Molecular Iodine ($A14$) Structure: A_oC8_64_f-003

This structure originally had the label `A_oC8_64_f.I`. Calls to that address will be redirected here.

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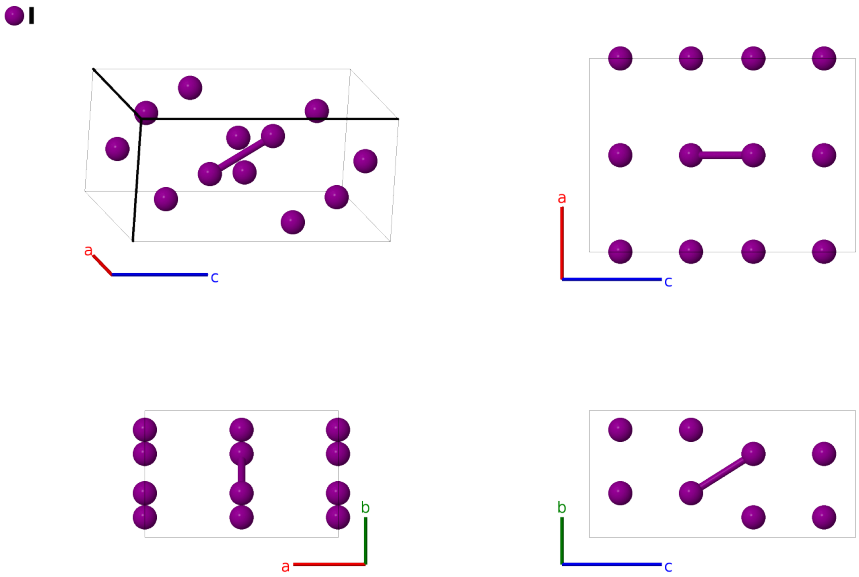
https://aflow.org/p/234K

https://aflow.org/p/A_oC8_64_f-003



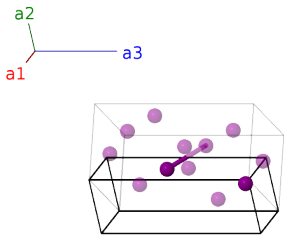
Prototype	I
AFLOW prototype label	A_oC8_64_f-003
***Strukturbericht* designation**	$A14$
ICSD	657497
Pearson symbol	oC8
Space group number	64
Space group symbol	$Cmce$
AFLOW prototype command	`aflow --proto=A_oC8_64_f-003 --params=`$a, b/a, c/a, y_1, z_1$

Other compounds with this structure
Br_2, Cl_2

- α-gallium ($A11$), molecular iodine ($A14$), and black phosphorous ($A17$) all share the same AFLOW label, A_oC8_64_f. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

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
$\mathbf{B_1}$	=	$-y_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$by_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(8f)	I I
$\mathbf{B_2}$	=	$\left(y_1 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	I I
$\mathbf{B_3}$	=	$-\left(y_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	I I
$\mathbf{B_4}$	=	$y_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-by_1\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(8f)	I I

References

[1] C. Petrillo, O. Moze, and R. M. Ibberson, *High resolution neutron powder diffraction investigation of the low temperature crystal structure of molecular iodine (I_2)*, Physica B **180**, 639–641 (1992), doi:10.1016/0921-4526(92)90420-W.

Found in

[1] M. Winter, *WebElements: the periodic table on the WWW (1993–2015)*. The University of Sheffield and WebElements Ltd.