

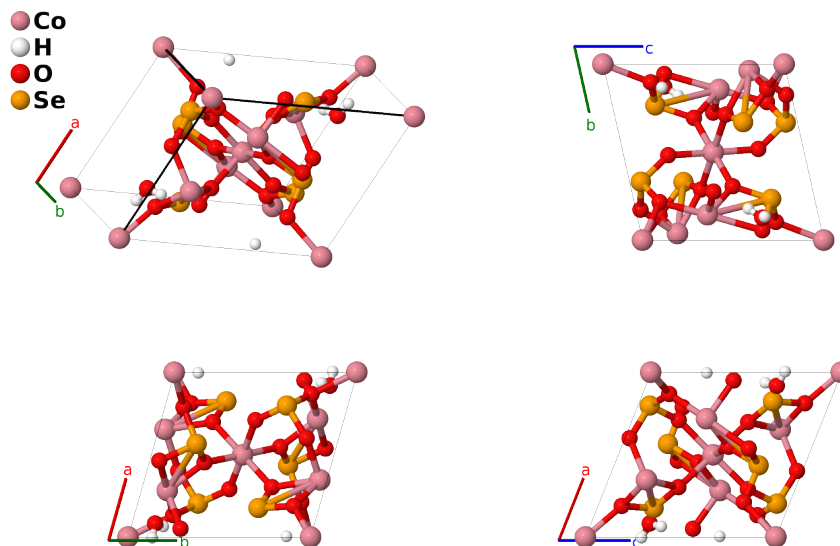
Co₃(SeO₃)₃·H₂O Structure: A3B2C10D3_aP36_2_be2i_2i_10i_3i-001

This structure originally had the label A3B2C10D3_aP36_2_ah2i_2i_10i_3i. Calls to that address will be redirected here.

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<https://aflow.org/p/0ZM1>

https://aflow.org/p/A3B2C10D3_aP36_2_be2i_2i_10i_3i-001



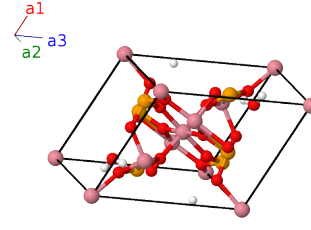
Prototype	Co ₃ H ₂ O ₁₀ Se ₃
AFLOW prototype label	A3B2C10D3_aP36_2_be2i_2i_10i_3i-001
ICSD	66717
Pearson symbol	aP36
Space group number	2
Space group symbol	$P\bar{1}$
AFLOW prototype command	<pre>aflow --proto=A3B2C10D3_aP36_2_be2i_2i_10i_3i-001 --params=a,b/a,c/a,α,β,γ,x₃,y₃,z₃,x₄,y₄,z₄,x₅,y₅,z₅,x₆,y₆,z₆,x₇,y₇,z₇,x₈,y₈, z₈,x₉,y₉,z₉,x₁₀,y₁₀,z₁₀,x₁₁,y₁₁,z₁₁,x₁₂,y₁₂,z₁₂,x₁₃,y₁₃,z₁₃,x₁₄,y₁₄,z₁₄,x₁₅,y₁₅,z₁₅,x₁₆, y₁₆,z₁₆,x₁₇,y₁₇,z₁₇,x₁₈,y₁₈,z₁₈,x₁₉,y₁₉,z₁₉</pre>

