$U_2Mn_3Si_5$ Structure: A3B5C2_tP40_128_dh_egh_h-001

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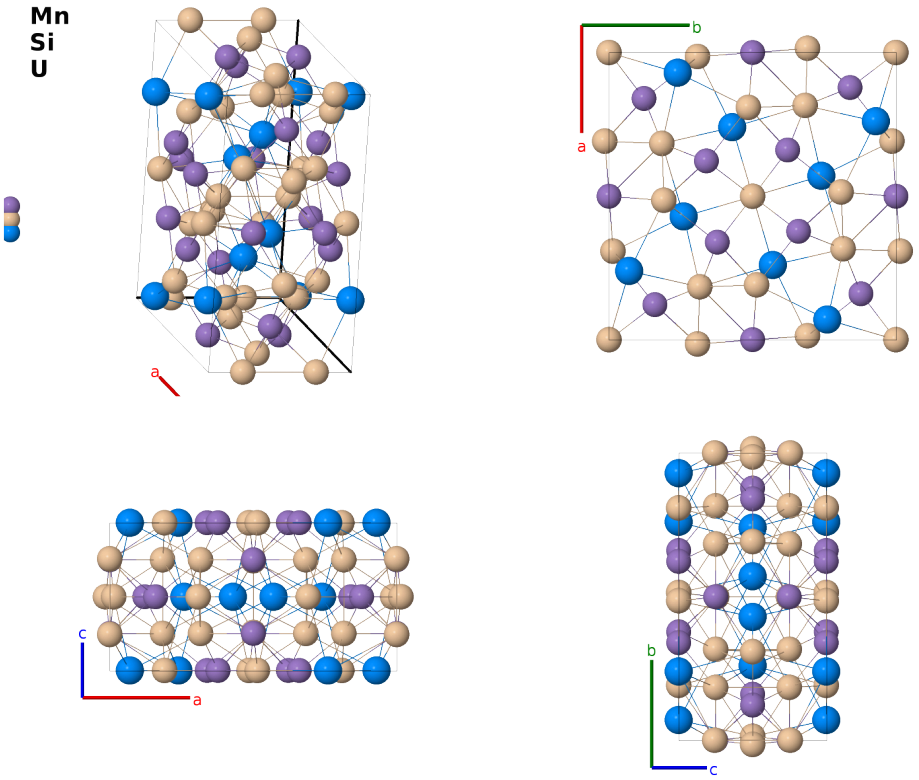
https://aflow.org/prototype-encyclopedia/P4UA

https://aflow.org/prototype-encyclopedia/A3B5C2_tP40_128_dh_egh_h-001



Prototype	$Mn_3Si_5U_2$
AFLOW prototype label	A3B5C2_tP40_128_dh_egh_h-001
ICSD	20929
CCDC	1598654
Pearson symbol	tP40
Space group number	128
Space group symbol	$P4/mnc$
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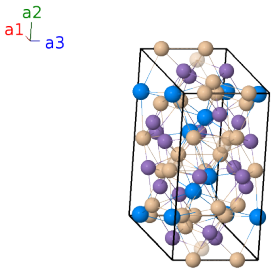
Other compounds with this structure

$Ce_2Co_3Si_5$, $Ce_2Ni_3Si_5$, $Ce_2Ru_3Ga_5$, $Dy_2Ni_3Si_5$, $Dy_2Ru_3Ge_5$, $Dy_2Ru_3Si_5$, $Er_2Mn_3Si_5$, $Gd_2Re_3Si_5$, $La_2Ru_3Ga_5$, $Lu_2Fe_3Si_5$, $Lu_2Ru_3Si_5$, $Nd_2Os_3Ga_5$, $Nd_2Ru_3Ga_5$, $Np_2Re_3Ga_5$, $Pr_2Ru_3Ga_5$, $Pr_2Ru_3Ge_5$, $Pu_2Fe_3Ga_5$, $Pu_2Re_3Ga_5$, $Pu_2Tc_3Ga_5$, $Rb_2Os_3Si_5$, $Sc_2Fe_3Si_5$, $Sm_2Ru_3Ga_5$, $Sm_2Ru_3Ge_5$, $Tb_2Mn_3Si_5$, $U_2Tc_3Ga_5$, $Y_2Ni_3Si_5$

- Some authors refer to this as the $Sc_2Fe_3Si_5$ type.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Mn I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4d)	Mn I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	Mn I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4d)	Mn I
$\mathbf{B_5}$	=	$z_2\,\mathbf{a}_3$	=	$cz_2\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_7}$	=	$-z_2\,\mathbf{a}_3$	=	$-cz_2\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Si I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Si II
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Si II
$\mathbf{B_{11}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Si II
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8g)	Si II
$\mathbf{B_{13}}$	=	$-x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	Si II
$\mathbf{B_{14}}$	=	$x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	Si II
$\mathbf{B_{15}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	Si II
$\mathbf{B_{16}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8g)	Si II
$\mathbf{B_{17}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}}$	(8h)	Mn II
$\mathbf{B_{18}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}}$	(8h)	Mn II
$\mathbf{B_{19}}$	=	$-y_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2$	=	$-ay_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(8h)	Mn II
$\mathbf{B_{20}}$	=	$y_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$ay_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(8h)	Mn II
$\mathbf{B_{21}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + a\left(y_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8h)	Mn II

