$Co_3(SeO_3)_3{\cdot}H_2O$ Structure: A3B2C10D3_aP36_2_be2i_2i_10i_3i-001

This structure previously used the label(s) `A3B2C10D3_aP36_2_ah2i_2i_10i_3i`. Calls to these addresses will be redirected here.

Cite this page as:

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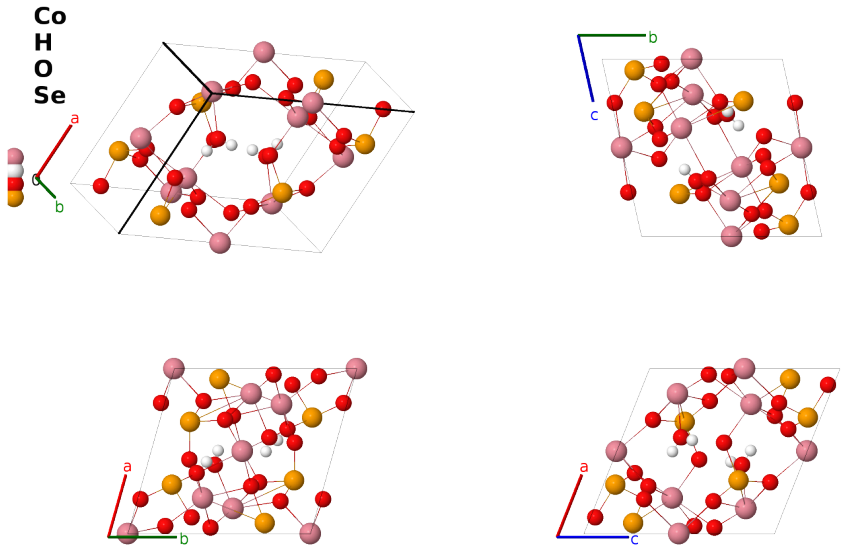
https://aflow.org/prototype-encyclopedia/0ZM1

https://aflow.org/prototype-encyclopedia/A3B2C10D3_aP36_2_be2i_2i_10i_3i-001



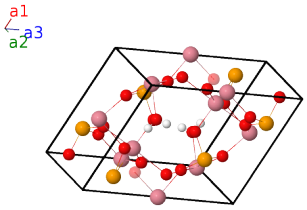
Prototype	$Co_3H_2O_{10}Se_3$
AFLOW prototype label	A3B2C10D3_aP36_2_be2i_2i_10i_3i-001
ICSD	66717
CCDC	1628781
Pearson symbol	aP36
Space group number	2
Space group symbol	$P\bar{1}$
AFLOW prototype command	`aflow --proto=A3B2C10D3_aP36_2_be2i_2i_10i_3i-001 --params=`$a, b/a, c/a, \alpha, \beta, \gamma, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}$

Other compounds with this structure

$Mn_3(SeO_3)_3{\cdot}H_2O$, $Ni_3(SeO_3)_3{\cdot}H_2O$

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

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

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[1] M. Wildner, *Crystal structures of $Co_3(SeO_3)_3{\cdot}H_2O$ and $Ni_3(SeO_3)_3{\cdot}H_2O$, two new isotypic compounds*, Monatsh. Chem. **122**, 585–594 (1991), doi:10.1007/BF00811457.

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[1] K. M. Taddei, L. D. Sanjeewa, J. Xing, Q. Zhang, D. Parker, A. Podleznyak, D. dela Cruz, and A. S. Sefat, *Tunable magnetic order in low-symmetry SeO_3 ligand linked $TM_3(SeO_3)_3H_2O$ (TM = Mn, Co and Ni) compounds*, Phys. Rev. Materials **4**, 024410 (2020), doi:10.1103/PhysRevMaterials.4.024410.

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