

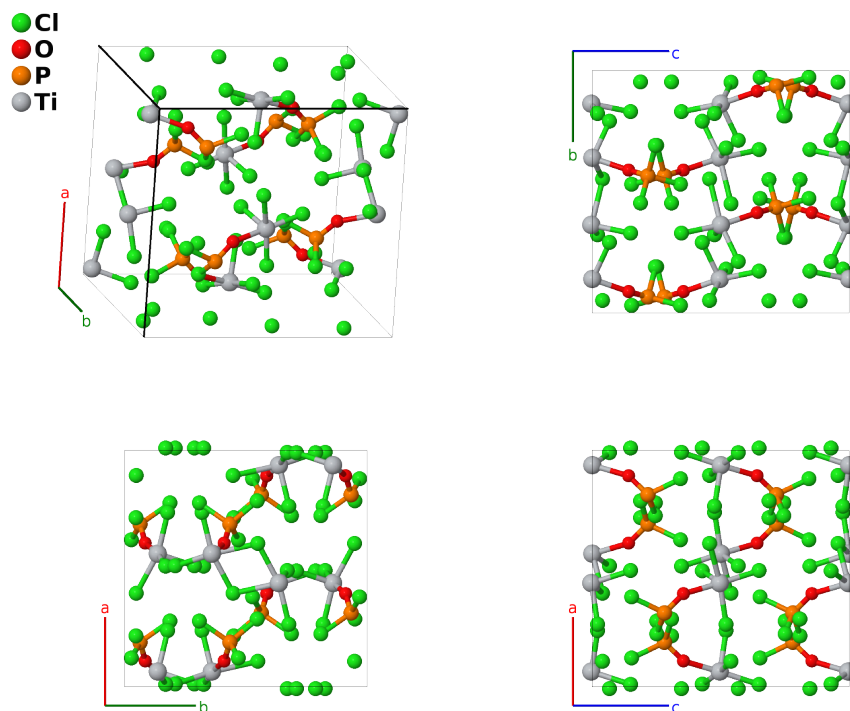
# $(\text{TiCl}_4 \cdot \text{POCl}_3)_2$ Structure: A7BCD\_oP80\_61\_7c\_c\_c\_c-001

This structure originally had the label A7BCD\_oP80\_61\_7c\_c\_c\_c. Calls to that address will be redirected here.

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<https://aflow.org/p/Q18C>

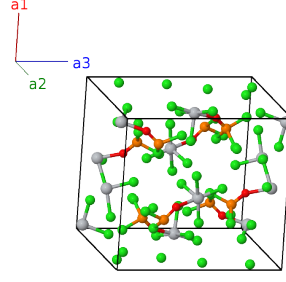
[https://aflow.org/p/A7BCD\\_oP80\\_61\\_7c\\_c\\_c\\_c-001](https://aflow.org/p/A7BCD_oP80_61_7c_c_c_c-001)



Prototype	$\text{Cl}_7\text{OPTi}$
AFLOW prototype label	A7BCD_oP80_61_7c_c_c_c-001
ICSD	27520
Pearson symbol	oP80
Space group number	61
Space group symbol	$Pbca$
AFLOW prototype command	<pre>aflow --proto=A7BCD_oP80_61_7c_c_c_c-001 --params=a, b/a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, x10, y10, z10</pre>

