β-$Ca_2P_2O_7$ Structure: A2B7C2_tP88_76_4a_14a_4a-001

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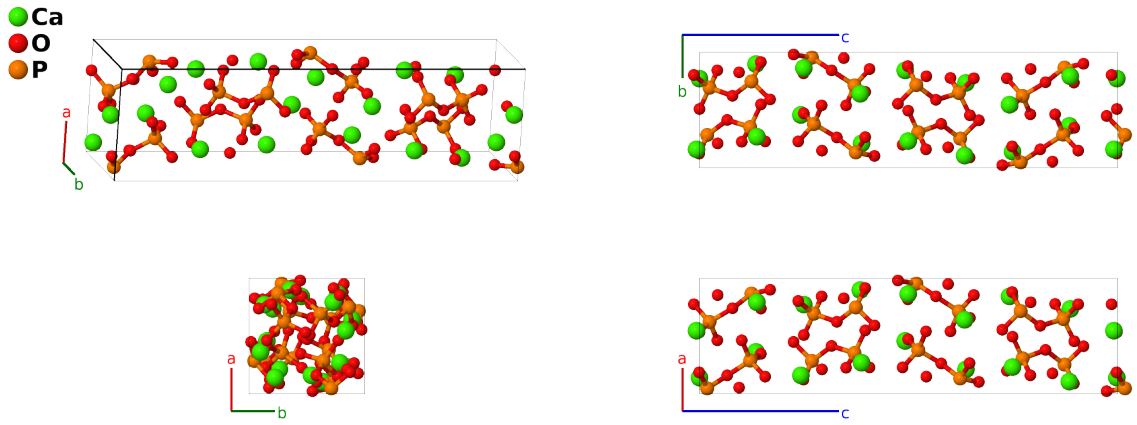
https://aflow.org/p/BAJJ

https://aflow.org/p/A2B7C2_tP88_76_4a_14a_4a-001



Prototype	$Ca_2O_7P_2$
AFLOW prototype label	A2B7C2_tP88_76_4a_14a_4a-001
ICSD	73712
Pearson symbol	tP88
Space group number	76
Space group symbol	$P4_1$
AFLOW prototype command	`aflow --proto=A2B7C2_tP88_76_4a_14a_4a-001 --params=`$a, c/a, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15}, y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}, x_{20}, y_{20}, z_{20}, x_{21}, y_{21}, z_{21}, x_{22}, y_{22}, z_{22}$

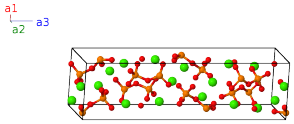
Other compounds with this structure

$Eu_2Si_2O_7$, $La_2Si_2O_7$, $Nd_2Si_2O_7$, $Pr_2Si_2O_7$, $Sm_2Si_2O_7$

- (Felsche, 1970) refers to this as the "A-$RE_2Si_2O_7$ structure, where "RE" is a rare-earth element.
- This is the low-temperature form of $Ca_2P_2O_7$. At higher temperatures it transforms into the monoclinic α-$Ca_2P_2O_7$ structure.
- The origin of the z-axis in space group $P4_1$ #76 is not specified. We fix it by setting $z_1 = 0$.

