

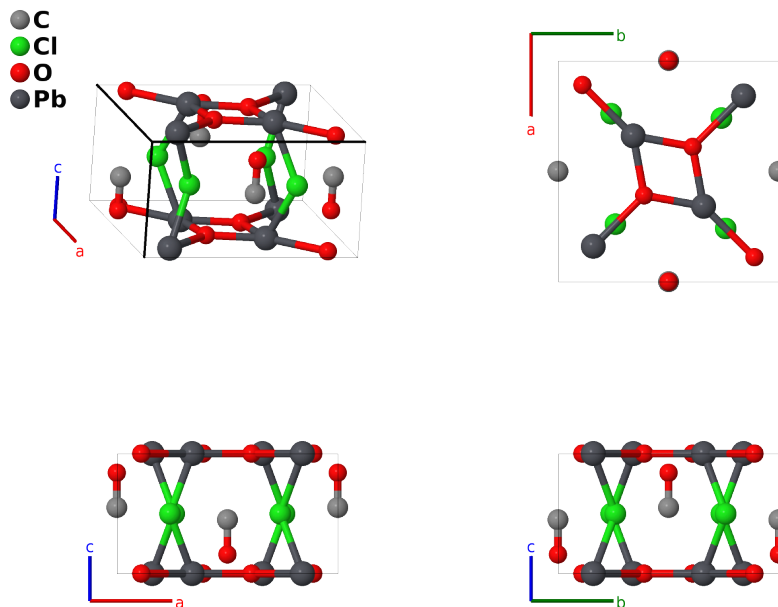
$G7_5$ ($\text{PbCO}_3 \cdot \text{PbCl}_2$, Phosgenite) (*Obsolete*) Structure: AB2C3D2_tP16_90_c_f_ce_e-001

This structure originally had the label AB2C3D2_tP16_90_c_f_ce_e. Calls to that address will be redirected here.

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

https://aflow.org/p/AB2C3D2_tP16_90_c_f_ce_e-001



Prototype	$\text{CCl}_2\text{O}_3\text{Pb}_2$
AFLOW prototype label	AB2C3D2_tP16_90_c_f_ce_e-001
<i>Strukturbericht</i> designation	$G7_5$
Mineral name	phosgenite
ICSD	none
Pearson symbol	tP16
Space group number	90
Space group symbol	$P4_212$
AFLOW prototype command	<code>aflow --proto=AB2C3D2_tP16_90_c_f_ce_e-001 --params=a, c/a, z1, z2, x3, x4, x5</code>

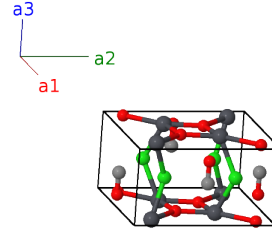
- (Onotaro, 1934) made an early determination of the structure of phosgenite, and (Gottfried, 1937) assigned it the *Strukturbericht* designation $G7_5$. However, the “proposed structure [was] based on photographic data and partly on steric considerations” (Giuseppetti, 1974). Subsequent investigations showed that the true phosgenite structure was in space group $P4/mbm$ #127. We list the original structure here as part of the historical record.

Simple Tetragonal primitive vectors

$$\mathbf{a}_1 = a \hat{\mathbf{x}}$$

$$\mathbf{a}_2 = a \hat{\mathbf{y}}$$

$$\mathbf{a}_3 = c \hat{\mathbf{z}}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= \frac{1}{2} \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(2c)	C I
\mathbf{B}_2	$= \frac{1}{2} \mathbf{a}_1 - z_1 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - cz_1 \hat{\mathbf{z}}$	(2c)	C I
\mathbf{B}_3	$= \frac{1}{2} \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(2c)	O I
\mathbf{B}_4	$= \frac{1}{2} \mathbf{a}_1 - z_2 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - cz_2 \hat{\mathbf{z}}$	(2c)	O I
\mathbf{B}_5	$= x_3 \mathbf{a}_1 + x_3 \mathbf{a}_2$	$=$	$ax_3 \hat{\mathbf{x}} + ax_3 \hat{\mathbf{y}}$	(4e)	O II
\mathbf{B}_6	$= -x_3 \mathbf{a}_1 - x_3 \mathbf{a}_2$	$=$	$-ax_3 \hat{\mathbf{x}} - ax_3 \hat{\mathbf{y}}$	(4e)	O II
\mathbf{B}_7	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (x_3 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_3 + \frac{1}{2}) \hat{\mathbf{y}}$	(4e)	O II
\mathbf{B}_8	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (x_3 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_3 - \frac{1}{2}) \hat{\mathbf{y}}$	(4e)	O II
\mathbf{B}_9	$= x_4 \mathbf{a}_1 + x_4 \mathbf{a}_2$	$=$	$ax_4 \hat{\mathbf{x}} + ax_4 \hat{\mathbf{y}}$	(4e)	Pb I
\mathbf{B}_{10}	$= -x_4 \mathbf{a}_1 - x_4 \mathbf{a}_2$	$=$	$-ax_4 \hat{\mathbf{x}} - ax_4 \hat{\mathbf{y}}$	(4e)	Pb I
\mathbf{B}_{11}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + (x_4 + \frac{1}{2}) \mathbf{a}_2$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_4 + \frac{1}{2}) \hat{\mathbf{y}}$	(4e)	Pb I
\mathbf{B}_{12}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - (x_4 - \frac{1}{2}) \mathbf{a}_2$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_4 - \frac{1}{2}) \hat{\mathbf{y}}$	(4e)	Pb I
\mathbf{B}_{13}	$= x_5 \mathbf{a}_1 + x_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + ax_5 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	Cl I
\mathbf{B}_{14}	$= -x_5 \mathbf{a}_1 - x_5 \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - ax_5 \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	Cl I
\mathbf{B}_{15}	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + (x_5 + \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + a(x_5 + \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	Cl I
\mathbf{B}_{16}	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - (x_5 - \frac{1}{2}) \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - a(x_5 - \frac{1}{2}) \hat{\mathbf{y}} + \frac{1}{2} c \hat{\mathbf{z}}$	(4f)	Cl I

References

- [1] E. Onotaro, *La struttura della Fosgenite*, Period. d. Mineral. **5**, 1-27 (1934).
- [2] C. Gottfried and F. Schosberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

Found in

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