

Pb₃TeCo₃P₂O₁₄ Structure:

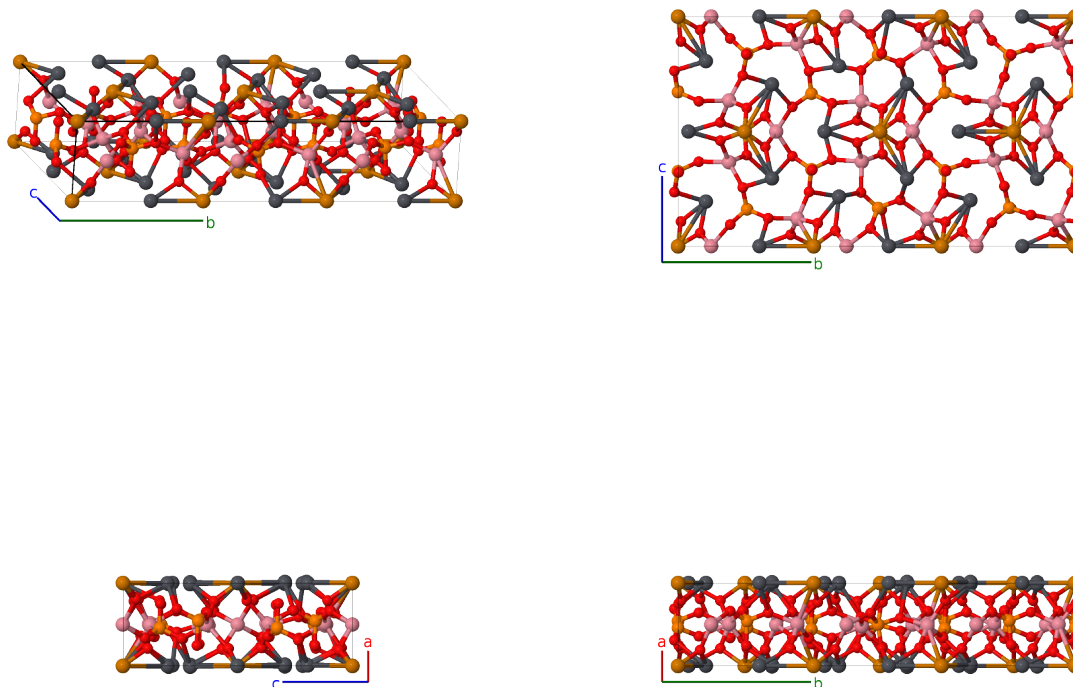
A3B14C2D3E_mP138_3_3c3d6e_42e_6e_3a3b6e_3a3b-001

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<https://aflow.org/p/TBT2>

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● Co
● O
● P
● Pb
● Te



Prototype	Co ₃ O ₁₄ P ₂ Pb ₃ Te
AFLOW prototype label	A3B14C2D3E_mP138_3_3c3d6e_42e_6e_3a3b6e_3a3b-001
ICSD	425850
Pearson symbol	mP138
Space group number	3
Space group symbol	<i>P</i> 2
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$y_{33}, z_{33}, x_{34}, y_{34}, z_{34}, x_{35}, y_{35}, z_{35}, x_{36}, y_{36}, z_{36}, x_{37}, y_{37}, z_{37}, x_{38}, y_{38}, z_{38}, x_{39}, y_{39}, z_{39}, x_{40}, y_{40}, z_{40}, x_{41}, y_{41}, z_{41}, x_{42}, y_{42}, z_{42}, x_{43}, y_{43}, z_{43}, x_{44}, y_{44}, z_{44}, x_{45}, y_{45}, z_{45}, x_{46}, y_{46}, z_{46}, x_{47}, y_{47}, z_{47}, x_{48}, y_{48}, z_{48}, x_{49}, y_{49}, z_{49}, x_{50}, y_{50}, z_{50}, x_{51}, y_{51}, z_{51}, x_{52}, y_{52}, z_{52}, x_{53}, y_{53}, z_{53}, x_{54}, y_{54}, z_{54}, x_{55}, y_{55}, z_{55}, x_{56}, y_{56}, z_{56}, x_{57}, y_{57}, z_{57}, x_{58}, y_{58}, z_{58}, x_{59}, y_{59}, z_{59}, x_{60}, y_{60}, z_{60}, x_{61}, y_{61}, z_{61}, x_{62}, y_{62}, z_{62}, x_{63}, y_{63}, z_{63}, x_{64}, y_{64}, z_{64}, x_{65}, y_{65}, z_{65}, x_{66}, y_{66}, z_{66}, x_{67}, y_{67}, z_{67}, x_{68}, y_{68}, z_{68}, x_{69}, y_{69}, z_{69}, x_{70}, y_{70}, z_{70}, x_{71}, y_{71}, z_{71}, x_{72}, y_{72}, z_{72}, x_{73}, y_{73}, z_{73}, x_{74}, y_{74}, z_{74}, x_{75}, y_{75}, z_{75}, x_{76}, y_{76}, z_{76}, x_{77}, y_{77}, z_{77}, x_{78}, y_{78}, z_{78}$

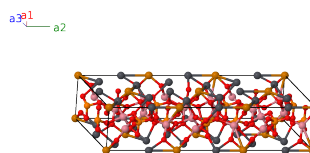
Other compounds with this structure

$\text{Pb}_3\text{TeCo}_3\text{V}_2\text{O}_{14}$

- This is a derivative of the dugganite/langasite structure.