Other compounds with this structure

Mn₃(SeO₃)₃·H₂O, Ni₃(SeO₃)₃·H₂O

Triclinic primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= a \hat{\mathbf{x}} \\
\mathbf{a}_2 &= b \cos \gamma \hat{\mathbf{x}} + b \sin \gamma \hat{\mathbf{y}} \\
\mathbf{a}_3 &= c_x \hat{\mathbf{x}} + c_y \hat{\mathbf{y}} + c_z \hat{\mathbf{z}} \\
c_x &= c \cos \beta \\
c_y &= c(\cos \alpha - \cos \beta \cos \gamma) / \sin \gamma \\
c_z &= \sqrt{c^2 - c_x^2 - c_y^2}
\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c_x \hat{\mathbf{x}} + \frac{1}{2} c_y \hat{\mathbf{y}} + \frac{1}{2} c_z \hat{\mathbf{z}}$	(1b)	Co I
\mathbf{B}_2	$= \frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} (a + b \cos \gamma) \hat{\mathbf{x}} + \frac{1}{2} b \sin \gamma \hat{\mathbf{y}}$	(1e)	Co II
\mathbf{B}_3	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + by_3 \cos \gamma + c_x z_3) \hat{\mathbf{x}} + (by_3 \sin \gamma + c_y z_3) \hat{\mathbf{y}} + c_z z_3 \hat{\mathbf{z}}$	(2i)	Co III
\mathbf{B}_4	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + by_3 \cos \gamma + c_x z_3) \hat{\mathbf{x}} - (by_3 \sin \gamma + c_y z_3) \hat{\mathbf{y}} - c_z z_3 \hat{\mathbf{z}}$	(2i)	Co III
\mathbf{B}_5	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + by_4 \cos \gamma + c_x z_4) \hat{\mathbf{x}} + (by_4 \sin \gamma + c_y z_4) \hat{\mathbf{y}} + c_z z_4 \hat{\mathbf{z}}$	(2i)	Co IV
\mathbf{B}_6	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + by_4 \cos \gamma + c_x z_4) \hat{\mathbf{x}} - (by_4 \sin \gamma + c_y z_4) \hat{\mathbf{y}} - c_z z_4 \hat{\mathbf{z}}$	(2i)	Co IV
\mathbf{B}_7	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + by_5 \cos \gamma + c_x z_5) \hat{\mathbf{x}} + (by_5 \sin \gamma + c_y z_5) \hat{\mathbf{y}} + c_z z_5 \hat{\mathbf{z}}$	(2i)	H I
\mathbf{B}_8	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + by_5 \cos \gamma + c_x z_5) \hat{\mathbf{x}} - (by_5 \sin \gamma + c_y z_5) \hat{\mathbf{y}} - c_z z_5 \hat{\mathbf{z}}$	(2i)	H I
\mathbf{B}_9	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + by_6 \cos \gamma + c_x z_6) \hat{\mathbf{x}} + (by_6 \sin \gamma + c_y z_6) \hat{\mathbf{y}} + c_z z_6 \hat{\mathbf{z}}$	(2i)	H II
\mathbf{B}_{10}	$= -x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + by_6 \cos \gamma + c_x z_6) \hat{\mathbf{x}} - (by_6 \sin \gamma + c_y z_6) \hat{\mathbf{y}} - c_z z_6 \hat{\mathbf{z}}$	(2i)	H II
\mathbf{B}_{11}	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + by_7 \cos \gamma + c_x z_7) \hat{\mathbf{x}} + (by_7 \sin \gamma + c_y z_7) \hat{\mathbf{y}} + c_z z_7 \hat{\mathbf{z}}$	(2i)	O I
\mathbf{B}_{12}	$= -x_7 \mathbf{a}_1 - y_7 \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + by_7 \cos \gamma + c_x z_7) \hat{\mathbf{x}} - (by_7 \sin \gamma + c_y z_7) \hat{\mathbf{y}} - c_z z_7 \hat{\mathbf{z}}$	(2i)	O I
\mathbf{B}_{13}	$= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + by_8 \cos \gamma + c_x z_8) \hat{\mathbf{x}} + (by_8 \sin \gamma + c_y z_8) \hat{\mathbf{y}} + c_z z_8 \hat{\mathbf{z}}$	(2i)	O II
\mathbf{B}_{14}	$= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + by_8 \cos \gamma + c_x z_8) \hat{\mathbf{x}} - (by_8 \sin \gamma + c_y z_8) \hat{\mathbf{y}} - c_z z_8 \hat{\mathbf{z}}$	(2i)	O II
\mathbf{B}_{15}	$= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + by_9 \cos \gamma + c_x z_9) \hat{\mathbf{x}} + (by_9 \sin \gamma + c_y z_9) \hat{\mathbf{y}} + c_z z_9 \hat{\mathbf{z}}$	(2i)	O III
\mathbf{B}_{16}	$= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$-(ax_9 + by_9 \cos \gamma + c_x z_9) \hat{\mathbf{x}} - (by_9 \sin \gamma + c_y z_9) \hat{\mathbf{y}} - c_z z_9 \hat{\mathbf{z}}$	(2i)	O III
\mathbf{B}_{17}	$= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + by_{10} \cos \gamma + c_x z_{10}) \hat{\mathbf{x}} + (by_{10} \sin \gamma + c_y z_{10}) \hat{\mathbf{y}} + c_z z_{10} \hat{\mathbf{z}}$	(2i)	O IV
\mathbf{B}_{18}	$= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$-(ax_{10} + by_{10} \cos \gamma + c_x z_{10}) \hat{\mathbf{x}} - (by_{10} \sin \gamma + c_y z_{10}) \hat{\mathbf{y}} - c_z z_{10} \hat{\mathbf{z}}$	(2i)	O IV
\mathbf{B}_{19}	$= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + by_{11} \cos \gamma + c_x z_{11}) \hat{\mathbf{x}} + (by_{11} \sin \gamma + c_y z_{11}) \hat{\mathbf{y}} + c_z z_{11} \hat{\mathbf{z}}$	(2i)	O V

