Caesium hexafluoridoiridate(IV)

Anton I. Smolentsev,[a]* Alexander I. Gubanov,[a,b] Dmitry Yu. Naumov[a] and Andrey M. Danilenko[a]

[a]Nikolaev Institute of Inorganic Chemistry, SB Russian Academy of Sciences, Akademician Lavrentiev Prospekt 3, Novosibirsk 90, 630090, Russian Federation, and [b]Novosibirsk State University, Pirogova Street 2, Novosibirsk 90, 630090, Russian Federation

Correspondence e-mail: smolentsev@ngs.ru

$Cs_2[IrF_6]$ possesses a framework structure constructed from Cs^+ cations and $[IrF_6]^{2-}$ complex anions. The cation is 12-coordinated by F atoms, forming a slightly distorted anti-cuboctahedron; the anion has the shape of an almost ideal octahedron. Cs, Ir and F atoms are located on special positions of $3m$, $\overline{3}m$ 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 analogue, $K_2[IrF_6]$ (Fitz *et al.*, 2002). The stucture of $Rb_2[IrF_6]$ has also been reported (Smolentsev, Gubanov, Naumov & Danilenko, 2007). The precursor, $H_2[IrF_6]$, was prepared as described by Smolentsev, Gubanov & Danilenko (2007).

Experimental

Crystal data

$Cs_2[IrF_6]$	$Z = 1$
$M_r = 572.02$	Mo $K\alpha$ radiation
Trigonal, $P\overline{3}m1$	$\mu = 30.40$ mm^{-1}
$a = 6.2421$ (3) Å	$T = 296$ (2) K
$c = 5.0084$ (5) Å	$0.08 \times 0.06 \times 0.04$ mm
$V = 169.00$ (2) Å^3	

Data collection

Bruker–Nonius X8 APEXII diffractometer	1513 measured reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)	211 independent reflections
$T_{min} = 0.134$, $T_{max} = 0.288$	207 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.019$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.013$	13 parameters
$wR(F^2) = 0.028$	$\Delta\rho_{max} = 1.03$ e Å^{-3}
$S = 1.06$	$\Delta\rho_{min} = -0.49$ e Å^{-3}
211 reflections	

Table 1
Selected bond lengths (Å).

Ir1—F1	1.941 (2)	Cs1—F1	3.1564 (4)
Cs1—F1^i	3.140 (2)	Cs1—F1^{ii}	3.252 (3)

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*.

References

Babel, D. (1967). *Structure and Bonding*, Vol. 3, pp. 1–87. Berlin, Heidelberg, New York: Springer-Verlag.

Bruker (2004). *APEX2* (Version 1.08), *SAINT* (Version 7.03), *SADABS* (Version 2.11) and *SHELXTL* (Version 6.12). Bruker AXS Inc., Madison, Wisconsin, USA.

Cason, C. J. (2002). *POV-RAY for Windows*. Version 3.5. http://www.povray.org.

Fitz, H., Müller, B. G., Graudejus, O. & Bartlett, N. (2002). *Z. Anorg. Allg. Chem.* **628**, 133–137.

Ozawa, T. C. & Kang, S. J. (2004). *Balls & Sticks (BS)*. Version 1.51. http://www.softbug.com/toycrate/bs.

Smolentsev, A. I., Gubanov, A. I. & Danilenko, A. M. (2007). *Acta Cryst.* C63, i99–i101.

Smolentsev, A. I., Gubanov, A. I., Naumov, D. Yu. & Danilenko, A. M. (2007). *Acta Cryst.* E63, i200.

supplementary materials

Caesium hexafluoridoiridate(IV)

A. I. Smolentsev, A. I. Gubanov, D. Y. Naumov and A. M. Danilenko

Comment

For general discussion and comments on the figures, see Smolentsev, Gubanov, Naumov & Danilenko (2007).

Experimental

Cs_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

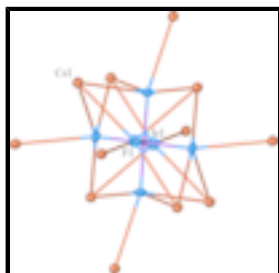The maximum peak and deepest hole are located 0.82 Å and 0.70 Å, both from Ir1.

