10-3-8 $[Ca_{10}(Pt_3As_8)(Fe_2As_2)_5]$ Superconductor Structure: A9B5C5D2_aP42_2_9i_5i_5i_aei-001

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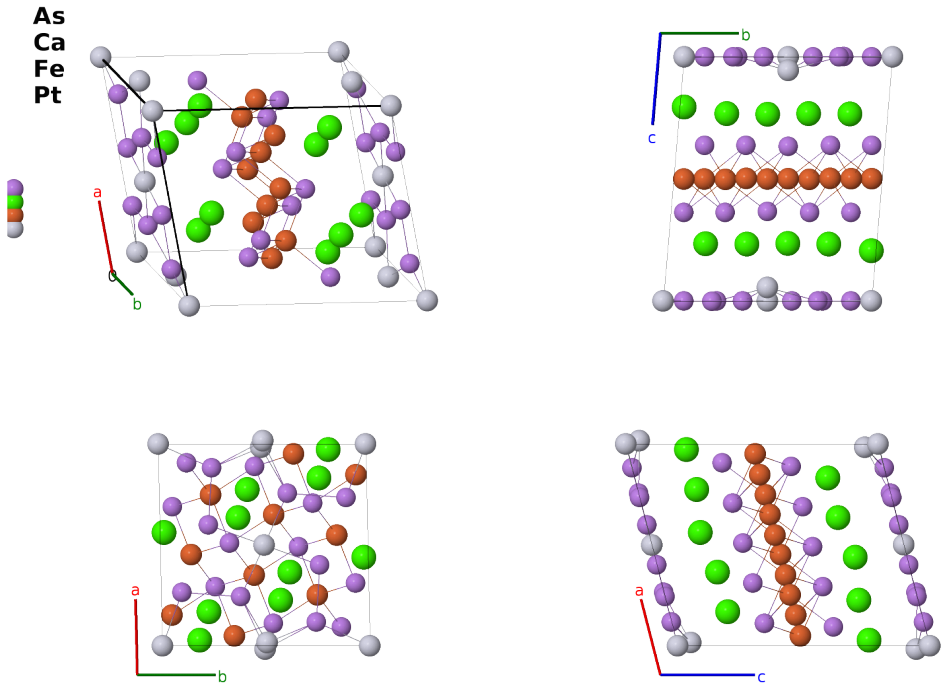
https://aflow.org/prototype-encyclopedia/4M4Y

https://aflow.org/prototype-encyclopedia/A9B5C5D2_aP42_2_9i_5i_5i_aei-001



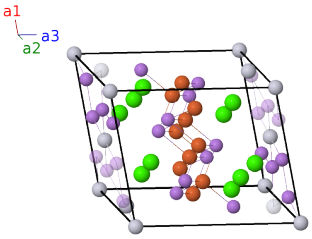
Prototype	$As_{18}Ca_{10}Fe_{10}Pt_3$
AFLOW prototype label	A9B5C5D2_aP42_2_9i_5i_5i_aei-001
Pearson symbol	aP42
Space group number	2
Space group symbol	$P\bar{1}$
AFLOW prototype command	`aflow --proto=A9B5C5D2_aP42_2_9i_5i_5i_aei-001 --params=`$a, b/a, c/a, \alpha, \beta, \gamma, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}, x_{20}, y_{20}, z_{20}, x_{21}, y_{21}, z_{21}, x_{22}, y_{22}, z_{22}$

- This is a high-temperature superconducting structure from the iron-arsenide family. The designation 10-3-8 comes from the stoichiometry of the Ca-Pt-As substitutions to the FeAs structure.
- The data for this structure was taken at 100K.

- The sites labled Fe actually are $Fe_{0.96}Pt_{0.04}$. The Pt-III (2i) site is only 50% occupied.

