C17 (Fe_2B) Structure (*Obsolete*): AB2_tI12_121_ab_i-001

This structure originally had the label `AB2_tI12_121_ab_i`. Calls to that address will be redirected here.

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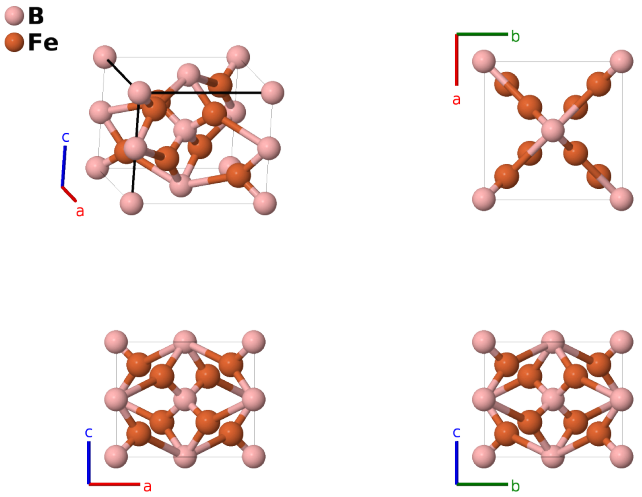
https://aflow.org/p/1BSH

https://aflow.org/p/AB2_tI12_121_ab_i-001

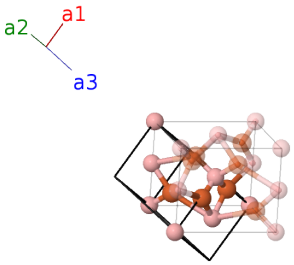


Prototype	BFe_2
AFLOW prototype label	AB2_tI12_121_ab_i-001
***Strukturbericht* designation**	$C17$
ICSD	16809
Pearson symbol	tI12
Space group number	121
Space group symbol	$I\bar{4}2m$
AFLOW prototype command	`aflow --proto=AB2_tI12_121_ab_i-001 --params=`$a, c/a, x_3, z_3$

- (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 Al_2Cu, *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

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



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.