Figures

Fig. 1. A fragment of the $Cs_2[IrF_6]$ structure showing the complex anion surrounded by the cations. Displacement ellipsoids are drawn at the 50% probability level.
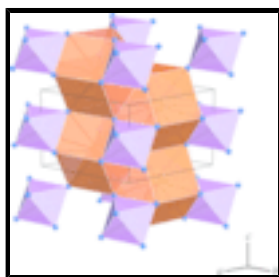

Fig. 2. Packing diagram for $Cs_2[IrF_6]$, viewed in perspective, with Cs-centered anticuboctahedra (orange) and Ir-centered octahedra (purple).

Caesium hexafluoridoiridate(IV)

Crystal data

$Cs_2[IrF_6]$	$Z = 1$
$M_r = 572.02$	$F_{000} = 241$
Trigonal, $P\bar{3}m1$	$D_x = 5.620$ Mg m^{-3}

Hall symbol: -P 3 2"

a = 6.2421 (3) Å

b = 6.2421 (3) Å

c = 5.0084 (5) Å

α = 90º

β = 90º

γ = 120º

V = 169.00 (2) Å^3

Mo $K\alpha$ radiation
λ = 0.71073 Å

Cell parameters from 982 reflections

θ = 3.8–30.0º

μ = 30.40 mm^{-1}

T = 296 (2) K

Needle, light-pink

0.08 × 0.06 × 0.04 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} = 0.134, T_{max} = 0.288

1513 measured reflections

211 independent reflections

207 reflections with $I > 2\sigma(I)$

R_{int} = 0.019

θ_{max} = 30.0º

θ_{min} = 3.8º

$h = -8\rightarrow8$

$k = -8\rightarrow5$

$l = -7\rightarrow7$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.013

$wR(F^2)$ = 0.028

S = 1.06

211 reflections

13 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

$w = 1/[\sigma^2(F_o^2) + (0.0133P)^2 + 0.3436P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max}$ = 1.04 e Å^{-3}

$\Delta\rho_{min}$ = −0.49 e Å^{-3}

Extinction correction: SHELXL97,
$Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0058 (8)

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 calculat-

ing *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	0.01382 (13)
Cs1	0.6667	0.3333	0.19957 (9)	0.02036 (14)
F1	0.1497 (2)	0.2995 (4)	0.2862 (5)	0.0233 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ir1	0.01221 (14)	0.01221 (14)	0.0171 (2)	0.00610 (7)	0.000	0.000
Cs1	0.01903 (16)	0.01903 (16)	0.0230 (3)	0.00951 (8)	0.000	0.000
F1	0.0245 (10)	0.0171 (12)	0.0258 (13)	0.0085 (6)	0.0037 (5)	0.0075 (10)

Geometric parameters (Å, °)

Ir1—F1^i	1.941 (2)	Cs1—F1^{xii}	3.140 (2)
Ir1—F1^{ii}	1.941 (2)	Cs1—F1^{xiii}	3.1564 (4)
Ir1—F1^{iii}	1.941 (2)	Cs1—F1^{xiv}	3.1564 (4)
Ir1—F1^{iv}	1.941 (2)	Cs1—F1^{xv}	3.1564 (4)
Ir1—F1	1.941 (2)	Cs1—F1	3.1564 (4)
Ir1—F1^v	1.941 (2)	Cs1—F1^v	3.1564 (4)
Ir1—Cs1^{vi}	3.9054 (2)	Cs1—F1^{xvi}	3.1564 (4)
Ir1—Cs1^{vii}	3.9054 (2)	Cs1—F1^{xvii}	3.252 (3)
Ir1—Cs1^{viii}	3.9054 (2)	Cs1—F1^{viii}	3.252 (3)
Ir1—Cs1^{ix}	3.9054 (2)	Cs1—F1^i	3.252 (3)
Ir1—Cs1	3.9054 (2)	F1—Cs1^{xii}	3.140 (2)
Ir1—Cs1^{iv}	3.9054 (2)	F1—Cs1^{vii}	3.1564 (4)
Cs1—F1^x	3.140 (2)	F1—Cs1^{viii}	3.252 (3)
Cs1—F1^{xi}	3.140 (2)		
F1^i—Ir1—F1^{ii}	180.00 (11)	F1^{xii}—Cs1—F1^{xiii}	129.02 (2)
F1^i—Ir1—F1^{iii}	92.50 (10)	F1^x—Cs1—F1^{xiv}	98.23 (4)
F1^{ii}—Ir1—F1^{iii}	87.50 (10)	F1^{xi}—Cs1—F1^{xiv}	129.02 (2)
F1^i—Ir1—F1^{iv}	92.50 (10)	F1^{xii}—Cs1—F1^{xiv}	63.06 (8)
F1^{ii}—Ir1—F1^{iv}	87.50 (10)	F1^{xiii}—Cs1—F1^{xiv}	118.14 (2)
F1^{iii}—Ir1—F1^{iv}	92.50 (10)	F1^x—Cs1—F1^{xv}	63.06 (8)
F1^i—Ir1—F1	87.50 (10)	F1^{xi}—Cs1—F1^{xv}	129.02 (2)
F1^{ii}—Ir1—F1	92.50 (10)	F1^{xii}—Cs1—F1^{xv}	98.23 (4)
F1^{iii}—Ir1—F1	87.50 (10)	F1^{xiii}—Cs1—F1^{xv}	52.74 (9)
F1^{iv}—Ir1—F1	180.00 (11)	F1^{xiv}—Cs1—F1^{xv}	66.00 (9)