Triclinic primitive vectors

$$
\begin{aligned}
\mathbf{a_1} &= a\,\hat{\mathbf{x}} \\
\mathbf{a_2} &= b\cos\gamma\,\hat{\mathbf{x}} + b\sin\gamma\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c_x\,\hat{\mathbf{x}} + c_y\,\hat{\mathbf{y}} + c_z\,\hat{\mathbf{z}} \\
c_x &= c\cos\beta \\
c_y &= c(\cos\alpha - \cos\beta\cos\gamma)/\sin\gamma \\
c_z &= \sqrt{c^2 - c_x^2 - c_y^2}
\end{aligned}
$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Pt I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}\,(a + b\cos\gamma)\,\hat{\mathbf{x}} + \frac{1}{2}b\sin\gamma\,\hat{\mathbf{y}}$	(1e)	Pt II
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + by_3\cos\gamma + c_xz_3)\,\hat{\mathbf{x}} + (by_3\sin\gamma + c_yz_3)\,\hat{\mathbf{y}} + c_zz_3\,\hat{\mathbf{z}}$	(2i)	As I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + by_3\cos\gamma + c_xz_3)\,\hat{\mathbf{x}} - (by_3\sin\gamma + c_yz_3)\,\hat{\mathbf{y}} - c_zz_3\,\hat{\mathbf{z}}$	(2i)	As I
$\mathbf{B_5}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + by_4\cos\gamma + c_xz_4)\,\hat{\mathbf{x}} + (by_4\sin\gamma + c_yz_4)\,\hat{\mathbf{y}} + c_zz_4\,\hat{\mathbf{z}}$	(2i)	As II
$\mathbf{B_6}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + by_4\cos\gamma + c_xz_4)\,\hat{\mathbf{x}} - (by_4\sin\gamma + c_yz_4)\,\hat{\mathbf{y}} - c_zz_4\,\hat{\mathbf{z}}$	(2i)	As II
$\mathbf{B_7}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + by_5\cos\gamma + c_xz_5)\,\hat{\mathbf{x}} + (by_5\sin\gamma + c_yz_5)\,\hat{\mathbf{y}} + c_zz_5\,\hat{\mathbf{z}}$	(2i)	As III
$\mathbf{B_8}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + by_5\cos\gamma + c_xz_5)\,\hat{\mathbf{x}} - (by_5\sin\gamma + c_yz_5)\,\hat{\mathbf{y}} - c_zz_5\,\hat{\mathbf{z}}$	(2i)	As III
$\mathbf{B_9}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + by_6\cos\gamma + c_xz_6)\,\hat{\mathbf{x}} + (by_6\sin\gamma + c_yz_6)\,\hat{\mathbf{y}} + c_zz_6\,\hat{\mathbf{z}}$	(2i)	As IV
$\mathbf{B_{10}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + by_6\cos\gamma + c_xz_6)\,\hat{\mathbf{x}} - (by_6\sin\gamma + c_yz_6)\,\hat{\mathbf{y}} - c_zz_6\,\hat{\mathbf{z}}$	(2i)	As IV
$\mathbf{B_{11}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$(ax_7 + by_7\cos\gamma + c_xz_7)\,\hat{\mathbf{x}} + (by_7\sin\gamma + c_yz_7)\,\hat{\mathbf{y}} + c_zz_7\,\hat{\mathbf{z}}$	(2i)	As V
$\mathbf{B_{12}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-(ax_7 + by_7\cos\gamma + c_xz_7)\,\hat{\mathbf{x}} - (by_7\sin\gamma + c_yz_7)\,\hat{\mathbf{y}} - c_zz_7\,\hat{\mathbf{z}}$	(2i)	As V
$\mathbf{B_{13}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$(ax_8 + by_8\cos\gamma + c_xz_8)\,\hat{\mathbf{x}} + (by_8\sin\gamma + c_yz_8)\,\hat{\mathbf{y}} + c_zz_8\,\hat{\mathbf{z}}$	(2i)	As VI
$\mathbf{B_{14}}$	=	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	=	$-(ax_8 + by_8\cos\gamma + c_xz_8)\,\hat{\mathbf{x}} - (by_8\sin\gamma + c_yz_8)\,\hat{\mathbf{y}} - c_zz_8\,\hat{\mathbf{z}}$	(2i)	As VI
$\mathbf{B_{15}}$	=	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$(ax_9 + by_9\cos\gamma + c_xz_9)\,\hat{\mathbf{x}} + (by_9\sin\gamma + c_yz_9)\,\hat{\mathbf{y}} + c_zz_9\,\hat{\mathbf{z}}$	(2i)	As VII
$\mathbf{B_{16}}$	=	$-x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3$	=	$-(ax_9 + by_9\cos\gamma + c_xz_9)\,\hat{\mathbf{x}} - (by_9\sin\gamma + c_yz_9)\,\hat{\mathbf{y}} - c_zz_9\,\hat{\mathbf{z}}$	(2i)	As VII
$\mathbf{B_{17}}$	=	$x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3$	=	$(ax_{10} + by_{10}\cos\gamma + c_xz_{10})\,\hat{\mathbf{x}} + (by_{10}\sin\gamma + c_yz_{10})\,\hat{\mathbf{y}} + c_zz_{10}\,\hat{\mathbf{z}}$	(2i)	As VIII

