (16)
F1^{ii}—Ir1—F1^{iii}	86.99 (8)	F1^{xi}—Rb1—F1	118.542 (16)
F1^{i}—Ir1—F1^{iv}	86.99 (8)	F1^{iii}—Rb1—F1	55.52 (7)
F1^{ii}—Ir1—F1^{iv}	93.01 (8)	F1^{xii}—Rb1—F1	63.49 (7)

F1^{iii}—Ir1—F1^{iv}	180.0	F1^{vi}—Rb1—F1^{xiii}	105.27 (6)
F1^{i}—Ir1—F1	93.01 (8)	F1^{vii}—Rb1—F1^{xiii}	144.63 (2)
F1^{ii}—Ir1—F1	86.99 (8)	F1^{viii}—Rb1—F1^{xiii}	144.63 (2)
F1^{iii}—Ir1—F1	93.01 (8)	F1^{ix}—Rb1—F1^{xiii}	51.80 (6)
F1^{iv}—Ir1—F1	86.99 (8)	F1^{x}—Rb1—F1^{xiii}	51.80 (6)
F1^{i}—Ir1—F1^{v}	86.99 (8)	F1^{xi}—Rb1—F1^{xiii}	85.57 (4)
F1^{ii}—Ir1—F1^{v}	93.01 (8)	F1^{iii}—Rb1—F1^{xiii}	85.57 (4)
F1^{iii}—Ir1—F1^{v}	86.99 (8)	F1^{xii}—Rb1—F1^{xiii}	113.70 (3)
F1^{iv}—Ir1—F1^{v}	93.01 (8)	F1—Rb1—F1^{xiii}	113.70 (3)
F1—Ir1—F1^{v}	180.00 (9)	F1^{vi}—Rb1—F1^{xiv}	144.63 (2)
F1^{vi}—Rb1—F1^{vii}	64.92 (6)	F1^{vii}—Rb1—F1^{xiv}	144.63 (2)
F1^{vi}—Rb1—F1^{viii}	64.92 (6)	F1^{viii}—Rb1—F1^{xiv}	105.27 (6)
F1^{vii}—Rb1—F1^{viii}	64.92 (6)	F1^{ix}—Rb1—F1^{xiv}	85.57 (4)