Simple Orthorhombic primitive vectors

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



## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$a x_1 \hat{\mathbf{x}} + b y_1 \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(8c)	Cl I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - b y_1 \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cl I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_1 \hat{\mathbf{x}} + b \left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cl I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(8c)	Cl I
$\mathbf{B}_5$	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-a x_1 \hat{\mathbf{x}} - b y_1 \hat{\mathbf{y}} - c z_1 \hat{\mathbf{z}}$	(8c)	Cl I
$\mathbf{B}_6$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 + y_1 \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} + b y_1 \hat{\mathbf{y}} - c \left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cl I
$\mathbf{B}_7$	$= x_1 \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a x_1 \hat{\mathbf{x}} - b \left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cl I
$\mathbf{B}_8$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$-a \left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} + c z_1 \hat{\mathbf{z}}$	(8c)	Cl I
$\mathbf{B}_9$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(8c)	Cl II
$\mathbf{B}_{10}$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cl II
$\mathbf{B}_{11}$	$= -x_2 \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} + b \left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cl II
$\mathbf{B}_{12}$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(8c)	Cl II
$\mathbf{B}_{13}$	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-a x_2 \hat{\mathbf{x}} - b y_2 \hat{\mathbf{y}} - c z_2 \hat{\mathbf{z}}$	(8c)	Cl II
$\mathbf{B}_{14}$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 + y_2 \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} + b y_2 \hat{\mathbf{y}} - c \left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cl II
$\mathbf{B}_{15}$	$= x_2 \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a x_2 \hat{\mathbf{x}} - b \left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cl II
$\mathbf{B}_{16}$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$-a \left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} + b \left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} + c z_2 \hat{\mathbf{z}}$	(8c)	Cl II
$\mathbf{B}_{17}$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} + c z_3 \hat{\mathbf{z}}$	(8c)	Cl III
$\mathbf{B}_{18}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a \left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cl III
$\mathbf{B}_{19}$	$= -x_3 \mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} + b \left(y_3 + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cl III
$\mathbf{B}_{20}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} - b \left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(8c)	Cl III
$\mathbf{B}_{21}$	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-a x_3 \hat{\mathbf{x}} - b y_3 \hat{\mathbf{y}} - c z_3 \hat{\mathbf{z}}$	(8c)	Cl III
$\mathbf{B}_{22}$	$= \left(x_3 + \frac{1}{2}\right) \mathbf{a}_1 + y_3 \mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a \left(x_3 + \frac{1}{2}\right) \hat{\mathbf{x}} + b y_3 \hat{\mathbf{y}} - c \left(z_3 - \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cl III
$\mathbf{B}_{23}$	$= x_3 \mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$a x_3 \hat{\mathbf{x}} - b \left(y_3 - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	(8c)	Cl III