$$\mathbf{B_{22}} = \left(x_4 + \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_4 - \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 = a\left(x_4 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_4 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}c\hat{\mathbf{z}} \quad \text{(8h)} \quad \text{Mn II}$$

$$\mathbf{B_{23}} = \left(y_4 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_4 + \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 = a\left(y_4 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_4 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}c\hat{\mathbf{z}} \quad \text{(8h)} \quad \text{Mn II}$$

$$\mathbf{B_{24}} = -\left(y_4 - \tfrac{1}{2}\right)\mathbf{a}_1 - \left(x_4 - \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 = -a\left(y_4 - \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_4 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}c\hat{\mathbf{z}} \quad \text{(8h)} \quad \text{Mn II}$$

$$\mathbf{B_{25}} = x_5\mathbf{a}_1 + y_5\mathbf{a}_2 = ax_5\hat{\mathbf{x}} + ay_5\hat{\mathbf{y}} \quad \text{(8h)} \quad \text{Si III}$$

$$\mathbf{B_{26}} = -x_5\mathbf{a}_1 - y_5\mathbf{a}_2 = -ax_5\hat{\mathbf{x}} - ay_5\hat{\mathbf{y}} \quad \text{(8h)} \quad \text{Si III}$$

$$\mathbf{B_{27}} = -y_5\mathbf{a}_1 + x_5\mathbf{a}_2 = -ay_5\hat{\mathbf{x}} + ax_5\hat{\mathbf{y}} \quad \text{(8h)} \quad \text{Si III}$$

$$\mathbf{B_{28}} = y_5\mathbf{a}_1 - x_5\mathbf{a}_2 = ay_5\hat{\mathbf{x}} - ax_5\hat{\mathbf{y}} \quad \text{(8h)} \quad \text{Si III}$$

$$\mathbf{B_{29}} = -\left(x_5 - \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_5 + \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 = -a\left(x_5 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_5 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}c\hat{\mathbf{z}} \quad \text{(8h)} \quad \text{Si III}$$

$$\mathbf{B_{30}} = \left(x_5 + \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_5 - \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 = a\left(x_5 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_5 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}c\hat{\mathbf{z}} \quad \text{(8h)} \quad \text{Si III}$$

$$\mathbf{B_{31}} = \left(y_5 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_5 + \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 = a\left(y_5 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_5 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}c\hat{\mathbf{z}} \quad \text{(8h)} \quad \text{Si III}$$

$$\mathbf{B_{32}} = -\left(y_5 - \tfrac{1}{2}\right)\mathbf{a}_1 - \left(x_5 - \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 = -a\left(y_5 - \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_5 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}c\hat{\mathbf{z}} \quad \text{(8h)} \quad \text{Si III}$$

$$\mathbf{B_{33}} = x_6\mathbf{a}_1 + y_6\mathbf{a}_2 = ax_6\hat{\mathbf{x}} + ay_6\hat{\mathbf{y}} \quad \text{(8h)} \quad \text{U I}$$

$$\mathbf{B_{34}} = -x_6\mathbf{a}_1 - y_6\mathbf{a}_2 = -ax_6\hat{\mathbf{x}} - ay_6\hat{\mathbf{y}} \quad \text{(8h)} \quad \text{U I}$$

$$\mathbf{B_{35}} = -y_6\mathbf{a}_1 + x_6\mathbf{a}_2 = -ay_6\hat{\mathbf{x}} + ax_6\hat{\mathbf{y}} \quad \text{(8h)} \quad \text{U I}$$

$$\mathbf{B_{36}} = y_6\mathbf{a}_1 - x_6\mathbf{a}_2 = ay_6\hat{\mathbf{x}} - ax_6\hat{\mathbf{y}} \quad \text{(8h)} \quad \text{U I}$$

$$\mathbf{B_{37}} = -\left(x_6 - \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_6 + \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 = -a\left(x_6 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_6 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}c\hat{\mathbf{z}} \quad \text{(8h)} \quad \text{U I}$$

$$\mathbf{B_{38}} = \left(x_6 + \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_6 - \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 = a\left(x_6 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_6 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}c\hat{\mathbf{z}} \quad \text{(8h)} \quad \text{U I}$$

$$\mathbf{B_{39}} = \left(y_6 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(x_6 + \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 = a\left(y_6 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(x_6 + \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}c\hat{\mathbf{z}} \quad \text{(8h)} \quad \text{U I}$$

$$\mathbf{B_{40}} = -\left(y_6 - \tfrac{1}{2}\right)\mathbf{a}_1 - \left(x_6 - \tfrac{1}{2}\right)\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3 = -a\left(y_6 - \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(x_6 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + \tfrac{1}{2}c\hat{\mathbf{z}} \quad \text{(8h)} \quad \text{U I}$$

References

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