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + ay_1\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4a)	Ca I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} - ay_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Ca I
$\mathbf{B_3}$	=	$-y_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + \left(z_1 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ay_1\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(4a)	Ca I
$\mathbf{B_4}$	=	$y_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 + \left(z_1 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$ay_1\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(4a)	Ca I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4a)	Ca II
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Ca II
$\mathbf{B_7}$	=	$-y_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \left(z_2 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(4a)	Ca II
$\mathbf{B_8}$	=	$y_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \left(z_2 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(4a)	Ca II
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4a)	Ca III
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Ca III
$\mathbf{B_{11}}$	=	$-y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(4a)	Ca III
$\mathbf{B_{12}}$	=	$y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \left(z_3 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(4a)	Ca III
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(4a)	Ca IV
$\mathbf{B_{14}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	Ca IV
$\mathbf{B_{15}}$	=	$-y_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(4a)	Ca IV
$\mathbf{B_{16}}$	=	$y_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + \left(z_4 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(4a)	Ca IV
$\mathbf{B_{17}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_{18}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_{19}}$	=	$-y_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_{20}}$	=	$y_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + \left(z_5 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}} + c\left(z_5 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B_{21}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_{22}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_{23}}$	=	$-y_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + \left(z_6 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_{24}}$	=	$y_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + \left(z_6 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} + c\left(z_6 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B_{25}}$	=	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(4a)	O III
$\mathbf{B_{26}}$	=	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - ay_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O III
$\mathbf{B_{27}}$	=	$-y_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + \left(z_7 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ay_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(4a)	O III
$\mathbf{B_{28}}$	=	$y_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 + \left(z_7 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$ay_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} + c\left(z_7 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(4a)	O III
$\mathbf{B_{29}}$	=	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(4a)	O IV
$\mathbf{B_{30}}$	=	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} - ay_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O IV
