Phosgenite [$Pb_2Cl_2(CO_3)$] Structure: AB2C3D2_tP32_127_g_eh_gk_k-001

This structure previously used the label(s) `AB2C3D2_tP32_127_g_eh_gk_k`. Calls to these addresses will be redirected here.

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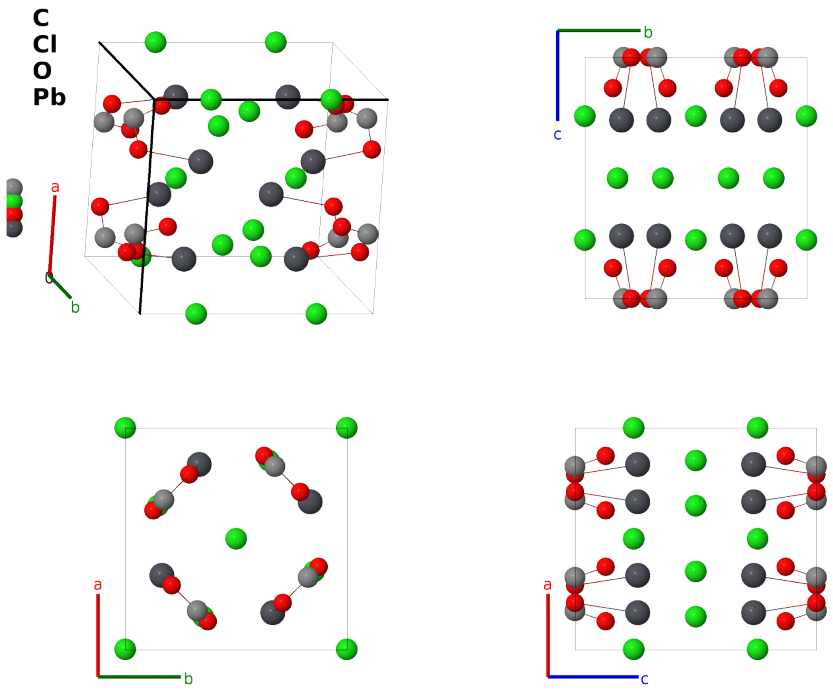
https://aflow.org/prototype-encyclopedia/URTV

https://aflow.org/prototype-encyclopedia/AB2C3D2_tP32_127_g_eh_gk_k-001

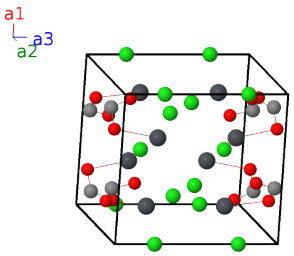


Prototype	$CCl_2O_3Pb_2$
AFLOW prototype label	AB2C3D2_tP32_127_g_eh_gk_k-001
Mineral name	phosgenite
ICSD	4240
CCDC	1592915
Pearson symbol	tP32
Space group number	127
Space group symbol	$P4/mbm$
AFLOW prototype command	`aflow --proto=AB2C3D2_tP32_127_g_eh_gk_k-001 --params=`$a, c/a, z_1, x_2, x_3, x_4, x_5, z_5, x_6, z_6$

- (Onotaro, 1934) made the first determination of the structure of phosgenite, which was given *Strukturbericht* designation $G7_5$ by (Gottfried). (Giuseppetti, 1974) and others found that the actual structure has a unit cell twice that of $G7_5$. This newer structure is presented here.

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(4e)	Cl I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4e)	Cl I
$\mathbf{B_3}$	=	$-z_1\,\mathbf{a}_3$	=	$-cz_1\,\hat{\mathbf{z}}$	(4e)	Cl I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4e)	Cl I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}} + a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	C I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	C I
$\mathbf{B_7}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}}$	(4g)	C I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}}$	(4g)	C I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B_{11}}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B_{12}}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(4g)	O I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + \left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Cl II
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a}_1 - \left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Cl II
$\mathbf{B_{15}}$	=	$-\left(x_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Cl II
$\mathbf{B_{16}}$	=	$\left(x_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4h)	Cl II
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8k)	O II
$\mathbf{B_{18}}$	=	$-x_5\,\mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8k)	O II
$\mathbf{B_{19}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8k)	O II
$\mathbf{B_{20}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(8k)	O II
$\mathbf{B_{21}}$	=	$-\left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8k)	O II
$\mathbf{B_{22}}$	=	$\left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8k)	O II
$\mathbf{B_{23}}$	=	$x_5\,\mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + a\left(x_5 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8k)	O II
$\mathbf{B_{24}}$	=	$-x_5\,\mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - a\left(x_5 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(8k)	O II
$\mathbf{B_{25}}$	=	$x_6\,\mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8k)	Pb I
$\mathbf{B_{26}}$	=	$-x_6\,\mathbf{a}_1 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8k)	Pb I

$\mathbf{B_{27}}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8k)	Pb I
$\mathbf{B_{28}}$	=	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(8k)	Pb I
$\mathbf{B_{29}}$	=	$-\left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8k)	Pb I
$\mathbf{B_{30}}$	=	$\left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8k)	Pb I
$\mathbf{B_{31}}$	=	$x_6\,\mathbf{a}_1 + \left(x_6 + \frac{1}{2}\right)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + a\left(x_6 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8k)	Pb I
$\mathbf{B_{32}}$	=	$-x_6\,\mathbf{a}_1 - \left(x_6 - \frac{1}{2}\right)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - a\left(x_6 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$	(8k)	Pb I

References

[1] G. Giuseppetti and C. Tadini, *Reexamination of the crystal structure of phosgenite, $Pb_2Cl_2(CO_3)$*, TMPM **21**, 101–109 (1974), doi:10.1007/BF01081262.

[2] E. Onotaro, *La struttura della Fosgenite*, Period. d. Mineral. **5**, 1–27 (1934).

[3] C. Gottfried and F. Schossberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

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