$$\begin{aligned}
\mathbf{B}_{20} &= -x_{11} \mathbf{a}_1 - y_{11} \mathbf{a}_2 - z_{11} \mathbf{a}_3 &= & -(ax_{11} + by_{11} \cos \gamma + c_x z_{11}) \hat{\mathbf{x}} - & (2i) & \text{O V} \\
&&& (by_{11} \sin \gamma + c_y z_{11}) \hat{\mathbf{y}} - c_z z_{11} \hat{\mathbf{z}} \\
\mathbf{B}_{21} &= x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3 &= & (ax_{12} + by_{12} \cos \gamma + c_x z_{12}) \hat{\mathbf{x}} + & (2i) & \text{O VI} \\
&&& (by_{12} \sin \gamma + c_y z_{12}) \hat{\mathbf{y}} + c_z z_{12} \hat{\mathbf{z}} \\
\mathbf{B}_{22} &= -x_{12} \mathbf{a}_1 - y_{12} \mathbf{a}_2 - z_{12} \mathbf{a}_3 &= & -(ax_{12} + by_{12} \cos \gamma + c_x z_{12}) \hat{\mathbf{x}} - & (2i) & \text{O VI} \\
&&& (by_{12} \sin \gamma + c_y z_{12}) \hat{\mathbf{y}} - c_z z_{12} \hat{\mathbf{z}} \\
\mathbf{B}_{23} &= x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3 &= & (ax_{13} + by_{13} \cos \gamma + c_x z_{13}) \hat{\mathbf{x}} + & (2i) & \text{O VII} \\
&&& (by_{13} \sin \gamma + c_y z_{13}) \hat{\mathbf{y}} + c_z z_{13} \hat{\mathbf{z}} \\
\mathbf{B}_{24} &= -x_{13} \mathbf{a}_1 - y_{13} \mathbf{a}_2 - z_{13} \mathbf{a}_3 &= & -(ax_{13} + by_{13} \cos \gamma + c_x z_{13}) \hat{\mathbf{x}} - & (2i) & \text{O VII} \\
&&& (by_{13} \sin \gamma + c_y z_{13}) \hat{\mathbf{y}} - c_z z_{13} \hat{\mathbf{z}} \\
\mathbf{B}_{25} &= x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3 &= & (ax_{14} + by_{14} \cos \gamma + c_x z_{14}) \hat{\mathbf{x}} + & (2i) & \text{O VIII} \\
&&& (by_{14} \sin \gamma + c_y z_{14}) \hat{\mathbf{y}} + c_z z_{14} \hat{\mathbf{z}} \\
\mathbf{B}_{26} &= -x_{14} \mathbf{a}_1 - y_{14} \mathbf{a}_2 - z_{14} \mathbf{a}_3 &= & -(ax_{14} + by_{14} \cos \gamma + c_x z_{14}) \hat{\mathbf{x}} - & (2i) & \text{O VIII} \\
&&& (by_{14} \sin \gamma + c_y z_{14}) \hat{\mathbf{y}} - c_z z_{14} \hat{\mathbf{z}} \\
\mathbf{B}_{27} &= x_{15} \mathbf{a}_1 + y_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3 &= & (ax_{15} + by_{15} \cos \gamma + c_x z_{15}) \hat{\mathbf{x}} + & (2i) & \text{O IX} \\
&&& (by_{15} \sin \gamma + c_y z_{15}) \hat{\mathbf{y}} + c_z z_{15} \hat{\mathbf{z}} \\
\mathbf{B}_{28} &= -x_{15} \mathbf{a}_1 - y_{15} \mathbf{a}_2 - z_{15} \mathbf{a}_3 &= & -(ax_{15} + by_{15} \cos \gamma + c_x z_{15}) \hat{\mathbf{x}} - & (2i) & \text{O IX} \\
&&& (by_{15} \sin \gamma + c_y z_{15}) \hat{\mathbf{y}} - c_z z_{15} \hat{\mathbf{z}} \\
\mathbf{B}_{29} &= x_{16} \mathbf{a}_1 + y_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3 &= & (ax_{16} + by_{16} \cos \gamma + c_x z_{16}) \hat{\mathbf{x}} + & (2i) & \text{O X} \\