$$\mathbf{B_{18}} = -x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 - z_{10}\,\mathbf{a}_3 = -\left(ax_{10} + by_{10}\cos\gamma + c_x z_{10}\right)\hat{\mathbf{x}} - \left(by_{10}\sin\gamma + c_y z_{10}\right)\hat{\mathbf{y}} - c_z z_{10}\,\hat{\mathbf{z}}$$ (2i) As VIII

$$\mathbf{B_{19}} = x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 = \left(ax_{11} + by_{11}\cos\gamma + c_x z_{11}\right)\hat{\mathbf{x}} + \left(by_{11}\sin\gamma + c_y z_{11}\right)\hat{\mathbf{y}} + c_z z_{11}\,\hat{\mathbf{z}}$$ (2i) As IX

$$\mathbf{B_{20}} = -x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 - z_{11}\,\mathbf{a}_3 = -\left(ax_{11} + by_{11}\cos\gamma + c_x z_{11}\right)\hat{\mathbf{x}} - \left(by_{11}\sin\gamma + c_y z_{11}\right)\hat{\mathbf{y}} - c_z z_{11}\,\hat{\mathbf{z}}$$ (2i) As IX

$$\mathbf{B_{21}} = x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 = \left(ax_{12} + by_{12}\cos\gamma + c_x z_{12}\right)\hat{\mathbf{x}} + \left(by_{12}\sin\gamma + c_y z_{12}\right)\hat{\mathbf{y}} + c_z z_{12}\,\hat{\mathbf{z}}$$ (2i) Ca I

$$\mathbf{B_{22}} = -x_{12}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 - z_{12}\,\mathbf{a}_3 = -\left(ax_{12} + by_{12}\cos\gamma + c_x z_{12}\right)\hat{\mathbf{x}} - \left(by_{12}\sin\gamma + c_y z_{12}\right)\hat{\mathbf{y}} - c_z z_{12}\,\hat{\mathbf{z}}$$ (2i) Ca I

$$\mathbf{B_{23}} = x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3 = \left(ax_{13} + by_{13}\cos\gamma + c_x z_{13}\right)\hat{\mathbf{x}} + \left(by_{13}\sin\gamma + c_y z_{13}\right)\hat{\mathbf{y}} + c_z z_{13}\,\hat{\mathbf{z}}$$ (2i) Ca II

$$\mathbf{B_{24}} = -x_{13}\,\mathbf{a}_1 - y_{13}\,\mathbf{a}_2 - z_{13}\,\mathbf{a}_3 = -\left(ax_{13} + by_{13}\cos\gamma + c_x z_{13}\right)\hat{\mathbf{x}} - \left(by_{13}\sin\gamma + c_y z_{13}\right)\hat{\mathbf{y}} - c_z z_{13}\,\hat{\mathbf{z}}$$ (2i) Ca II

$$\mathbf{B_{25}} = x_{14}\,\mathbf{a}_1 + y_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3 = \left(ax_{14} + by_{14}\cos\gamma + c_x z_{14}\right)\hat{\mathbf{x}} + \left(by_{14}\sin\gamma + c_y z_{14}\right)\hat{\mathbf{y}} + c_z z_{14}\,\hat{\mathbf{z}}$$ (2i) Ca III

$$\mathbf{B_{26}} = -x_{14}\,\mathbf{a}_1 - y_{14}\,\mathbf{a}_2 - z_{14}\,\mathbf{a}_3 = -\left(ax_{14} + by_{14}\cos\gamma + c_x z_{14}\right)\hat{\mathbf{x}} - \left(by_{14}\sin\gamma + c_y z_{14}\right)\hat{\mathbf{y}} - c_z z_{14}\,\hat{\mathbf{z}}$$ (2i) Ca III