$\mathbf{B_{31}}$	=	$-y_8\,\mathbf{a}_1 + x_8\,\mathbf{a}_2 + \left(z_8 + \frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ay_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{4}\right)\,\hat{\mathbf{z}}$	(4a)	O IV
$\mathbf{B_{32}}$	=	$y_8\,\mathbf{a}_1 - x_8\,\mathbf{a}_2 + \left(z_8 + \frac{3}{4}\right)\,\mathbf{a}_3$	=	$ay_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} + c\left(z_8 + \frac{3}{4}\right)\,\hat{\mathbf{z}}$	(4a)	O IV
$\mathbf{B_{33}}$	=	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} + ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(4a)	O V
$\mathbf{B_{34}}$	=	$-x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 + \left(z_9 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} - ay_9\,\hat{\mathbf{y}} + c\left(z_9 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	O V

$$
\begin{array}{lcccccc}
\mathbf{B_{35}} & = & -y_9\,\mathbf{a}_1 + x_9\,\mathbf{a}_2 + \left(z_9+\frac{1}{4}\right)\,\mathbf{a}_3 & = & -ay_9\,\hat{\mathbf{x}} + ax_9\,\hat{\mathbf{y}} + c\left(z_9+\frac{1}{4}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O V} \\
\mathbf{B_{36}} & = & y_9\,\mathbf{a}_1 - x_9\,\mathbf{a}_2 + \left(z_9+\frac{3}{4}\right)\,\mathbf{a}_3 & = & ay_9\,\hat{\mathbf{x}} - ax_9\,\hat{\mathbf{y}} + c\left(z_9+\frac{3}{4}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O V} \\
\mathbf{B_{37}} & = & x_{10}\,\mathbf{a}_1 + y_{10}\,\mathbf{a}_2 + z_{10}\,\mathbf{a}_3 & = & ax_{10}\,\hat{\mathbf{x}} + ay_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O VI} \\
\mathbf{B_{38}} & = & -x_{10}\,\mathbf{a}_1 - y_{10}\,\mathbf{a}_2 + \left(z_{10}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_{10}\,\hat{\mathbf{x}} - ay_{10}\,\hat{\mathbf{y}} + c\left(z_{10}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O VI} \\
\mathbf{B_{39}} & = & -y_{10}\,\mathbf{a}_1 + x_{10}\,\mathbf{a}_2 + \left(z_{10}+\frac{1}{4}\right)\,\mathbf{a}_3 & = & -ay_{10}\,\hat{\mathbf{x}} + ax_{10}\,\hat{\mathbf{y}} + c\left(z_{10}+\frac{1}{4}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O VI} \\
\mathbf{B_{40}} & = & y_{10}\,\mathbf{a}_1 - x_{10}\,\mathbf{a}_2 + \left(z_{10}+\frac{3}{4}\right)\,\mathbf{a}_3 & = & ay_{10}\,\hat{\mathbf{x}} - ax_{10}\,\hat{\mathbf{y}} + c\left(z_{10}+\frac{3}{4}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O VI} \\
\mathbf{B_{41}} & = & x_{11}\,\mathbf{a}_1 + y_{11}\,\mathbf{a}_2 + z_{11}\,\mathbf{a}_3 & = & ax_{11}\,\hat{\mathbf{x}} + ay_{11}\,\hat{\mathbf{y}} + cz_{11}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O VII} \\
\mathbf{B_{42}} & = & -x_{11}\,\mathbf{a}_1 - y_{11}\,\mathbf{a}_2 + \left(z_{11}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_{11}\,\hat{\mathbf{x}} - ay_{11}\,\hat{\mathbf{y}} + c\left(z_{11}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O VII} \\
\mathbf{B_{43}} & = & -y_{11}\,\mathbf{a}_1 + x_{11}\,\mathbf{a}_2 + \left(z_{11}+\frac{1}{4}\right)\,\mathbf{a}_3 & = & -ay_{11}\,\hat{\mathbf{x}} + ax_{11}\,\hat{\mathbf{y}} + c\left(z_{11}+\frac{1}{4}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O VII} \\
\mathbf{B_{44}} & = & y_{11}\,\mathbf{a}_1 - x_{11}\,\mathbf{a}_2 + \left(z_{11}+\frac{3}{4}\right)\,\mathbf{a}_3 & = & ay_{11}\,\hat{\mathbf{x}} - ax_{11}\,\hat{\mathbf{y}} + c\left(z_{11}+\frac{3}{4}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O VII} \\
\mathbf{B_{45}} & = & x_{12}\,\mathbf{a}_1 + y_{12}\,\mathbf{a}_2 + z_{12}\,\mathbf{a}_3 & = & ax_{12}\,\hat{\mathbf{x}} + ay_{12}\,\hat{\mathbf{y}} + cz_{12}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O VIII} \\
