

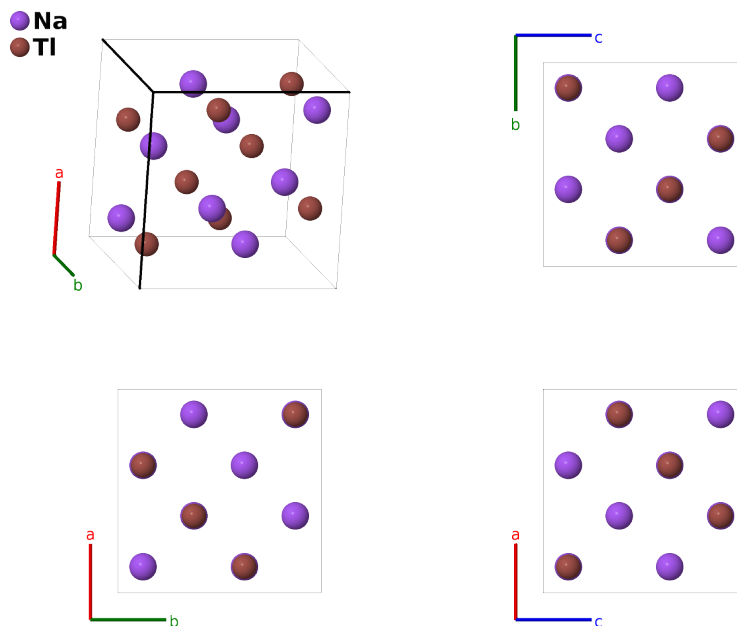
# NaTl (*B32*) Structure: AB\_cF16\_227\_a\_b-001

This structure originally had the label AB\_cF16\_227\_a\_b. Calls to that address will be redirected here.

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<https://aflow.org/p/CHL9>

[https://aflow.org/p/AB\\_cF16\\_227\\_a\\_b-001](https://aflow.org/p/AB_cF16_227_a_b-001)



Prototype	NaTl
AFLOW prototype label	AB_cF16_227_a_b-001
<i>Strukturbericht</i> designation	<i>B32</i>
ICSD	645049
Pearson symbol	cF16
Space group number	227
Space group symbol	$Fd\bar{3}m$
AFLOW prototype command	<code>aflow --proto=AB_cF16_227_a_b-001 --params=a</code>

## Other compounds with this structure

LiAl,  $\gamma$ -LiCd, LiGa, LiIn,  $\delta'$ -LiZn, NaIn

- This is an example of a Zintl Phase.

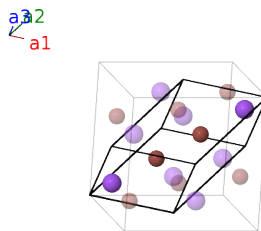
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## Face-centered Cubic primitive vectors

$$\mathbf{a}_1 = \frac{1}{2}a\hat{y} + \frac{1}{2}a\hat{z}$$

$$\mathbf{a}_2 = \frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{z}$$

$$\mathbf{a}_3 = \frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{y}$$



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## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{8}\mathbf{a}_1 + \frac{1}{8}\mathbf{a}_2 + \frac{1}{8}\mathbf{a}_3$	$=$	$\frac{1}{8}a\hat{x} + \frac{1}{8}a\hat{y} + \frac{1}{8}a\hat{z}$	(8a)	Na I
$\mathbf{B}_2$	$= \frac{7}{8}\mathbf{a}_1 + \frac{7}{8}\mathbf{a}_2 + \frac{7}{8}\mathbf{a}_3$	$=$	$\frac{7}{8}a\hat{x} + \frac{7}{8}a\hat{y} + \frac{7}{8}a\hat{z}$	(8a)	Na I
$\mathbf{B}_3$	$= \frac{3}{8}\mathbf{a}_1 + \frac{3}{8}\mathbf{a}_2 + \frac{3}{8}\mathbf{a}_3$	$=$	$\frac{3}{8}a\hat{x} + \frac{3}{8}a\hat{y} + \frac{3}{8}a\hat{z}$	(8b)	Tl I
$\mathbf{B}_4$	$= \frac{5}{8}\mathbf{a}_1 + \frac{5}{8}\mathbf{a}_2 + \frac{5}{8}\mathbf{a}_3$	$=$	$\frac{5}{8}a\hat{x} + \frac{5}{8}a\hat{y} + \frac{5}{8}a\hat{z}$	(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.