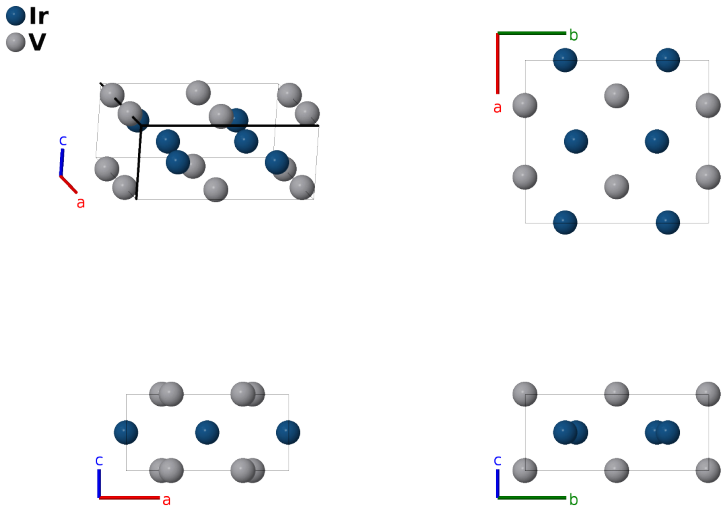
α-IrV Structure: AB_oC8_65_g_j-001

This structure originally had the label `AB_oC8_65_j_g`. Calls to that address will be redirected here.

Cite this page as: M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017

https://aflow.org/p/S2CY

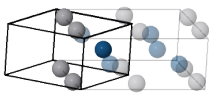
https://aflow.org/p/AB_oC8_65_g_j-001



Prototype	IrV
AFLOW prototype label	AB_oC8_65_g_j-001
ICSD	104590
Pearson symbol	oC8
Space group number	65
Space group symbol	$Cmmm$
AFLOW prototype command	`aflow --proto=AB_oC8_65_g_j-001 --params=`$a, b/a, c/a, x_1, y_2$

Base-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2$	=	$ax_1\,\hat{\mathbf{x}}$	(4g)	Ir I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2$	=	$-ax_1\,\hat{\mathbf{x}}$	(4g)	Ir I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4j)	V I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4j)	V I

References

[1] B. C. Giessen and N. J. Grant, *New intermediate phases in transition metal systems, III*, Acta Cryst. **18**, 1080–1081 (1965), doi:10.1107/S0365110X65002566.

Found in

[1] P. Villars and L. Calvert, *Pearson's Handbook of Crystallographic Data for Intermetallic Phases* (ASM International, Materials Park, OH, 1991), 2nd edn.