&&& (by_{16} \sin \gamma + c_y z_{16}) \hat{\mathbf{y}} + c_z z_{16} \hat{\mathbf{z}} \\
\mathbf{B}_{30} &= -x_{16} \mathbf{a}_1 - y_{16} \mathbf{a}_2 - z_{16} \mathbf{a}_3 &= & -(ax_{16} + by_{16} \cos \gamma + c_x z_{16}) \hat{\mathbf{x}} - & (2i) & \text{O X} \\
&&& (by_{16} \sin \gamma + c_y z_{16}) \hat{\mathbf{y}} - c_z z_{16} \hat{\mathbf{z}} \\
\mathbf{B}_{31} &= x_{17} \mathbf{a}_1 + y_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3 &= & (ax_{17} + by_{17} \cos \gamma + c_x z_{17}) \hat{\mathbf{x}} + & (2i) & \text{Se I} \\
&&& (by_{17} \sin \gamma + c_y z_{17}) \hat{\mathbf{y}} + c_z z_{17} \hat{\mathbf{z}} \\
\mathbf{B}_{32} &= -x_{17} \mathbf{a}_1 - y_{17} \mathbf{a}_2 - z_{17} \mathbf{a}_3 &= & -(ax_{17} + by_{17} \cos \gamma + c_x z_{17}) \hat{\mathbf{x}} - & (2i) & \text{Se I} \\
&&& (by_{17} \sin \gamma + c_y z_{17}) \hat{\mathbf{y}} - c_z z_{17} \hat{\mathbf{z}} \\
\mathbf{B}_{33} &= x_{18} \mathbf{a}_1 + y_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3 &= & (ax_{18} + by_{18} \cos \gamma + c_x z_{18}) \hat{\mathbf{x}} + & (2i) & \text{Se II} \\
&&& (by_{18} \sin \gamma + c_y z_{18}) \hat{\mathbf{y}} + c_z z_{18} \hat{\mathbf{z}} \\
\mathbf{B}_{34} &= -x_{18} \mathbf{a}_1 - y_{18} \mathbf{a}_2 - z_{18} \mathbf{a}_3 &= & -(ax_{18} + by_{18} \cos \gamma + c_x z_{18}) \hat{\mathbf{x}} - & (2i) & \text{Se II} \\
&&& (by_{18} \sin \gamma + c_y z_{18}) \hat{\mathbf{y}} - c_z z_{18} \hat{\mathbf{z}} \\
\mathbf{B}_{35} &= x_{19} \mathbf{a}_1 + y_{19} \mathbf{a}_2 + z_{19} \mathbf{a}_3 &= & (ax_{19} + by_{19} \cos \gamma + c_x z_{19}) \hat{\mathbf{x}} + & (2i) & \text{Se III} \\
&&& (by_{19} \sin \gamma + c_y z_{19}) \hat{\mathbf{y}} + c_z z_{19} \hat{\mathbf{z}} \\
\mathbf{B}_{36} &= -x_{19} \mathbf{a}_1 - y_{19} \mathbf{a}_2 - z_{19} \mathbf{a}_3 &= & -(ax_{19} + by_{19} \cos \gamma + c_x z_{19}) \hat{\mathbf{x}} - & (2i) & \text{Se III} \\
&&& (by_{19} \sin \gamma + c_y z_{19}) \hat{\mathbf{y}} - c_z z_{19} \hat{\mathbf{z}}
\end{aligned}$$

References

- [1] M. Wildner, *Crystal structures of $\text{Co}_3(\text{SeO}_3)_3 \cdot \text{H}_2\text{O}$ and $\text{Ni}_3(\text{SeO}_3)_3 \cdot \text{H}_2\text{O}$, two new isotypic compounds*, *Monatsh. Chem.* **122**, 585–594 (1991), doi:10.1007/BF00811457.

Found in

- [1] K. M. Taddei, L. D. Sanjeeva, J. King, Q. Zhang, D. Parker, A. Podleznyak, D. dela Cruz, and A. S. Sefat, *Tunable magnetic order in low-symmetry SeO_3 ligand linked $\text{TM}_3(\text{SeO}_3)_3 \text{H}_2\text{O}$ ($\text{TM} = \text{Mn}, \text{Co}$ and Ni) compounds*, *Phys. Rev. Materials* **4**, 024410 (2020), doi:10.1103/PhysRevMaterials.4.024410.