Dugganite ($Pb_3Zn_3TeAs_2O_{14}$) Structure: A2B14C3DE3_hP23_150_d_d2g_e_a_f-001

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https://aflow.org/p/8A06

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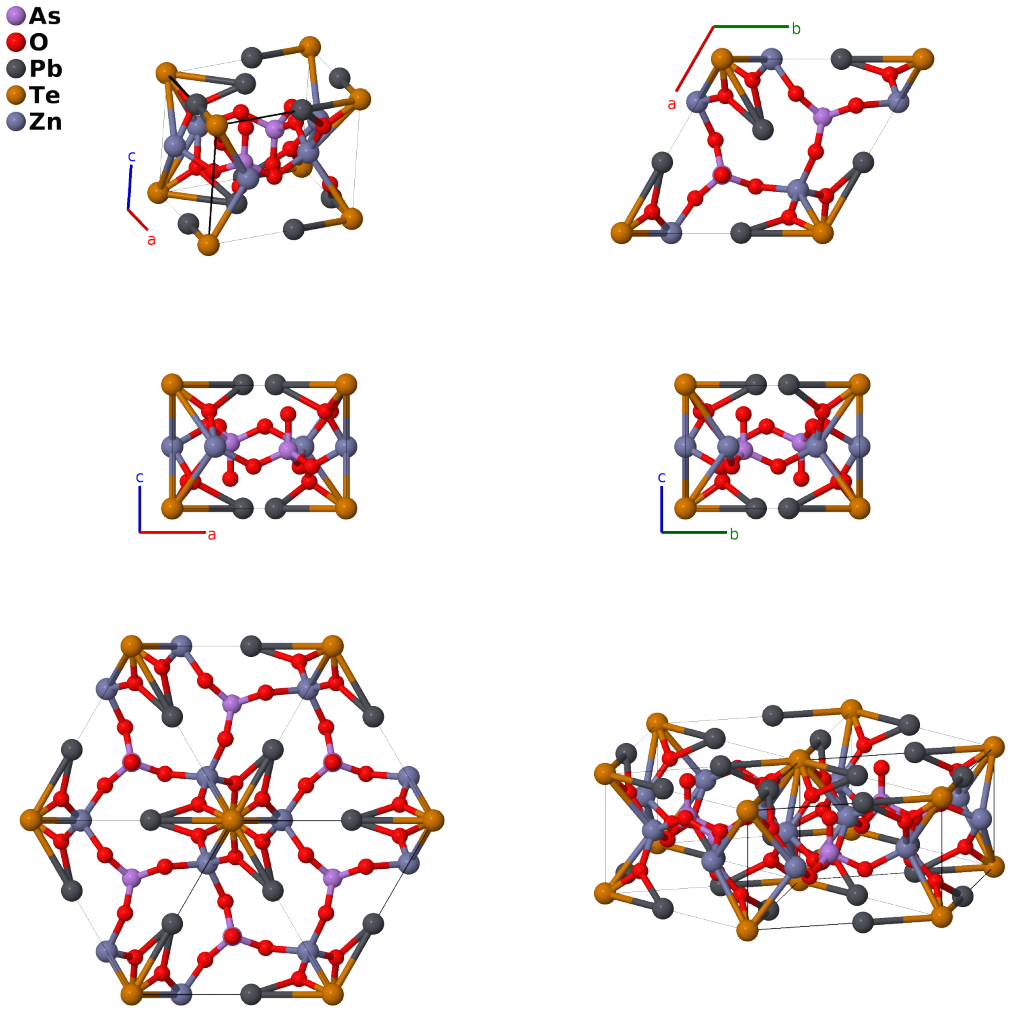


Prototype	$As_2O_{14}Pb_3TeZn_3$
AFLOW prototype label	A2B14C3DE3_hP23_150_d_d2g_e_a_f-001
Mineral name	dugganite
ICSD	85574
Pearson symbol	hP23
Space group number	150
Space group symbol	$P321$

AFLOW prototype command `aflow --proto=A2B14C3DE3_hP23_150_d_d2g_e_a_f-001 --params=`$a, c/a, z_2, z_3, x_4, x_5, x_6, y_6, z_6, x_7, y_7, z_7$

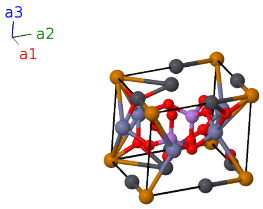
Other compounds with this structure

$Ba_3Co_3P_2TeO_{14}$, $Ca_3NbGa_3Si_2O_{14}$, $Ca_3Ga_2Ge_4O_{14}$ (langasite), $La_3Ga_3(Ga, Si)_2GaO_{14}$, $La_3Ga_5SiO_{14}$, $Pb_3Mn_3P_2TeO_{14}$, $Ba_3TeCo_3P_2O$ $Pb_3TeCo_3P_2O_{14}$, $Pb_3TeCo_3V_2O_{14}$

- Some authors use langasite, $Ca_3Ga_2Ge_4O_{14}$, as the prototype for this structure, however in langasite the (1a) and (3f) Wyckoff positions are a mixture of gallium and germanium atoms (Dudka, 2013). None of the Wyckoff positions in dugganite are disordered, so we use it as the prototype.

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Te I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2d)	As I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2d)	As I
$\mathbf{B_4}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2d)	O I
$\mathbf{B_5}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2d)	O I
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}$	(3e)	Pb I
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_2$	=	$\frac{1}{2}ax_4\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}}$	(3e)	Pb I
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2$	=	$-ax_4\,\hat{\mathbf{x}}$	(3e)	Pb I
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_5\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3f)	Zn I
$\mathbf{B_{10}}$	=	$x_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_5\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3f)	Zn I
$\mathbf{B_{11}}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3f)	Zn I
$\mathbf{B_{12}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{13}}$	=	$-y_6\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - 2y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{14}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{15}}$	=	$y_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 + y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{16}}$	=	$(x_6 - y_6)\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - 2y_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{17}}$	=	$-x_6\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_6 - y_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(6g)	O II
$\mathbf{B_{18}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 + y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,(x_7 - y_7)\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(6g)	O III
$\mathbf{B_{19}}$	=	$-y_7\,\mathbf{a}_1 + (x_7 - y_7)\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - 2y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(6g)	O III
$\mathbf{B_{20}}$	=	$-(x_7 - y_7)\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_7 - y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(6g)	O III
$\mathbf{B_{21}}$	=	$y_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 + y_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,(x_7 - y_7)\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(6g)	O III
$\mathbf{B_{22}}$	=	$(x_7 - y_7)\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - 2y_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(6g)	O III

$$\mathbf{B_{23}} = -x_7\,\mathbf{a}_1 - (x_7 - y_7)\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 = -\tfrac{1}{2}a\,(2x_7 - y_7)\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}ay_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \quad \text{(6g)} \quad \text{O III}$$

References

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[2] A. P. Dudka and B. V. Mill, *Accurate Crystal Structure Refinement of $Ca_3Ga_2Ge_4O_{14}$ at 295 and 100 K and Analysis of the Disorder in the Atomic Positions*, Crystallogr. Rep. **58**, 594–603 (2013), doi:10.1134/S1063774513040081. Published in Kristallografiya, 2013, Vol. 58, No. 4, pp. 593–602.

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