$$\begin{aligned}
\mathbf{B}_{56} &= -\left(x_7 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right) \mathbf{a}_2 + z_7 \mathbf{a}_3 &= & -a\left(x_7 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}} & (8c) & \text{Cl VII} \\
\mathbf{B}_{57} &= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3 &= & ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8c) & \text{O I} \\
\mathbf{B}_{58} &= -\left(x_8 - \frac{1}{2}\right) \mathbf{a}_1 - y_8 \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3 &= & -a\left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{O I} \\
\mathbf{B}_{59} &= -x_8 \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3 &= & -ax_8 \hat{\mathbf{x}} + b\left(y_8 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{O I} \\
\mathbf{B}_{60} &= \left(x_8 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right) \mathbf{a}_2 - z_8 \mathbf{a}_3 &= & a\left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_8 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (8c) & \text{O I} \\
\mathbf{B}_{61} &= -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 &= & -ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (8c) & \text{O I} \\
\mathbf{B}_{62} &= \left(x_8 + \frac{1}{2}\right) \mathbf{a}_1 + y_8 \mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right) \mathbf{a}_3 &= & a\left(x_8 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{O I} \\
\mathbf{B}_{63} &= x_8 \mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right) \mathbf{a}_3 &= & ax_8 \hat{\mathbf{x}} - b\left(y_8 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{O I} \\
\mathbf{B}_{64} &= -\left(x_8 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right) \mathbf{a}_2 + z_8 \mathbf{a}_3 &= & -a\left(x_8 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_8 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8c) & \text{O I} \\
\mathbf{B}_{65} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 &= & ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (8c) & \text{P I} \\
\mathbf{B}_{66} &= -\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 - y_9 \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 &= & -a\left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{P I} \\
\mathbf{B}_{67} &= -x_9 \mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3 &= & -ax_9 \hat{\mathbf{x}} + b\left(y_9 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{P I} \\
\mathbf{B}_{68} &= \left(x_9 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 - z_9 \mathbf{a}_3 &= & a\left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_9 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (8c) & \text{P I} \\
\mathbf{B}_{69} &= -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 &= & -ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (8c) & \text{P I} \\
\mathbf{B}_{70} &= \left(x_9 + \frac{1}{2}\right) \mathbf{a}_1 + y_9 \mathbf{a}_2 - \left(z_9 - \frac{1}{2}\right) \mathbf{a}_3 &= & a\left(x_9 + \frac{1}{2}\right) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - c\left(z_9 - \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{P I} \\
\mathbf{B}_{71} &= x_9 \mathbf{a}_1 - \left(y_9 - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right) \mathbf{a}_3 &= & ax_9 \hat{\mathbf{x}} - b\left(y_9 - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{P I} \\
\mathbf{B}_{72} &= -\left(x_9 - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_9 + \frac{1}{2}\right) \mathbf{a}_2 + z_9 \mathbf{a}_3 &= & -a\left(x_9 - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_9 + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (8c) & \text{P I} \\
\mathbf{B}_{73} &= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= & ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (8c) & \text{Ti I} \\
\mathbf{B}_{74} &= -\left(x_{10} - \frac{1}{2}\right) \mathbf{a}_1 - y_{10} \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 &= & -a\left(x_{10} - \frac{1}{2}\right) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{Ti I} \\
\mathbf{B}_{75} &= -x_{10} \mathbf{a}_1 + \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_3 &= & -ax_{10} \hat{\mathbf{x}} + b\left(y_{10} + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_{10} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{Ti I} \\
\mathbf{B}_{76} &= \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_{10} - \frac{1}{2}\right) \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= & a\left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_{10} - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} & (8c) & \text{Ti I} \\
\mathbf{B}_{77} &= -x_{10} \mathbf{a}_1 - y_{10} \mathbf{a}_2 - z_{10} \mathbf{a}_3 &= & -ax_{10} \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}} & (8c) & \text{Ti I} \\
\mathbf{B}_{78} &= \left(x_{10} + \frac{1}{2}\right) \mathbf{a}_1 + y_{10} \mathbf{a}_2 - \left(z_{10} - \frac{1}{2}\right) \mathbf{a}_3 &= & a\left(x_{10} + \frac{1}{2}\right) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} - c\left(z_{10} - \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{Ti I} \\
\mathbf{B}_{79} &= x_{10} \mathbf{a}_1 - \left(y_{10} - \frac{1}{2}\right) \mathbf{a}_2 + \left(z_{10} + \frac{1}{2}\right) \mathbf{a}_3 &= & ax_{10} \hat{\mathbf{x}} - b\left(y_{10} - \frac{1}{2}\right) \hat{\mathbf{y}} + c\left(z_{10} + \frac{1}{2}\right) \hat{\mathbf{z}} & (8c) & \text{Ti I} \\
\mathbf{B}_{80} &= -\left(x_{10} - \frac{1}{2}\right) \mathbf{a}_1 + \left(y_{10} + \frac{1}{2}\right) \mathbf{a}_2 + z_{10} \mathbf{a}_3 &= & -a\left(x_{10} - \frac{1}{2}\right) \hat{\mathbf{x}} + b\left(y_{10} + \frac{1}{2}\right) \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}} & (8c) & \text{Ti I}
\end{aligned}$$

## References

- [1] C.-I. Brändén and I. Lindqvist, *The Crystal Structure of  $(\text{TiCl}_4 \cdot \text{POCl}_3)_2$* , Acta Chem. Scand. **14**, 726–732 (1960), doi:10.3891/acta.chem.scand.14-0726.