F1^{vi}—Rb1—F1^{ix}	63.40 (7)	F1^{x}—Rb1—F1^{xiv}	113.70 (3)
F1^{vii}—Rb1—F1^{ix}	128.10 (2)	F1^{xi}—Rb1—F1^{xiv}	51.80 (6)
F1^{viii}—Rb1—F1^{ix}	96.72 (4)	F1^{iii}—Rb1—F1^{xiv}	113.70 (3)
F1^{vi}—Rb1—F1^{x}	63.40 (7)	F1^{xii}—Rb1—F1^{xiv}	51.80 (6)
F1^{vii}—Rb1—F1^{x}	96.72 (4)	F1—Rb1—F1^{xiv}	85.57 (4)
F1^{viii}—Rb1—F1^{x}	128.10 (2)	F1^{xiii}—Rb1—F1^{xiv}	61.90 (6)
F1^{ix}—Rb1—F1^{x}	55.52 (7)	F1^{vi}—Rb1—F1^{ii}	144.63 (2)
F1^{vi}—Rb1—F1^{xi}	96.72 (4)	F1^{vii}—Rb1—F1^{ii}	105.27 (6)
F1^{vii}—Rb1—F1^{xi}	128.10 (2)	F1^{viii}—Rb1—F1^{ii}	144.63 (2)
F1^{viii}—Rb1—F1^{xi}	63.40 (7)	F1^{ix}—Rb1—F1^{ii}	113.70 (3)
F1^{ix}—Rb1—F1^{xi}	63.49 (7)	F1^{x}—Rb1—F1^{ii}	85.57 (4)
F1^{x}—Rb1—F1^{xi}	118.542 (16)	F1^{xi}—Rb1—F1^{ii}	113.70 (3)
F1^{vi}—Rb1—F1^{iii}	96.72 (4)	F1^{iii}—Rb1—F1^{ii}	51.80 (6)
F1^{vii}—Rb1—F1^{iii}	63.40 (7)	F1^{xii}—Rb1—F1^{ii}	85.57 (4)
F1^{viii}—Rb1—F1^{iii}	128.10 (2)	F1—Rb1—F1^{ii}	51.80 (6)