F1^i—Ir1—F1^v	87.50 (10)	F1^x—Cs1—F1	129.02 (2)
F1^{ii}—Ir1—F1^v	92.50 (10)	F1^{xi}—Cs1—F1	63.06 (8)
F1^{iii}—Ir1—F1^v	180.0	F1^{xii}—Cs1—F1	98.23 (4)
F1^{iv}—Ir1—F1^v	87.50 (10)	F1^{xiii}—Cs1—F1	118.14 (2)
F1—Ir1—F1^v	92.50 (10)	F1^{xiv}—Cs1—F1	118.14 (2)
F1^i—Ir1—Cs1^{vi}	53.317 (7)	F1^{xv}—Cs1—F1	162.83 (9)
F1^{ii}—Ir1—Cs1^{vi}	126.683 (7)	F1^x—Cs1—F1^v	98.23 (4)
F1^{iii}—Ir1—Cs1^{vi}	123.86 (8)	F1^{xi}—Cs1—F1^v	63.06 (8)
F1^{iv}—Ir1—Cs1^{vi}	53.317 (7)	F1^{xii}—Cs1—F1^v	129.02 (2)
F1—Ir1—Cs1^{vi}	126.683 (7)	F1^{xiii}—Cs1—F1^v	66.00 (9)
F1^v—Ir1—Cs1^{vi}	56.14 (8)	F1^{xiv}—Cs1—F1^v	162.83 (9)
F1^i—Ir1—Cs1^{vii}	126.683 (7)	F1^{xv}—Cs1—F1^v	118.14 (2)
F1^{ii}—Ir1—Cs1^{vii}	53.317 (7)	F1—Cs1—F1^v	52.74 (9)
F1^{iii}—Ir1—Cs1^{vii}	56.14 (8)	F1^x—Cs1—F1^{xvi}	129.02 (2)
F1^{iv}—Ir1—Cs1^{vii}	126.683 (7)	F1^{xi}—Cs1—F1^{xvi}	98.23 (4)
F1—Ir1—Cs1^{vii}	53.317 (7)	F1^{xii}—Cs1—F1^{xvi}	63.06 (8)
F1^v—Ir1—Cs1^{vii}	123.86 (8)	F1^{xiii}—Cs1—F1^{xvi}	162.83 (9)
Cs1^{vi}—Ir1—Cs1^{vii}	180.0	F1^{xiv}—Cs1—F1^{xvi}	52.74 (9)
F1^i—Ir1—Cs1^{viii}	53.317 (7)	F1^{xv}—Cs1—F1^{xvi}	118.14 (2)
F1^{ii}—Ir1—Cs1^{viii}	126.683 (7)	F1—Cs1—F1^{xvi}	66.00 (9)
F1^{iii}—Ir1—Cs1^{viii}	53.317 (7)	F1^v—Cs1—F1^{xvi}	118.14 (2)
F1^{iv}—Ir1—Cs1^{viii}	123.86 (8)	F1^x—Cs1—F1^{xvii}	103.17 (7)
F1—Ir1—Cs1^{viii}	56.14 (8)	F1^{xi}—Cs1—F1^{xvii}	143.77 (3)
F1^v—Ir1—Cs1^{viii}	126.683 (7)	F1^{xii}—Cs1—F1^{xvii}	143.77 (3)
Cs1^{vi}—Ir1—Cs1^{viii}	106.101 (7)	F1^{xiii}—Cs1—F1^{xvii}	49.50 (7)
Cs1^{vii}—Ir1—Cs1^{viii}	73.899 (7)	F1^{xiv}—Cs1—F1^{xvii}	85.78 (5)
F1^i—Ir1—Cs1^{ix}	126.683 (7)	F1^{xv}—Cs1—F1^{xvii}	49.50 (7)
F1^{ii}—Ir1—Cs1^{ix}	53.317 (7)	F1—Cs1—F1^{xvii}	113.34 (3)
F1^{iii}—Ir1—Cs1^{ix}	126.683 (7)	F1^v—Cs1—F1^{xvii}	85.78 (5)
F1^{iv}—Ir1—Cs1^{ix}	56.14 (8)	F1^{xvi}—Cs1—F1^{xvii}	113.34 (3)
F1—Ir1—Cs1^{ix}	123.86 (8)	F1^x—Cs1—F1^{viii}	143.77 (3)
F1^v—Ir1—Cs1^{ix}	53.317 (7)	F1^{xi}—Cs1—F1^{viii}	143.77 (3)
Cs1^{vi}—Ir1—Cs1^{ix}	73.899 (7)	F1^{xii}—Cs1—F1^{viii}	103.17 (7)
Cs1^{vii}—Ir1—Cs1^{ix}	106.101 (7)	F1^{xiii}—Cs1—F1^{viii}	113.34 (3)
Cs1^{viii}—Ir1—Cs1^{ix}	180.0	F1^{xiv}—Cs1—F1^{viii}	49.50 (7)
F1^i—Ir1—Cs1	56.14 (8)	F1^{xv}—Cs1—F1^{viii}	85.78 (5)
F1^{ii}—Ir1—Cs1	123.86 (8)	F1—Cs1—F1^{viii}	85.78 (5)
F1^{iii}—Ir1—Cs1	126.683 (7)	F1^v—Cs1—F1^{viii}	113.34 (3)
F1^{iv}—Ir1—Cs1	126.683 (7)	F1^{xvi}—Cs1—F1^{viii}	49.50 (7)
F1—Ir1—Cs1	53.317 (7)	F1^{xvii}—Cs1—F1^{viii}	63.83 (7)
F1^v—Ir1—Cs1	53.317 (7)	F1^x—Cs1—F1^i	143.77 (3)

