$GdSn_3$ Structure: AB3_oC16_38_ab_3a3b-001

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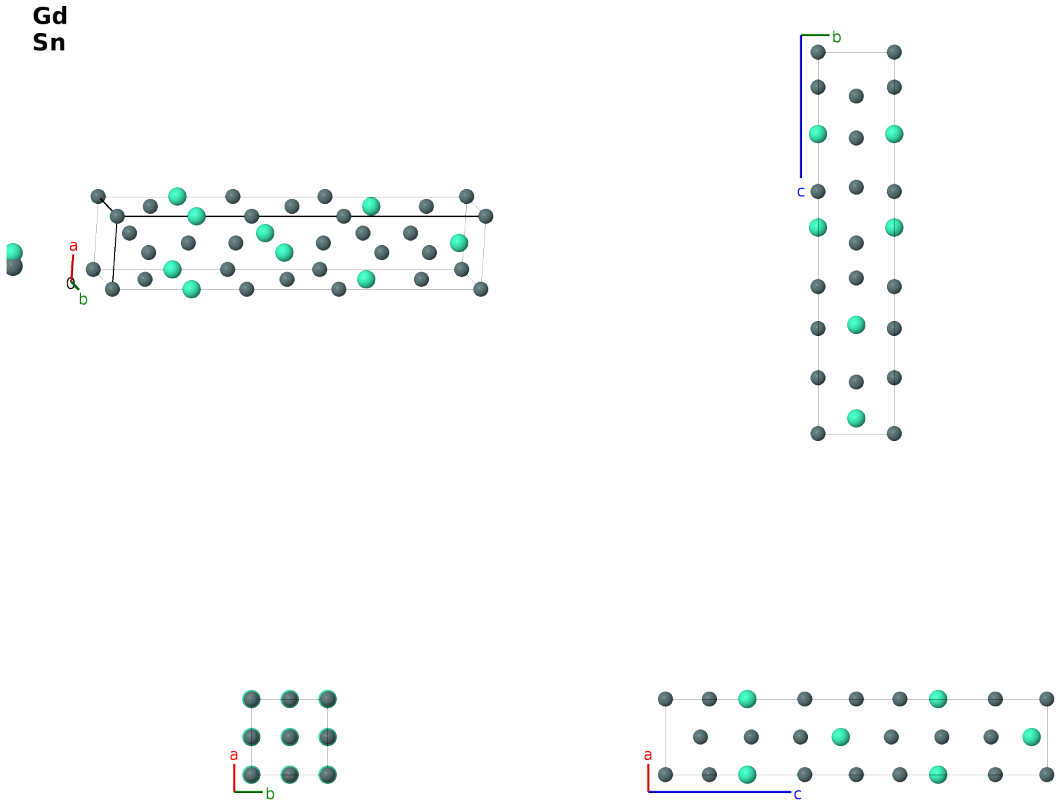
https://aflow.org/prototype-encyclopedia/L5S8

https://aflow.org/prototype-encyclopedia/AB3_oC16_38_ab_3a3b-001



Prototype	$GdSn_3$
AFLOW prototype label	AB3_oC16_38_ab_3a3b-001
ICSD	104154
CCDC	1662075
Pearson symbol	oC16
Space group number	38
Space group symbol	*Amm*2

AFLOW prototype command `aflow --proto=AB3_oC16_38_ab_3a3b-001 --params=`$a, b/a, c/a, z_1, z_2, z_3, z_4, z_5, z_6, z_7, z_8$

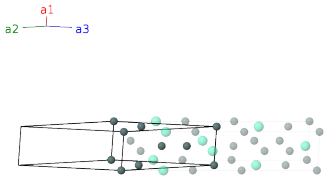
Other compounds with this structure

$DySn_3$, $HoSn_3$, $ReSn_3$, $TbSn_3$, $TmSn_3$, YSn_3

- (Palenzona, 1993) identify this as the low-temperature structure of $GdSn_3$, transforming into the $CuAu_3$ ($L1_2$) structure at high temperatures.
- (Palenzona, 1993) do not provide the coordinates for this structure within the paper, however ICSD entry 104154 gives the structure and lists this paper as the source.
- Space group $Amm2$ #38 does not specify the origin of the z-axis. Here it is fixed by setting $z_2 = 0$ for the Sn-I atom.

Base-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$-z_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Gd I
$\mathbf{B_2}$	=	$-z_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(2a)	Sn I
$\mathbf{B_3}$	=	$-z_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(2a)	Sn II
$\mathbf{B_4}$	=	$-z_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$cz_4\,\hat{\mathbf{z}}$	(2a)	Sn III
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_5\,\hat{\mathbf{z}}$	(2b)	Gd II
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_6\,\hat{\mathbf{z}}$	(2b)	Sn IV
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_7\,\hat{\mathbf{z}}$	(2b)	Sn V
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_8\,\hat{\mathbf{z}}$	(2b)	Sn VI

References

[1] A. Palenzona and P. Manfrinetti, *The tin-rich side of the rare earth-tin systems (R = Gd, Tb, Dy, Ho, Er, Tm, Lu and Y)*, J. Alloys Compd. **201**, 43–47 (1993), doi:10.1016/0925-8388(93)90859-L.

[2] F. Karlsruhe and NIST, *Inorganic Crystal Structure Database*, http://icsd.fiz-karlsruhe.de/.

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