F1^{ix}—Rb1—F1^{iii}	118.542 (16)	F1^{xiii}—Rb1—F1^{ii}	61.90 (6)
F1^{x}—Rb1—F1^{iii}	63.49 (7)	F1^{xiv}—Rb1—F1^{ii}	61.90 (6)
F1^{xi}—Rb1—F1^{iii}	165.46 (7)	Ir1—F1—Rb1^{xv}	161.40 (10)
F1^{vi}—Rb1—F1^{xii}	128.10 (2)	Ir1—F1—Rb1^{xvi}	95.49 (4)
F1^{vii}—Rb1—F1^{xii}	96.72 (4)	Rb1^{xv}—F1—Rb1^{xvi}	83.28 (4)
F1^{viii}—Rb1—F1^{xii}	63.40 (7)	Ir1—F1—Rb1	95.49 (4)
F1^{ix}—Rb1—F1^{xii}	118.542 (16)	Rb1^{xv}—F1—Rb1	83.28 (4)
F1^{x}—Rb1—F1^{xii}	165.46 (7)	Rb1^{xvi}—F1—Rb1	165.46 (7)
F1^{xi}—Rb1—F1^{xii}	55.52 (7)	Ir1—F1—Rb1^{xvii}	93.32 (7)
F1^{iii}—Rb1—F1^{xii}	118.542 (16)	Rb1^{xv}—F1—Rb1^{xvii}	105.27 (6)
F1^{vi}—Rb1—F1	128.10 (2)	Rb1^{xvi}—F1—Rb1^{xvii}	94.43 (4)
F1^{vii}—Rb1—F1	63.40 (7)	Rb1—F1—Rb1^{xvii}	94.43 (4)
F1^{viii}—Rb1—F1	96.72 (4)		

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

Fig. 1

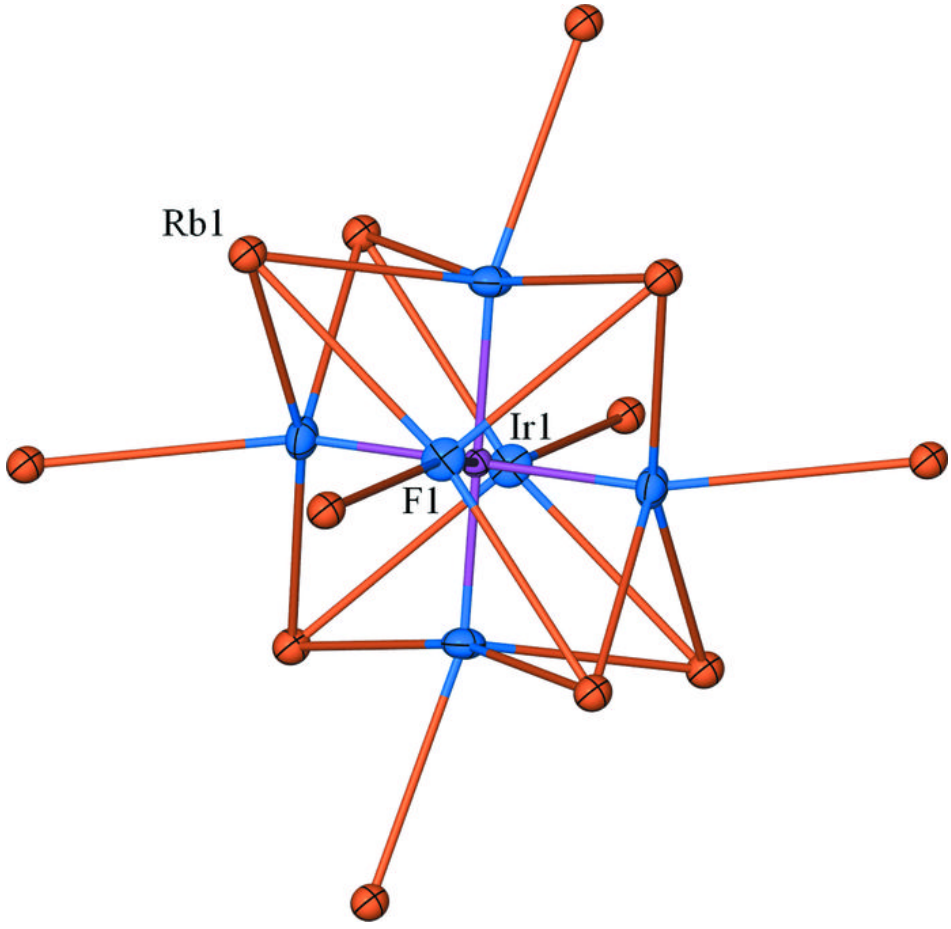
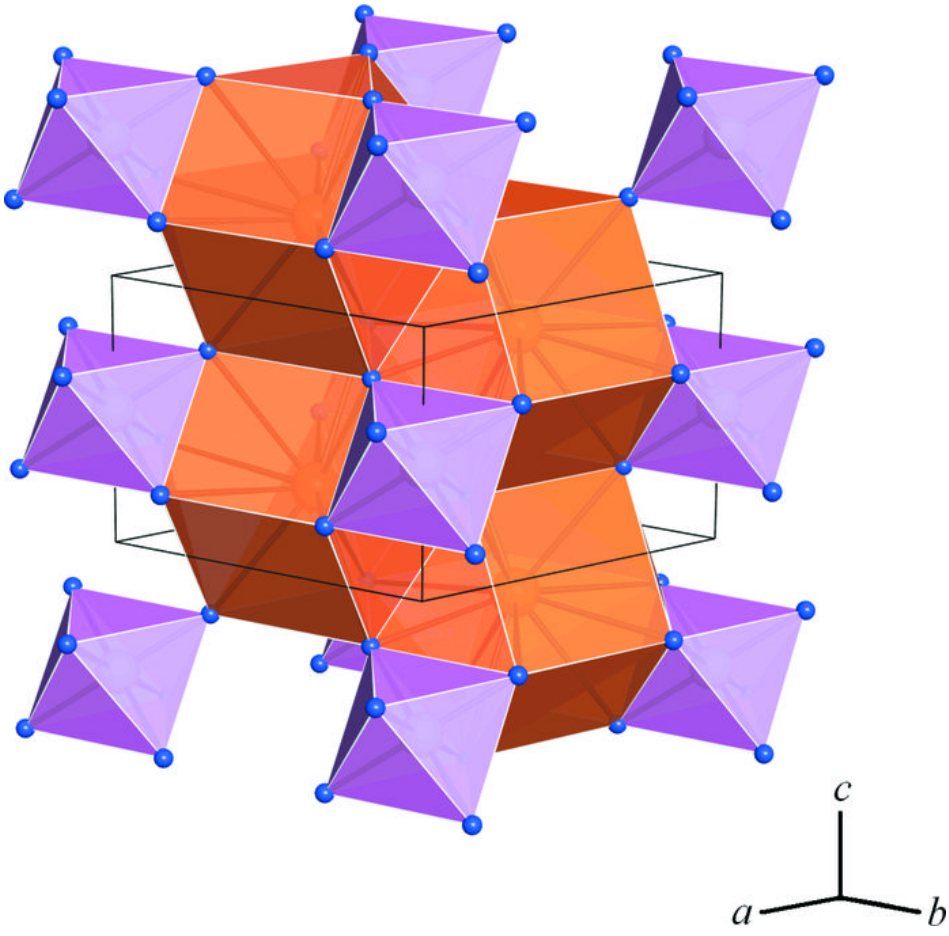
Fig. 2