Cs1^{vi}—Ir1—Cs1	73.899 (7)	F1^{xi}—Cs1—F1^{i}	103.17 (7)
Cs1^{vii}—Ir1—Cs1	106.101 (7)	F1^{xii}—Cs1—F1^{i}	143.77 (3)
Cs1^{viii}—Ir1—Cs1	73.899 (7)	F1^{xiii}—Cs1—F1^{i}	85.78 (5)
Cs1^{ix}—Ir1—Cs1	106.101 (7)	F1^{xiv}—Cs1—F1^{i}	113.34 (3)
F1^{i}—Ir1—Cs1^{iv}	123.86 (8)	F1^{xv}—Cs1—F1^{i}	113.34 (3)
F1^{ii}—Ir1—Cs1^{iv}	56.14 (8)	F1—Cs1—F1^{i}	49.50 (7)
F1^{iii}—Ir1—Cs1^{iv}	53.317 (7)	F1^{v}—Cs1—F1^{i}	49.50 (7)
F1^{iv}—Ir1—Cs1^{iv}	53.317 (7)	F1^{xvi}—Cs1—F1^{i}	85.78 (5)
F1—Ir1—Cs1^{iv}	126.683 (7)	F1^{xvii}—Cs1—F1^{i}	63.83 (7)
F1^{v}—Ir1—Cs1^{iv}	126.683 (7)	F1^{viii}—Cs1—F1^{i}	63.83 (7)
Cs1^{vi}—Ir1—Cs1^{iv}	106.101 (7)	Ir1—F1—Cs1^{xii}	162.69 (12)
Cs1^{vii}—Ir1—Cs1^{iv}	73.899 (7)	Ir1—F1—Cs1^{vii}	97.14 (4)
Cs1^{viii}—Ir1—Cs1^{iv}	106.101 (7)	Cs1^{xii}—F1—Cs1^{vii}	81.77 (4)
Cs1^{ix}—Ir1—Cs1^{iv}	73.899 (7)	Ir1—F1—Cs1	97.14 (4)
Cs1—Ir1—Cs1^{iv}	180.0	Cs1^{xii}—F1—Cs1	81.77 (4)
F1^{x}—Cs1—F1^{xi}	66.39 (7)	Cs1^{vii}—F1—Cs1	162.83 (9)
F1^{x}—Cs1—F1^{xii}	66.39 (7)	Ir1—F1—Cs1^{viii}	94.15 (9)
F1^{xi}—Cs1—F1^{xii}	66.39 (7)	Cs1^{xii}—F1—Cs1^{viii}	103.17 (7)
F1^{x}—Cs1—F1^{xiii}	63.06 (8)	Cs1^{vii}—F1—Cs1^{viii}	94.22 (5)
F1^{xi}—Cs1—F1^{xiii}	98.23 (4)	Cs1—F1—Cs1^{viii}	94.22 (5)

