NaTl ($B32$) Structure: AB_cF16_227_a_b-001

This structure previously used the label(s) `AB_cF16_227_a_b`. Calls to these addresses will be redirected here.

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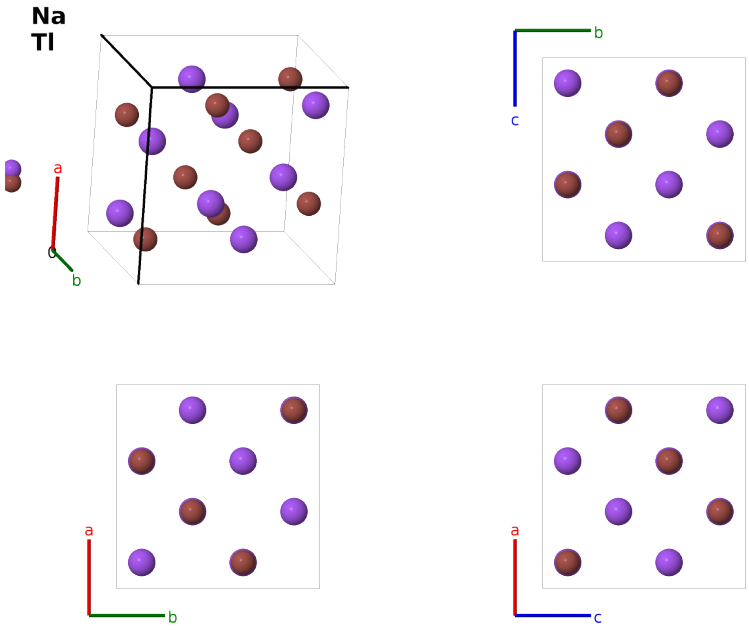
https://aflow.org/prototype-encyclopedia/CHL9

https://aflow.org/prototype-encyclopedia/AB_cF16_227_a_b-001



Prototype	NaTl
AFLOW prototype label	AB_cF16_227_a_b-001
***Strukturbericht* designation**	$B32$
ICSD	645049
CCDC	1761531
Pearson symbol	cF16
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	`aflow --proto=AB_cF16_227_a_b-001 --params=`a

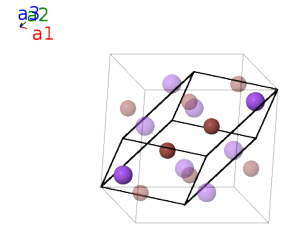
Other compounds with this structure

AlLi, AlMo, AlNb, AlTa, AlV, AlW, BLi, BaMg, CdLi (γ-LiCd), GaLi, InK, InLi, InNa, KNa, KTl, LaMg, LiZn (δ"), MgNd, MgSn, MoTa, MoV, MoW, NbMo, NbTa, NbV, NbW, TaV, TaW, VW

- This is an example of a Zintl Phase.

Face-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{8}\,\mathbf{a}_1 + \frac{1}{8}\,\mathbf{a}_2 + \frac{1}{8}\,\mathbf{a}_3$	=	$\frac{1}{8}a\,\hat{\mathbf{x}} + \frac{1}{8}a\,\hat{\mathbf{y}} + \frac{1}{8}a\,\hat{\mathbf{z}}$	(8a)	Na I
$\mathbf{B_2}$	=	$\frac{7}{8}\,\mathbf{a}_1 + \frac{7}{8}\,\mathbf{a}_2 + \frac{7}{8}\,\mathbf{a}_3$	=	$\frac{7}{8}a\,\hat{\mathbf{x}} + \frac{7}{8}a\,\hat{\mathbf{y}} + \frac{7}{8}a\,\hat{\mathbf{z}}$	(8a)	Na I
$\mathbf{B_3}$	=	$\frac{3}{8}\,\mathbf{a}_1 + \frac{3}{8}\,\mathbf{a}_2 + \frac{3}{8}\,\mathbf{a}_3$	=	$\frac{3}{8}a\,\hat{\mathbf{x}} + \frac{3}{8}a\,\hat{\mathbf{y}} + \frac{3}{8}a\,\hat{\mathbf{z}}$	(8b)	Tl I
$\mathbf{B_4}$	=	$\frac{5}{8}\,\mathbf{a}_1 + \frac{5}{8}\,\mathbf{a}_2 + \frac{5}{8}\,\mathbf{a}_3$	=	$\frac{5}{8}a\,\hat{\mathbf{x}} + \frac{5}{8}a\,\hat{\mathbf{y}} + \frac{5}{8}a\,\hat{\mathbf{z}}$	(8b)	Tl I

References

[1] K. Kuriyama, S. Saito, and K. Iwamura, *Ultrasonic study on the elastic moduli of the NaTl (B32) structure*, J. Phys. Chem. Solids **40**, 457–461 (1979), doi:10.1016/0022-3697(79)90062-3.

Found in

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

First cited in

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