$Ba_2Ti_2Fe_2As_4O$ Structure: A4B2C2DE2_tI22_139_2e_e_d_a_c-001

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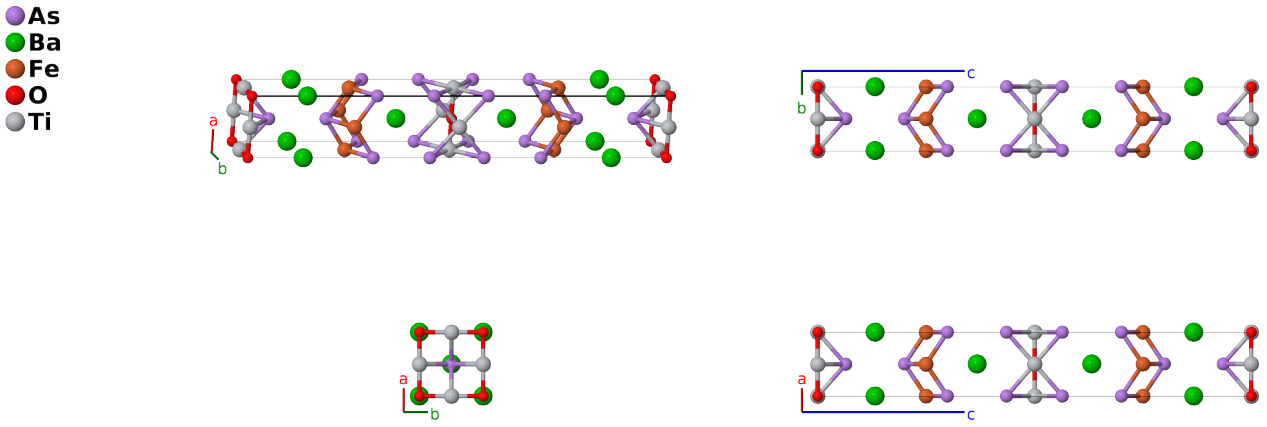
https://aflow.org/p/8C3Q

https://aflow.org/p/A4B2C2DE2_tI22_139_2e_e_d_a_c-001

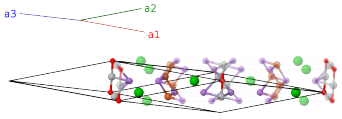


Prototype	$As_4Ba_2Fe_2OTi_2$
AFLOW prototype label	A4B2C2DE2_tI22_139_2e_e_d_a_c-001
ICSD	263018
Pearson symbol	tI22
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=A4B2C2DE2_tI22_139_2e_e_d_a_c-001 --params=`$a, c/a, z_4, z_5, z_6$

- (Sun, 2012) consider this to be intergrown layers of $BaFe_2As_2$, which has the $ThCr_2Si_2$ structure, and $BaTi_2As_2O$.

Body-centered Tetragonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$ =	0	=	0	(2a)	O I

$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}}$	(4c)	Ti I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(4c)	Ti I
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Fe I
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Fe I
$\mathbf{B_6}$	=	$z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$	=	$cz_4\,\hat{\mathbf{z}}$	(4e)	As I
$\mathbf{B_7}$	=	$-z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2$	=	$-cz_4\,\hat{\mathbf{z}}$	(4e)	As I
$\mathbf{B_8}$	=	$z_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2$	=	$cz_5\,\hat{\mathbf{z}}$	(4e)	As II
$\mathbf{B_9}$	=	$-z_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2$	=	$-cz_5\,\hat{\mathbf{z}}$	(4e)	As II
$\mathbf{B_{10}}$	=	$z_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2$	=	$cz_6\,\hat{\mathbf{z}}$	(4e)	Ba I
$\mathbf{B_{11}}$	=	$-z_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_2$	=	$-cz_6\,\hat{\mathbf{z}}$	(4e)	Ba I

References

[1] Y.-L. Sun, H. Jiang, H.-F. Zhai, J.-K. Bao, W.-H. Jiao, Q. Tao, C.-Y. Shen, Y.-W. Z., Z.-A. Xu, and G.-H. Cao, *$Ba_2Ti_2Fe_2As_4O$: A New Superconductor Containing Fe_2As_2 Layers and Ti_2O Sheets*, J. Am. Chem. Soc. **134**, 12893–12896 (2012), doi:10.1021/ja304315e.

Found in

[1] G. Wang, H. Zhang, L. Zhang, and C. Liu, *The electronic structure and magnetism of $BaTi_2Sb_2O$*, J. Appl. Phys. **113**, 243904 (2013), doi:10.1063/1.4812489.