\mathbf{B_{46}} & = & -x_{12}\,\mathbf{a}_1 - y_{12}\,\mathbf{a}_2 + \left(z_{12}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_{12}\,\hat{\mathbf{x}} - ay_{12}\,\hat{\mathbf{y}} + c\left(z_{12}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O VIII} \\
\mathbf{B_{47}} & = & -y_{12}\,\mathbf{a}_1 + x_{12}\,\mathbf{a}_2 + \left(z_{12}+\frac{1}{4}\right)\,\mathbf{a}_3 & = & -ay_{12}\,\hat{\mathbf{x}} + ax_{12}\,\hat{\mathbf{y}} + c\left(z_{12}+\frac{1}{4}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O VIII} \\
\mathbf{B_{48}} & = & y_{12}\,\mathbf{a}_1 - x_{12}\,\mathbf{a}_2 + \left(z_{12}+\frac{3}{4}\right)\,\mathbf{a}_3 & = & ay_{12}\,\hat{\mathbf{x}} - ax_{12}\,\hat{\mathbf{y}} + c\left(z_{12}+\frac{3}{4}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O VIII} \\
\mathbf{B_{49}} & = & x_{13}\,\mathbf{a}_1 + y_{13}\,\mathbf{a}_2 + z_{13}\,\mathbf{a}_3 & = & ax_{13}\,\hat{\mathbf{x}} + ay_{13}\,\hat{\mathbf{y}} + cz_{13}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O IX} \\
\mathbf{B_{50}} & = & -x_{13}\,\mathbf{a}_1 - y_{13}\,\mathbf{a}_2 + \left(z_{13}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_{13}\,\hat{\mathbf{x}} - ay_{13}\,\hat{\mathbf{y}} + c\left(z_{13}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O IX} \\
\mathbf{B_{51}} & = & -y_{13}\,\mathbf{a}_1 + x_{13}\,\mathbf{a}_2 + \left(z_{13}+\frac{1}{4}\right)\,\mathbf{a}_3 & = & -ay_{13}\,\hat{\mathbf{x}} + ax_{13}\,\hat{\mathbf{y}} + c\left(z_{13}+\frac{1}{4}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O IX} \\
\mathbf{B_{52}} & = & y_{13}\,\mathbf{a}_1 - x_{13}\,\mathbf{a}_2 + \left(z_{13}+\frac{3}{4}\right)\,\mathbf{a}_3 & = & ay_{13}\,\hat{\mathbf{x}} - ax_{13}\,\hat{\mathbf{y}} + c\left(z_{13}+\frac{3}{4}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O IX} \\
\mathbf{B_{53}} & = & x_{14}\,\mathbf{a}_1 + y_{14}\,\mathbf{a}_2 + z_{14}\,\mathbf{a}_3 & = & ax_{14}\,\hat{\mathbf{x}} + ay_{14}\,\hat{\mathbf{y}} + cz_{14}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O X} \\
\mathbf{B_{54}} & = & -x_{14}\,\mathbf{a}_1 - y_{14}\,\mathbf{a}_2 + \left(z_{14}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_{14}\,\hat{\mathbf{x}} - ay_{14}\,\hat{\mathbf{y}} + c\left(z_{14}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O X} \\
\mathbf{B_{55}} & = & -y_{14}\,\mathbf{a}_1 + x_{14}\,\mathbf{a}_2 + \left(z_{14}+\frac{1}{4}\right)\,\mathbf{a}_3 & = & -ay_{14}\,\hat{\mathbf{x}} + ax_{14}\,\hat{\mathbf{y}} + c\left(z_{14}+\frac{1}{4}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O X} \\
\mathbf{B_{56}} & = & y_{14}\,\mathbf{a}_1 - x_{14}\,\mathbf{a}_2 + \left(z_{14}+\frac{3}{4}\right)\,\mathbf{a}_3 & = & ay_{14}\,\hat{\mathbf{x}} - ax_{14}\,\hat{\mathbf{y}} + c\left(z_{14}+\frac{3}{4}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O X} \\
\mathbf{B_{57}} & = & x_{15}\,\mathbf{a}_1 + y_{15}\,\mathbf{a}_2 + z_{15}\,\mathbf{a}_3 & = & ax_{15}\,\hat{\mathbf{x}} + ay_{15}\,\hat{\mathbf{y}} + cz_{15}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XI} \\
\mathbf{B_{58}} & = & -x_{15}\,\mathbf{a}_1 - y_{15}\,\mathbf{a}_2 + \left(z_{15}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_{15}\,\hat{\mathbf{x}} - ay_{15}\,\hat{\mathbf{y}} + c\left(z_{15}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XI} \\
\mathbf{B_{59}} & = & -y_{15}\,\mathbf{a}_1 + x_{15}\,\mathbf{a}_2 + \left(z_{15}+\frac{1}{4}\right)\,\mathbf{a}_3 & = & -ay_{15}\,\hat{\mathbf{x}} + ax_{15}\,\hat{\mathbf{y}} + c\left(z_{15}+\frac{1}{4}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XI} \\
