

C17 (Fe₂B) Structure (*Obsolete*): AB2_tI12_121_ab_i-001

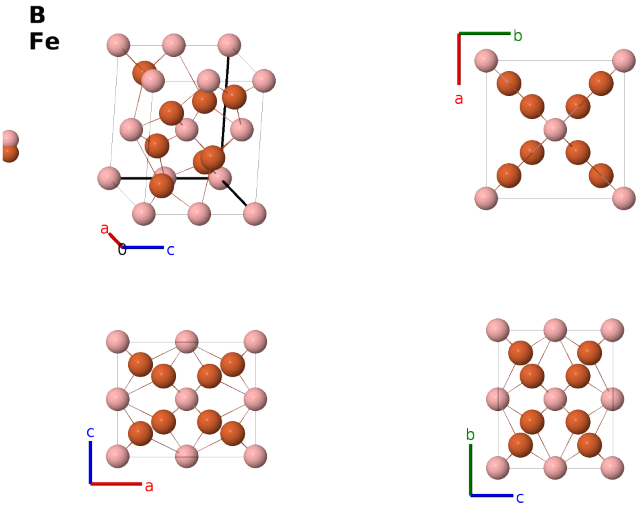
This structure previously used the label(s) **AB2_tI12_121_ab_i**. Calls to these addresses will be redirected here.

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<https://aflow.org/prototype-encyclopedia/1BSH>

https://aflow.org/prototype-encyclopedia/AB2_tI12_121_ab_i-001

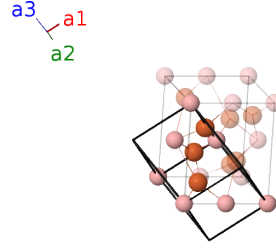


Prototype	BFe ₂
AFLOW prototype label	AB2_tI12_121_ab_i-001
<i>Strukturbericht</i> designation	C17
ICSD	16809
CCDC	1597347
Pearson symbol	tI12
Space group number	121
Space group symbol	$I\bar{4}2m$
AFLOW prototype command	<code>aflow --proto=AB2_tI12_121_ab_i-001 --params=a, c/a, x₃, z₃</code>

- (Wever, 1930) placed this structure in space group $I42m$ #121, and this was used to designate the structure as C17 in (Ewald, 1931). However, even then it was recognized that changing z_3 from the value of 0.2 assigned by Wever to 1/4 would add an inversion symmetry to the crystal, change the space group to $I4/mcm$ #140, and make the structure look very much like Al₂Cu, *Strukturbericht* C16. This has become the accepted structure, as in (Kapfenberger, 2006), so the label C17 is depreciated. We retain it here for historical interest.

Body-centered Tetragonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{1}{2}a \hat{\mathbf{y}} + \frac{1}{2}c \hat{\mathbf{z}} \\ \mathbf{a}_3 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{1}{2}a \hat{\mathbf{y}} - \frac{1}{2}c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	=	0	=	0	(2a) B I
$\mathbf{B}_2$	=	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	=	$\frac{1}{2}c \hat{\mathbf{z}}$	(2b) B II
$\mathbf{B}_3$	=	$(x_3 + z_3) \mathbf{a}_1 + (x_3 + z_3) \mathbf{a}_2 + 2x_3 \mathbf{a}_3$	=	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8i) Fe I
$\mathbf{B}_4$	=	$-(x_3 - z_3) \mathbf{a}_1 - (x_3 - z_3) \mathbf{a}_2 - 2x_3 \mathbf{a}_3$	=	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(8i) Fe I
$\mathbf{B}_5$	=	$-(x_3 + z_3) \mathbf{a}_1 + (x_3 - z_3) \mathbf{a}_2$	=	$ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8i) Fe I
$\mathbf{B}_6$	=	$(x_3 - z_3) \mathbf{a}_1 - (x_3 + z_3) \mathbf{a}_2$	=	$-ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(8i) Fe I

References

- [1] F. Wever and A. Müller, *Über das Zweistoffsystem Eisen-Bor und über die Struktur des Eisenborides Fe_4B_2* , Z. Anorganische und Allgemeine Chemie **192**, 317–336 (1930), doi:10.1002/zaac.19301920125.
- [2] P. P. Ewald and C. Hermann, eds., *Strukturbericht 1913-1928* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1931).
- [3] C. Kapfenberger, B. Albert, R. Pöttgen, and H. Huppertz, *Structure refinements of iron borides Fe_2B and FeB* , Z. Kristallgr. **221**, 477–481 (2006), doi:10.1524/zkri.2006.221.5-7.477.

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