GdSI Structure: ABC_hP12_174_aj_dk_ej-001

This structure originally had the label `ABC_hP12_174_cj_fk_aj`. Calls to that address will be redirected here.

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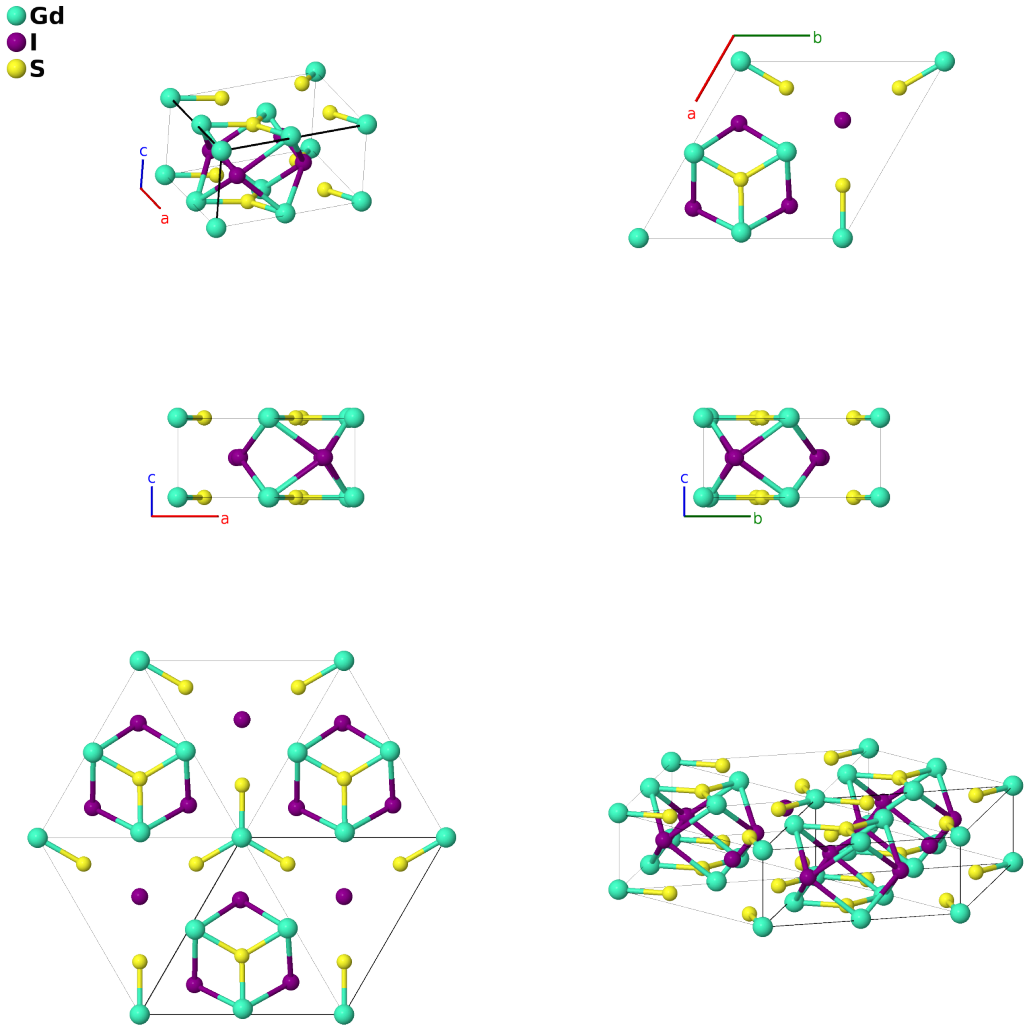
https://aflow.org/p/4BHM

https://aflow.org/p/ABC_hP12_174_aj_dk_ej-001



Prototype	GdIS
AFLOW prototype label	ABC_hP12_174_aj_dk_ej-001
ICSD	59203
Pearson symbol	hP12
Space group number	174
Space group symbol	$P\bar{6}$

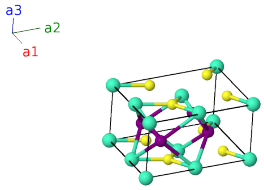
AFLOW prototype command `aflow --proto=ABC_hP12_174_aj_dk_ej-001 --params=`$a, c/a, x_4, y_4, x_5, y_5, x_6, y_6$

Other compounds with this structure
TbSI, DySI

- This is a major revision of the previously published version of this page in (Hicks, 2019), however the structure from that page is nearly identical to the structure found here. We have changed our reference from the original (Dagron, 1969) to the more accessible (Beck, 1986).
- This is a high-pressure phase of GdSI. At ambient pressure it is in the SmSI structure.
- The ICSD entry for this structure is incomplete, leaving out the (1a), (1d), and (1e) sites, apparently because of a misreading of Table 4 in (Beck, 1968).

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Gd I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(1d)	I I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}$	(1e)	S I
$\mathbf{B_4}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2$	=	$\frac{1}{2}a\,(x_4 + y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_4 - y_4)\,\hat{\mathbf{y}}$	(3j)	Gd II
$\mathbf{B_5}$	=	$-y_4\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2$	=	$\frac{1}{2}a\,(x_4 - 2y_4)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}$	(3j)	Gd II
$\mathbf{B_6}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$-\frac{1}{2}a\,(2x_4 - y_4)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}}$	(3j)	Gd II
$\mathbf{B_7}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2$	=	$\frac{1}{2}a\,(x_5 + y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_5 - y_5)\,\hat{\mathbf{y}}$	(3j)	S II
$\mathbf{B_8}$	=	$-y_5\,\mathbf{a}_1 + (x_5 - y_5)\,\mathbf{a}_2$	=	$\frac{1}{2}a\,(x_5 - 2y_5)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}}$	(3j)	S II
$\mathbf{B_9}$	=	$-(x_5 - y_5)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2$	=	$-\frac{1}{2}a\,(2x_5 - y_5)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_5\,\hat{\mathbf{y}}$	(3j)	S II
$\mathbf{B_{10}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3k)	I II
$\mathbf{B_{11}}$	=	$-y_6\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - 2y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3k)	I II
$\mathbf{B_{12}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3k)	I II

References

[1] H. P. Beck and C. Strobel, *Zur Hochdruckpolymorphie der Seltenerdsulfidiodide LnSI*, Z. Anorganische und Allgemeine Chemie **535**, 229–239 (1986), doi:10.1002/zaac.19865350427.

[2] C. Dagron and F. Thevet, *Répartition des types cristallins dans la série des iodosulfures et fluorosulfures des éléments des terres rares et d'yttrium*, C. R. Hebd. Séances Acad. Sci. C **268**, 1867–1869 (1969).

[3] D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1–S1011 (2019), doi:10.1016/j.commatsci.2018.10.043.

Found in

[1] P. Villars and K. Cenzual, *Pearson's Crystal Data – Crystal Structure Database for Inorganic Compounds* (2013). ASM International.