$ReSi_2$ Structure: AB2_oI6_71_a_e-002

This structure originally had the label `AB2_oI6_71_a_i`. Calls to that address will be redirected here.

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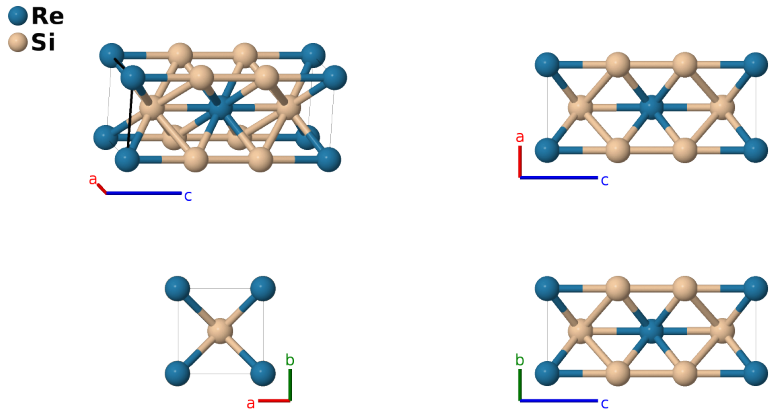
https://aflow.org/p/9FBX

https://aflow.org/p/AB2_oI6_71_a_e-002

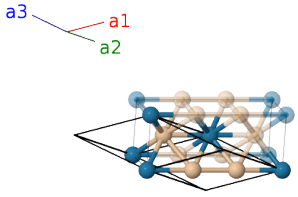


Prototype	$ReSi_2$
AFLOW prototype label	AB2_oI6_71_a_e-002
ICSD	38274
Pearson symbol	oI6
Space group number	71
Space group symbol	$Immm$
AFLOW prototype command	`aflow --proto=AB2_oI6_71_a_e-002 --params=`$a, b/a, c/a, x_2$

- The original references describe $MoPt_2$ and $ReSi_2$ in different orientations, so they have nominally different AFLOW prototype labels, AB2_oI6_71_a_g and AB2_oI6_71_a_i, respectively. When we apply our AFLOW prototype label rules, however, the label for both structures becomes AB2_oI6_71_a_e. The two structures are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Re I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}}$	(4e)	Si I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}}$	(4e)	Si I

References

[1] T. Siegrist, F. Hulliger, and G. Travaglini, *The crystal structure and some properties of $ReSi_2$*, J. Less-Common Met. **92**, 119–129 (1983), doi:10.1016/0022-5088(83)90233-3.