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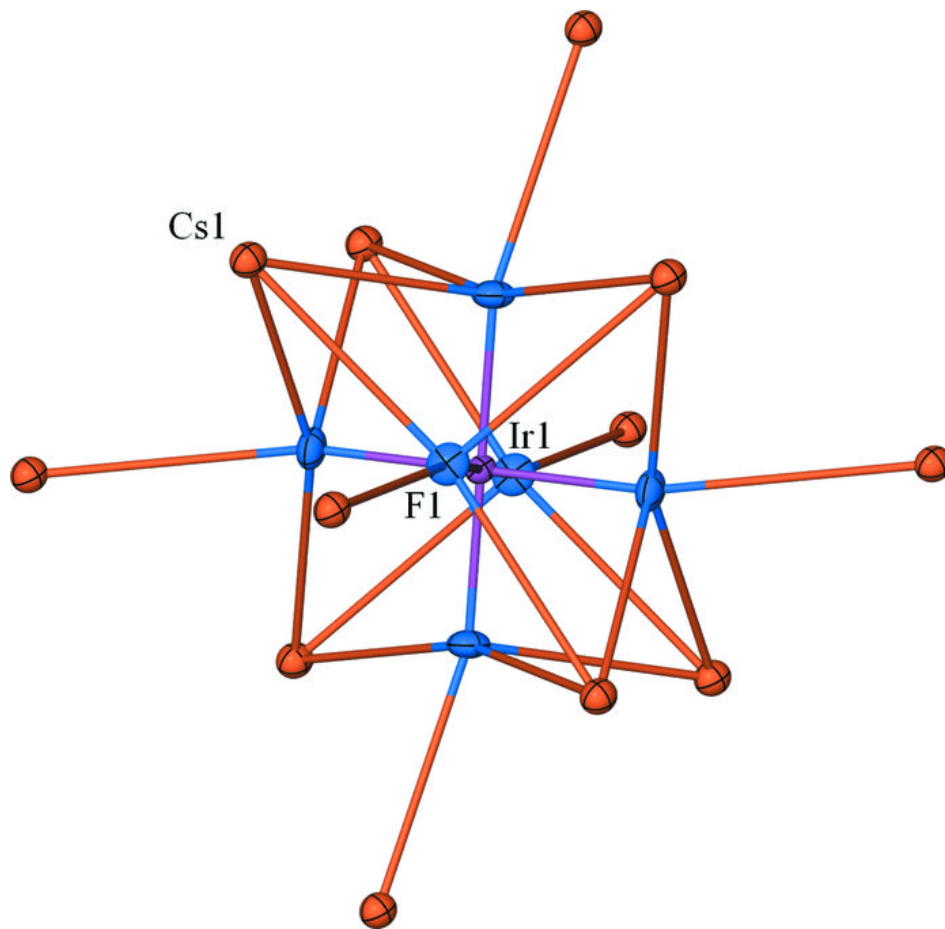
Fig. 1

Fig. 2