\mathbf{B_{60}} & = & y_{15}\,\mathbf{a}_1 - x_{15}\,\mathbf{a}_2 + \left(z_{15}+\frac{3}{4}\right)\,\mathbf{a}_3 & = & ay_{15}\,\hat{\mathbf{x}} - ax_{15}\,\hat{\mathbf{y}} + c\left(z_{15}+\frac{3}{4}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XI} \\
\mathbf{B_{61}} & = & x_{16}\,\mathbf{a}_1 + y_{16}\,\mathbf{a}_2 + z_{16}\,\mathbf{a}_3 & = & ax_{16}\,\hat{\mathbf{x}} + ay_{16}\,\hat{\mathbf{y}} + cz_{16}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XII} \\
\mathbf{B_{62}} & = & -x_{16}\,\mathbf{a}_1 - y_{16}\,\mathbf{a}_2 + \left(z_{16}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_{16}\,\hat{\mathbf{x}} - ay_{16}\,\hat{\mathbf{y}} + c\left(z_{16}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XII} \\
\mathbf{B_{63}} & = & -y_{16}\,\mathbf{a}_1 + x_{16}\,\mathbf{a}_2 + \left(z_{16}+\frac{1}{4}\right)\,\mathbf{a}_3 & = & -ay_{16}\,\hat{\mathbf{x}} + ax_{16}\,\hat{\mathbf{y}} + c\left(z_{16}+\frac{1}{4}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XII} \\
\mathbf{B_{64}} & = & y_{16}\,\mathbf{a}_1 - x_{16}\,\mathbf{a}_2 + \left(z_{16}+\frac{3}{4}\right)\,\mathbf{a}_3 & = & ay_{16}\,\hat{\mathbf{x}} - ax_{16}\,\hat{\mathbf{y}} + c\left(z_{16}+\frac{3}{4}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XII} \\
\mathbf{B_{65}} & = & x_{17}\,\mathbf{a}_1 + y_{17}\,\mathbf{a}_2 + z_{17}\,\mathbf{a}_3 & = & ax_{17}\,\hat{\mathbf{x}} + ay_{17}\,\hat{\mathbf{y}} + cz_{17}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XIII} \\
\mathbf{B_{66}} & = & -x_{17}\,\mathbf{a}_1 - y_{17}\,\mathbf{a}_2 + \left(z_{17}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_{17}\,\hat{\mathbf{x}} - ay_{17}\,\hat{\mathbf{y}} + c\left(z_{17}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XIII} \\
\mathbf{B_{67}} & = & -y_{17}\,\mathbf{a}_1 + x_{17}\,\mathbf{a}_2 + \left(z_{17}+\frac{1}{4}\right)\,\mathbf{a}_3 & = & -ay_{17}\,\hat{\mathbf{x}} + ax_{17}\,\hat{\mathbf{y}} + c\left(z_{17}+\frac{1}{4}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XIII} \\
\mathbf{B_{68}} & = & y_{17}\,\mathbf{a}_1 - x_{17}\,\mathbf{a}_2 + \left(z_{17}+\frac{3}{4}\right)\,\mathbf{a}_3 & = & ay_{17}\,\hat{\mathbf{x}} - ax_{17}\,\hat{\mathbf{y}} + c\left(z_{17}+\frac{3}{4}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XIII} \\
\mathbf{B_{69}} & = & x_{18}\,\mathbf{a}_1 + y_{18}\,\mathbf{a}_2 + z_{18}\,\mathbf{a}_3 & = & ax_{18}\,\hat{\mathbf{x}} + ay_{18}\,\hat{\mathbf{y}} + cz_{18}\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XIV} \\
\mathbf{B_{70}} & = & -x_{18}\,\mathbf{a}_1 - y_{18}\,\mathbf{a}_2 + \left(z_{18}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_{18}\,\hat{\mathbf{x}} - ay_{18}\,\hat{\mathbf{y}} + c\left(z_{18}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XIV} \\
\mathbf{B_{71}} & = & -y_{18}\,\mathbf{a}_1 + x_{18}\,\mathbf{a}_2 + \left(z_{18}+\frac{1}{4}\right)\,\mathbf{a}_3 & = & -ay_{18}\,\hat{\mathbf{x}} + ax_{18}\,\hat{\mathbf{y}} + c\left(z_{18}+\frac{1}{4}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XIV} \\
\mathbf{B_{72}} & = & y_{18}\,\mathbf{a}_1 - x_{18}\,\mathbf{a}_2 + \left(z_{18}+\frac{3}{4}\right)\,\mathbf{a}_3 & = & ay_{18}\,\hat{\mathbf{x}} - ax_{18}\,\hat{\mathbf{y}} + c\left(z_{18}+\frac{3}{4}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{O XIV} \\
\mathbf{B_{73}} & = & x_{19}\,\mathbf{a}_1 + y_{19}\,\mathbf{a}_2 + z_{19}\,\mathbf{a}_3 & = & ax_{19}\,\hat{\mathbf{x}} + ay_{19}\,\hat{\mathbf{y}} + cz_{19}\,\hat{\mathbf{z}} & \text{(4a)} & \text{P I} \\