Simple Monoclinic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= y_1 \mathbf{a}_2$	$=$	$by_1 \hat{\mathbf{y}}$	(1a)	Pb I
\mathbf{B}_2	$= y_2 \mathbf{a}_2$	$=$	$by_2 \hat{\mathbf{y}}$	(1a)	Pb II
\mathbf{B}_3	$= y_3 \mathbf{a}_2$	$=$	$by_3 \hat{\mathbf{y}}$	(1a)	Pb III
\mathbf{B}_4	$= y_4 \mathbf{a}_2$	$=$	$by_4 \hat{\mathbf{y}}$	(1a)	Te I
\mathbf{B}_5	$= y_5 \mathbf{a}_2$	$=$	$by_5 \hat{\mathbf{y}}$	(1a)	Te II
\mathbf{B}_6	$= y_6 \mathbf{a}_2$	$=$	$by_6 \hat{\mathbf{y}}$	(1a)	Te III
\mathbf{B}_7	$= y_7 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(1b)	Pb IV
\mathbf{B}_8	$= y_8 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(1b)	Pb V
\mathbf{B}_9	$= y_9 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(1b)	Pb VI
\mathbf{B}_{10}	$= y_{10} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(1b)	Te IV
\mathbf{B}_{11}	$= y_{11} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + by_{11} \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(1b)	Te V
\mathbf{B}_{12}	$= y_{12} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}c \cos \beta \hat{\mathbf{x}} + by_{12} \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(1b)	Te VI
\mathbf{B}_{13}	$= \frac{1}{2} \mathbf{a}_1 + y_{13} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_{13} \hat{\mathbf{y}}$	(1c)	Co I
\mathbf{B}_{14}	$= \frac{1}{2} \mathbf{a}_1 + y_{14} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}}$	(1c)	Co II
\mathbf{B}_{15}	$= \frac{1}{2} \mathbf{a}_1 + y_{15} \mathbf{a}_2$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + by_{15} \hat{\mathbf{y}}$	(1c)	Co III
\mathbf{B}_{16}	$= \frac{1}{2} \mathbf{a}_1 + y_{16} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}(a + c \cos \beta) \hat{\mathbf{x}} + by_{16} \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(1d)	Co IV
\mathbf{B}_{17}	$= \frac{1}{2} \mathbf{a}_1 + y_{17} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}(a + c \cos \beta) \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(1d)	Co V
\mathbf{B}_{18}	$= \frac{1}{2} \mathbf{a}_1 + y_{18} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2}(a + c \cos \beta) \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} + \frac{1}{2}c \sin \beta \hat{\mathbf{z}}$	(1d)	Co VI
\mathbf{B}_{19}	$= x_{19} \mathbf{a}_1 + y_{19} \mathbf{a}_2 + z_{19} \mathbf{a}_3$	$=$	$(ax_{19} + cz_{19} \cos \beta) \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} + cz_{19} \sin \beta \hat{\mathbf{z}}$	(2e)	Co VII
\mathbf{B}_{20}	$= -x_{19} \mathbf{a}_1 + y_{19} \mathbf{a}_2 - z_{19} \mathbf{a}_3$	$=$	$-(ax_{19} + cz_{19} \cos \beta) \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} - cz_{19} \sin \beta \hat{\mathbf{z}}$	(2e)	Co VII

$$\mathbf{B}_{138} = -x_{78} \mathbf{a}_1 + y_{78} \mathbf{a}_2 - z_{78} \mathbf{a}_3 = - (ax_{78} + cz_{78} \cos \beta) \hat{\mathbf{x}} + by_{78} \hat{\mathbf{y}} - cz_{78} \sin \beta \hat{\mathbf{z}} \quad (2e) \quad \text{Pb XII}$$

References

- [1] J. W. Krizan, C. de la Cruz, N. H. Andersen, and R. J. Cava, *Crystal structure and magnetic properties of the $Ba_3TeCo_3P_2O_{14}$, $Pb_3TeCo_3P_2O_{14}$, and $Pb_3TeCo_3V_2O_{14}$ langasites*, *Journal of Solid State Chemistry* **203**, 310–320 (2013), doi:10.1016/j.jssc.2013.04.035.