δ-Bi_2O_3 Structure: AB8_cF36_225_a_f-001

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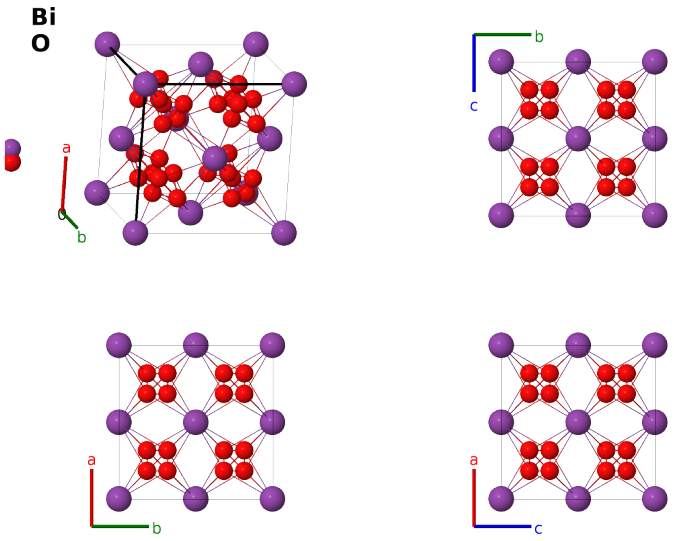
https://aflow.org/prototype-encyclopedia/X2Q7

https://aflow.org/prototype-encyclopedia/AB8_cF36_225_a_f-001



Prototype	Bi_2O_3
AFLOW prototype label	AB8_cF36_225_a_f-001
ICSD	2375
CCDC	1592277
Pearson symbol	cF36
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	`aflow --proto=AB8_cF36_225_a_f-001 --params=`a, x_2

Other compounds with this structure
α-CuI, γ-CuI

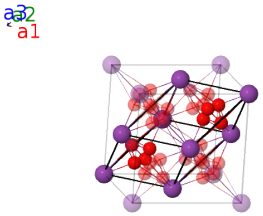
- Bi_2O_3 can be found in at least six forms (Harwig, 1978; Locherer, 2011):
  - monoclinic α-Bi_2O_3, the ground state, stable up to 729°,
  - tetragonal β-Bi_2O_3, $D5_{12}$, a metastable state observed at 650°C (this structure),

- body-centered cubic γ-Bi_2O_3, another metastable phase observed at 639°C,
- face-centered cubic δ-Bi_2O_3, the stable phase from 729° up to the melting point at 824°C (this structure),
- a high-pressure HP-Bi_2O_3, and
- a second "nonquenchable" high-pressure structure, HPC-Bi_2O_3.

- The oxygen sites are occupied 18.75% of the time. If $z_2 \to 1/4$, they coalesce on the (2c) Wyckoff position, and this becomes the fluorite ($C1$) structure.
- Other compounds with different stoichiometries have this structure. In copper(I) iodide both the high temperature α-CuI and the ground state γ-CuI phases are in this structure, with the copper atoms occupying 1/8 of the (32f) sites. (Keen, 1995)

Face-centered Cubic primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Bi I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(32f)	O I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 - 3x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(32f)	O I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 - 3x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(32f)	O I
$\mathbf{B_5}$	=	$-3x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(32f)	O I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + 3x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(32f)	O I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(32f)	O I
$\mathbf{B_8}$	=	$-x_2\,\mathbf{a}_1 + 3x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(32f)	O I
$\mathbf{B_9}$	=	$3x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(32f)	O I

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