$$\mathbf{B_{27}} = x_{15}\,\mathbf{a}_1 + y_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3 = \left(ax_{15} + by_{15}\cos\gamma + c_x z_{15}\right)\hat{\mathbf{x}} + \left(by_{15}\sin\gamma + c_y z_{15}\right)\hat{\mathbf{y}} + c_z z_{15}\,\hat{\mathbf{z}}$$ (2i) Ca IV

$$\mathbf{B_{28}} = -x_{15}\,\mathbf{a}_1 - y_{15}\,\mathbf{a}_2 - z_{15}\,\mathbf{a}_3 = -\left(ax_{15} + by_{15}\cos\gamma + c_x z_{15}\right)\hat{\mathbf{x}} - \left(by_{15}\sin\gamma + c_y z_{15}\right)\hat{\mathbf{y}} - c_z z_{15}\,\hat{\mathbf{z}}$$ (2i) Ca IV

$$\mathbf{B_{29}} = x_{16}\,\mathbf{a}_1 + y_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3 = \left(ax_{16} + by_{16}\cos\gamma + c_x z_{16}\right)\hat{\mathbf{x}} + \left(by_{16}\sin\gamma + c_y z_{16}\right)\hat{\mathbf{y}} + c_z z_{16}\,\hat{\mathbf{z}}$$ (2i) Ca V

$$\mathbf{B_{30}} = -x_{16}\,\mathbf{a}_1 - y_{16}\,\mathbf{a}_2 - z_{16}\,\mathbf{a}_3 = -\left(ax_{16} + by_{16}\cos\gamma + c_x z_{16}\right)\hat{\mathbf{x}} - \left(by_{16}\sin\gamma + c_y z_{16}\right)\hat{\mathbf{y}} - c_z z_{16}\,\hat{\mathbf{z}}$$ (2i) Ca V

$$\mathbf{B_{31}} = x_{17}\,\mathbf{a}_1 + y_{17}\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3 = \left(ax_{17} + by_{17}\cos\gamma + c_x z_{17}\right)\hat{\mathbf{x}} + \left(by_{17}\sin\gamma + c_y z_{17}\right)\hat{\mathbf{y}} + c_z z_{17}\,\hat{\mathbf{z}}$$ (2i) Fe I

$$\mathbf{B_{32}} = -x_{17}\,\mathbf{a}_1 - y_{17}\,\mathbf{a}_2 - z_{17}\,\mathbf{a}_3 = -\left(ax_{17} + by_{17}\cos\gamma + c_x z_{17}\right)\hat{\mathbf{x}} - \left(by_{17}\sin\gamma + c_y z_{17}\right)\hat{\mathbf{y}} - c_z z_{17}\,\hat{\mathbf{z}}$$ (2i) Fe I

$$\mathbf{B_{33}} = x_{18}\,\mathbf{a}_1 + y_{18}\,\mathbf{a}_2 + z_{18}\,\mathbf{a}_3 = \left(ax_{18} + by_{18}\cos\gamma + c_x z_{18}\right)\hat{\mathbf{x}} + \left(by_{18}\sin\gamma + c_y z_{18}\right)\hat{\mathbf{y}} + c_z z_{18}\,\hat{\mathbf{z}}$$ (2i) Fe II

$$\mathbf{B_{34}} = -x_{18}\,\mathbf{a}_1 - y_{18}\,\mathbf{a}_2 - z_{18}\,\mathbf{a}_3 = -\left(ax_{18} + by_{18}\cos\gamma + c_x z_{18}\right)\hat{\mathbf{x}} - \left(by_{18}\sin\gamma + c_y z_{18}\right)\hat{\mathbf{y}} - c_z z_{18}\,\hat{\mathbf{z}}$$ (2i) Fe II

$$\mathbf{B_{35}} = x_{19}\,\mathbf{a}_1 + y_{19}\,\mathbf{a}_2 + z_{19}\,\mathbf{a}_3 = \left(ax_{19} + by_{19}\cos\gamma + c_x z_{19}\right)\hat{\mathbf{x}} + \left(by_{19}\sin\gamma + c_y z_{19}\right)\hat{\mathbf{y}} + c_z z_{19}\,\hat{\mathbf{z}}$$ (2i) Fe III

