$MoSi_2$ ($C11_b$) Structure: AB2_tI6_139_a_e-001

This structure originally had the label `AB2_tI6_139_a_e`. Calls to that address will be redirected here.

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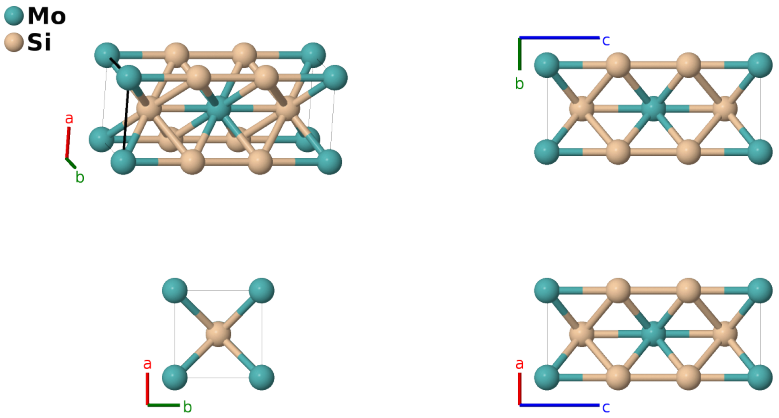
https://aflow.org/p/NG7F

https://aflow.org/p/AB2_tI6_139_a_e-001



Prototype	$MoSi_2$
AFLOW prototype label	AB2_tI6_139_a_e-001
***Strukturbericht* designation**	$C11_b$
ICSD	85756
Pearson symbol	tI6
Space group number	139
Space group symbol	$I4/mmm$
AFLOW prototype command	`aflow --proto=AB2_tI6_139_a_e-001 --params=`$a, c/a, z_2$

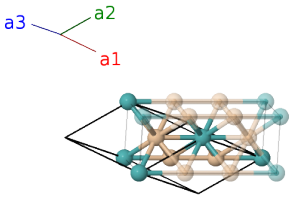
Other compounds with this structure

$AgZr_2$, $AuHf_2$, $AuMn_2$, $AuZr_2$, $BeAu_2$, $CdTi_2$, $CuHf_2$, $CuTl_2$, $CuZr_2$, $DyAg_2$, $DyAu_2$, $DyTl_2$, $ErAu_2$, $GdAg_2$, $GdAu_2$, $HfAu_2$, $LuAu_2$, $MnAu_2$, $MoGe_2$, MoU_2, β-$PdBi_2$, $PdHf_2$, $PdTi_2$, $PtHf_2$, $ReSi_2$, $TaNi_2$, $TiAu_2$, WSi_2, $ZrAu_2$, $ZrPd_2$

- When $c = 3a$ and $z_2 = 1/3$ the atoms are on the sites of a body-centered cubic ($A2$) lattice. For $MoSi_2$ itself, (Harada, 1998) gives $c/a = 2.45$ and $z_2 = 0.3353$. Other compounds in this structure have very different values of c/a and even z_2.

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)	Mo I
$\mathbf{B_2}$	=	$z_2\,\mathbf{a}_1 + z_2\,\mathbf{a}_2$	=	$cz_2\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_3}$	=	$-z_2\,\mathbf{a}_1 - z_2\,\mathbf{a}_2$	=	$-cz_2\,\hat{\mathbf{z}}$	(4e)	Si I

References

[1] Y. Harada, M. Morinaga, D. Saso, M. Takata, and M. Sakata, *Refinement of crystal structure in $MoSi_2$*, Intermetallics **6**, 523–527 (1998), doi:10.1016/S0966-9795(97)00102-7.