

Molecular Iodine (A14) Structure: A_oC8_64_f-003

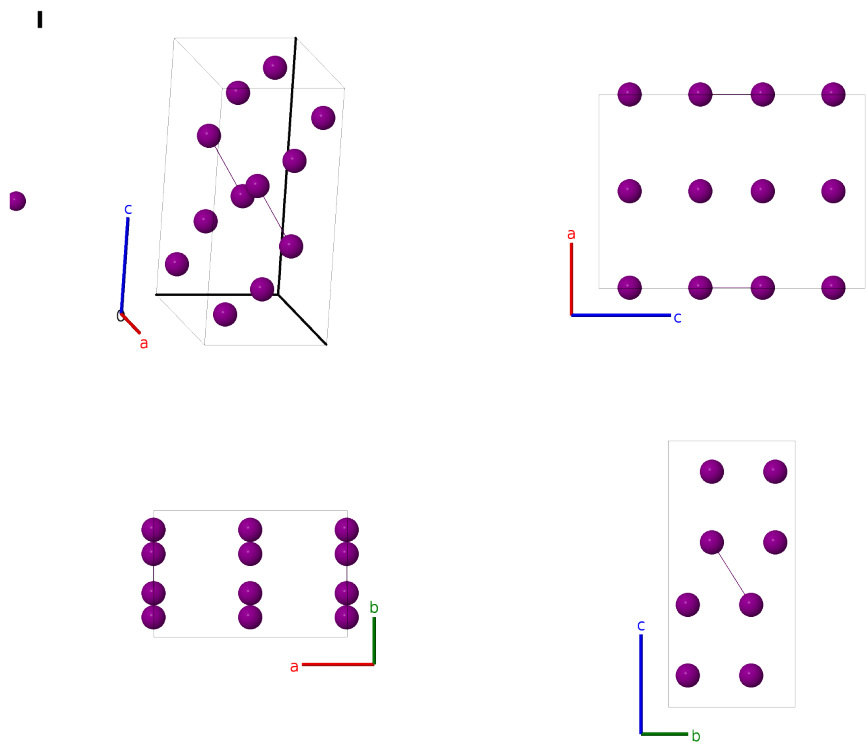
This structure previously used the label(s) **A_oC8_64_f.I**. Calls to these addresses will be redirected here.

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Osos, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/234K>

https://aflow.org/prototype-encyclopedia/A_oC8_64_f-003



Prototype	I
AFLOW prototype label	A_oC8_64_f-003
<i>Strukturbericht</i> designation	A14
ICSD	657497
CCDC	1766840
Pearson symbol	oC8
Space group number	64
Space group symbol	<i>Cmce</i>
AFLOW prototype command	<code>aflow --proto=A_oC8_64_f-003 --params=a, b/a, c/a, y₁, z₁</code>

Other compounds with this structure

Br₂, Cl₂

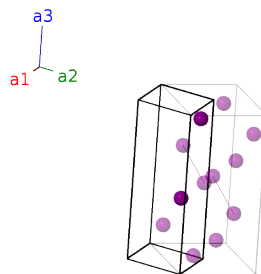
- α -gallium (A11), molecular iodine (A14), and black phosphorous (A17) all share the same AFLOW label, A_oC8_64.f. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

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.

First cited in

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. 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