

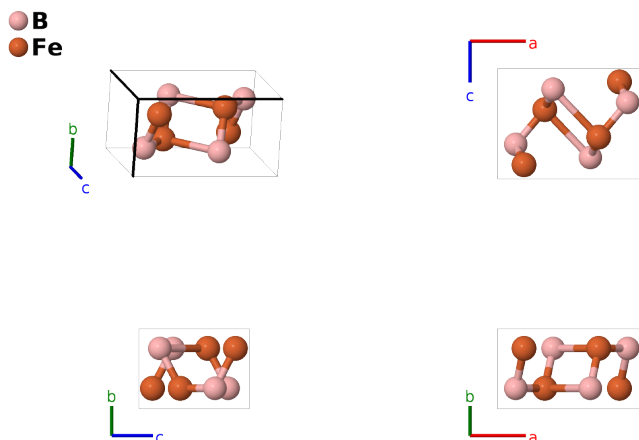
# FeB (*B27*) Structure: AB\_oP8\_62\_c\_c-003

This structure originally had the label AB\_oP8\_62\_c\_c.FeB. Calls to that address will be redirected here.

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<https://aflow.org/p/GH4J>

[https://aflow.org/p/AB\\_oP8\\_62\\_c\\_c-003](https://aflow.org/p/AB_oP8_62_c_c-003)



Prototype	BFe
AFLOW prototype label	AB_oP8_62_c_c-003
<i>Strukturbericht</i> designation	<i>B27</i>
ICSD	33577
Pearson symbol	oP8
Space group number	62
Space group symbol	<i>Pnma</i>
AFLOW prototype command	<code>aflow --proto=AB_oP8_62_c_c-003 --params=a, b/a, c/a, x<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, z<sub>2</sub></code>

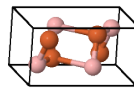
## Other compounds with this structure

CoB, CuCe, HfGe, MnB, NiDy, NiGd, NiHo, NiLu, NiTm, NiY, PdTh, PtDy, PtEr, PtGd, PtHo, PtLu, PtNd, PtPr, PtSm, PtTb, PtTm, PtY, PuSi, ThSi, TiSi, USi, ZrSi

- (Hermann, 1937), assigns the *Strukturbericht* designation *B15* to this structure. This was superseded by the current *B27* structure in (Gottfried, 1937). Here we follow (Parthé, 1993), who prefers the *B27* designation.
- FeAs (*B14*), GeS (*B16*), FeB (*B27*), SnS (*B29*), MnP (*B31*), and  $\eta$ -NiSi (*B<sub>d</sub>*) all share the same AFLOW label, AB\_oP8\_62\_c\_c. The structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

## Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4c)	B I
$\mathbf{B}_2$	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	B I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	(4c)	B I
$\mathbf{B}_4$	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	B I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4c)	Fe I
$\mathbf{B}_6$	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Fe I
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + \frac{3}{4} \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + \frac{3}{4}b \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	(4c)	Fe I
$\mathbf{B}_8$	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 + \frac{1}{4} \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + \frac{1}{4}b \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4c)	Fe I

## References

- [1] S. B. Hendricks and P. R. Kosting, *The Crystal Structure of Fe<sub>2</sub>P, Fe<sub>2</sub>N, Fe<sub>3</sub>N and FeB*, *Z. Kristallogr.* **74**, 511–533 (1930), doi:10.1524/zkri.1930.74.1.511.
- [2] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).
- [3] C. Gottfried and F. Schossberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).
- [4] E. Parthé, L. Gelato, B. Chabot, M. Penso, K. Cenzula, and R. Gladyshevskii, *Standardized Data and Crystal Chemical Characterization of Inorganic Structure Types, Gmelin Handbook of Inorganic and Organometallic Chemistry*, vol. 2 (Springer-Verlag, Berlin, Heidelberg, 1993), 8 edn., doi:10.1007/978-3-662-02909-1.3. See Table 4.3, pp. 363–371, for a comprehensive compilation of *Strukturbericht* symbols.

## Found in

- [1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, *Am. Mineral.* **88**, 247–250 (2003).