\mathbf{B_{74}} & = & -x_{19}\,\mathbf{a}_1 - y_{19}\,\mathbf{a}_2 + \left(z_{19}+\frac{1}{2}\right)\,\mathbf{a}_3 & = & -ax_{19}\,\hat{\mathbf{x}} - ay_{19}\,\hat{\mathbf{y}} + c\left(z_{19}+\frac{1}{2}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{P I} \\
\mathbf{B_{75}} & = & -y_{19}\,\mathbf{a}_1 + x_{19}\,\mathbf{a}_2 + \left(z_{19}+\frac{1}{4}\right)\,\mathbf{a}_3 & = & -ay_{19}\,\hat{\mathbf{x}} + ax_{19}\,\hat{\mathbf{y}} + c\left(z_{19}+\frac{1}{4}\right)\,\hat{\mathbf{z}} & \text{(4a)} & \text{P I}
\end{array}
$$

$\mathbf{B_{76}}$	=	$y_{19}\,\mathbf{a}_1 - x_{19}\,\mathbf{a}_2 + \left(z_{19}+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$ay_{19}\,\hat{\mathbf{x}} - ax_{19}\,\hat{\mathbf{y}} + c\left(z_{19}+\frac{3}{4}\right)\,\hat{\mathbf{z}}$	(4a)	P I
$\mathbf{B_{77}}$	=	$x_{20}\,\mathbf{a}_1 + y_{20}\,\mathbf{a}_2 + z_{20}\,\mathbf{a}_3$	=	$ax_{20}\,\hat{\mathbf{x}} + ay_{20}\,\hat{\mathbf{y}} + cz_{20}\,\hat{\mathbf{z}}$	(4a)	P II
$\mathbf{B_{78}}$	=	$-x_{20}\,\mathbf{a}_1 - y_{20}\,\mathbf{a}_2 + \left(z_{20}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_{20}\,\hat{\mathbf{x}} - ay_{20}\,\hat{\mathbf{y}} + c\left(z_{20}+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	P II
$\mathbf{B_{79}}$	=	$-y_{20}\,\mathbf{a}_1 + x_{20}\,\mathbf{a}_2 + \left(z_{20}+\frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ay_{20}\,\hat{\mathbf{x}} + ax_{20}\,\hat{\mathbf{y}} + c\left(z_{20}+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(4a)	P II
$\mathbf{B_{80}}$	=	$y_{20}\,\mathbf{a}_1 - x_{20}\,\mathbf{a}_2 + \left(z_{20}+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$ay_{20}\,\hat{\mathbf{x}} - ax_{20}\,\hat{\mathbf{y}} + c\left(z_{20}+\frac{3}{4}\right)\,\hat{\mathbf{z}}$	(4a)	P II
$\mathbf{B_{81}}$	=	$x_{21}\,\mathbf{a}_1 + y_{21}\,\mathbf{a}_2 + z_{21}\,\mathbf{a}_3$	=	$ax_{21}\,\hat{\mathbf{x}} + ay_{21}\,\hat{\mathbf{y}} + cz_{21}\,\hat{\mathbf{z}}$	(4a)	P III
$\mathbf{B_{82}}$	=	$-x_{21}\,\mathbf{a}_1 - y_{21}\,\mathbf{a}_2 + \left(z_{21}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_{21}\,\hat{\mathbf{x}} - ay_{21}\,\hat{\mathbf{y}} + c\left(z_{21}+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	P III
$\mathbf{B_{83}}$	=	$-y_{21}\,\mathbf{a}_1 + x_{21}\,\mathbf{a}_2 + \left(z_{21}+\frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ay_{21}\,\hat{\mathbf{x}} + ax_{21}\,\hat{\mathbf{y}} + c\left(z_{21}+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(4a)	P III
$\mathbf{B_{84}}$	=	$y_{21}\,\mathbf{a}_1 - x_{21}\,\mathbf{a}_2 + \left(z_{21}+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$ay_{21}\,\hat{\mathbf{x}} - ax_{21}\,\hat{\mathbf{y}} + c\left(z_{21}+\frac{3}{4}\right)\,\hat{\mathbf{z}}$	(4a)	P III
$\mathbf{B_{85}}$	=	$x_{22}\,\mathbf{a}_1 + y_{22}\,\mathbf{a}_2 + z_{22}\,\mathbf{a}_3$	=	$ax_{22}\,\hat{\mathbf{x}} + ay_{22}\,\hat{\mathbf{y}} + cz_{22}\,\hat{\mathbf{z}}$	(4a)	P IV
$\mathbf{B_{86}}$	=	$-x_{22}\,\mathbf{a}_1 - y_{22}\,\mathbf{a}_2 + \left(z_{22}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_{22}\,\hat{\mathbf{x}} - ay_{22}\,\hat{\mathbf{y}} + c\left(z_{22}+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4a)	P IV
$\mathbf{B_{87}}$	=	$-y_{22}\,\mathbf{a}_1 + x_{22}\,\mathbf{a}_2 + \left(z_{22}+\frac{1}{4}\right)\,\mathbf{a}_3$	=	$-ay_{22}\,\hat{\mathbf{x}} + ax_{22}\,\hat{\mathbf{y}} + c\left(z_{22}+\frac{1}{4}\right)\,\hat{\mathbf{z}}$	(4a)	P IV
$\mathbf{B_{88}}$	=	$y_{22}\,\mathbf{a}_1 - x_{22}\,\mathbf{a}_2 + \left(z_{22}+\frac{3}{4}\right)\,\mathbf{a}_3$	=	$ay_{22}\,\hat{\mathbf{x}} - ax_{22}\,\hat{\mathbf{y}} + c\left(z_{22}+\frac{3}{4}\right)\,\hat{\mathbf{z}}$	(4a)	P IV

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