$$\mathbf{B_{36}} = -x_{19}\,\mathbf{a}_1 - y_{19}\,\mathbf{a}_2 - z_{19}\,\mathbf{a}_3 = -\left(ax_{19} + by_{19}\cos\gamma + c_x z_{19}\right)\hat{\mathbf{x}} - \left(by_{19}\sin\gamma + c_y z_{19}\right)\hat{\mathbf{y}} - c_z z_{19}\,\hat{\mathbf{z}}$$ (2i) Fe III

$$\mathbf{B_{37}} = x_{20}\,\mathbf{a}_1 + y_{20}\,\mathbf{a}_2 + z_{20}\,\mathbf{a}_3 = \left(ax_{20} + by_{20}\cos\gamma + c_x z_{20}\right)\hat{\mathbf{x}} + \left(by_{20}\sin\gamma + c_y z_{20}\right)\hat{\mathbf{y}} + c_z z_{20}\,\hat{\mathbf{z}}$$ (2i) Fe IV

$$\mathbf{B_{38}} = -x_{20}\,\mathbf{a}_1 - y_{20}\,\mathbf{a}_2 - z_{20}\,\mathbf{a}_3 = -\left(ax_{20} + by_{20}\cos\gamma + c_x z_{20}\right)\hat{\mathbf{x}} - \left(by_{20}\sin\gamma + c_y z_{20}\right)\hat{\mathbf{y}} - c_z z_{20}\,\hat{\mathbf{z}}$$ (2i) Fe IV

$$\mathbf{B_{39}} = x_{21}\,\mathbf{a}_1 + y_{21}\,\mathbf{a}_2 + z_{21}\,\mathbf{a}_3 = \left(ax_{21} + by_{21}\cos\gamma + c_x z_{21}\right)\hat{\mathbf{x}} + \left(by_{21}\sin\gamma + c_y z_{21}\right)\hat{\mathbf{y}} + c_z z_{21}\,\hat{\mathbf{z}}$$ (2i) Fe V

$$\mathbf{B_{40}} = -x_{21}\,\mathbf{a}_1 - y_{21}\,\mathbf{a}_2 - z_{21}\,\mathbf{a}_3 = -\left(ax_{21} + by_{21}\cos\gamma + c_x z_{21}\right)\hat{\mathbf{x}} - \left(by_{21}\sin\gamma + c_y z_{21}\right)\hat{\mathbf{y}} - c_z z_{21}\,\hat{\mathbf{z}}$$ (2i) Fe V

$$\mathbf{B_{41}} = x_{22}\,\mathbf{a}_1 + y_{22}\,\mathbf{a}_2 + z_{22}\,\mathbf{a}_3 = \left(ax_{22} + by_{22}\cos\gamma + c_x z_{22}\right)\hat{\mathbf{x}} + \left(by_{22}\sin\gamma + c_y z_{22}\right)\hat{\mathbf{y}} + c_z z_{22}\,\hat{\mathbf{z}}$$ (2i) Pt III

$$\mathbf{B_{42}} = -x_{22}\,\mathbf{a}_1 - y_{22}\,\mathbf{a}_2 - z_{22}\,\mathbf{a}_3 = -\left(ax_{22} + by_{22}\cos\gamma + c_x z_{22}\right)\hat{\mathbf{x}} - \left(by_{22}\sin\gamma + c_y z_{22}\right)\hat{\mathbf{y}} - c_z z_{22}\,\hat{\mathbf{z}} \quad \text{(2i)} \quad \text{Pt III}$$

References

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[1] S. Cai, J. Zhao, N. Ni, J. Guo, R. Yang, P. Wang, J. Han, S. Long, Y. Zhou, Q. Wu, X. Qiu, T. Xiang, R. J. Cava, and L. Sun, *The breakdown of both strange metal and superconducting states at a pressure-induced quantum critical point in iron-pnictide superconductors*, Nat. Commun. **14**, 3116 (2023), doi:10.1038/s41467-023-38763-4.

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