95.545 Stimets Oct. 23, 2009 Meg Ann Noah

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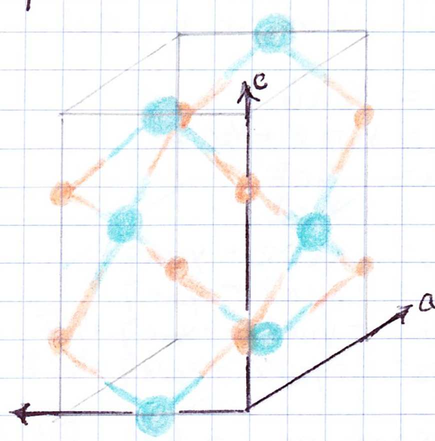
PtS

From the website: http://dave.nrl.navy.mil/lattice/struck/b17.html
The lattice vectors for the primative system are

$\vec{a}_1 = 3.4701\,\hat{x}$ $\quad a = 3.4701\,Å = b$
$\vec{a}_2 = 3.4701\,\hat{y}$ $\quad c = 6.1092\,Å$
$\vec{a}_3 = 6.1092\,\hat{z}$

The basis vectors are:

Pt $\vec{b}_1 = \frac{1}{2}a\hat{y}$
Pt $\vec{b}_2 = \frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{z}$
S $\vec{b}_3 = \frac{1}{4}c\hat{z}$
S $\vec{b}_4 = \frac{3}{4}c\hat{z}$



* there's a type-o in the basis vectors on the site for S atoms
$\frac{1}{4}a\hat{z} \rightarrow \frac{1}{4}c\hat{z}$
$\frac{3}{4}a\hat{z} \rightarrow \frac{3}{4}c\hat{z}$

PtS is in space group #131 $P4_2/mmc$
The long name is $P\ 4_2/m\ 2/m\ 2/c$
$4_2/m$ - 4-fold screw axis along the c-axis and an mirror plane perpendicular to c axis
$2/m$ - mirror plane perpendicular to the a axis, mirror plane perpendicular to b axis
$2/c$ - c-glide perpendicular to the diagonal formed by the a and b axis

Screw Axis Operators: (at origin oriented in $+\hat{z}$ direction)

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \frac{1}{2} \end{bmatrix} = \begin{bmatrix} -y \\ x \\ z+\frac{1}{2} \end{bmatrix} \qquad \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \frac{1}{2} \end{bmatrix} = \begin{bmatrix} y \\ -x \\ z+\frac{1}{2} \end{bmatrix}$$

Mirror Plane Operators: (perpendicular to c axis, a axis, and b axis resp.)

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} \cancel{x}\ x \\ \cancel{y}\ y \\ \cancel{z}\ -z \end{bmatrix} \qquad \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -x \\ y \\ z \end{bmatrix} \qquad \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x \\ -y \\ z \end{bmatrix}$$

Glide Planes: along the plane formed by $(\hat{a}+\hat{b})$

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \frac{1}{2} \end{bmatrix} = \begin{bmatrix} -y \\ -x \\ z+\frac{1}{2} \end{bmatrix} \qquad \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \frac{1}{2} \end{bmatrix} = \begin{bmatrix} y \\ x \\ z+\frac{1}{2} \end{bmatrix}$$

applying any of these operators to any basis vector of Pt produces that vector again ~~on~~ or the other Pt basis vector.
applying to any S basis vector produces that vector again or the other ~~P~~S vector

PdS

From the website http://dave.nrl.navy.mil/lattice/struk/b34.html
The lattice parameters are $a = 6.429\,Å$ and $6.661\,Å$
There are 16 atoms in the cell

Pd-I	$\vec{b}_1 = \frac{1}{2}a\hat{y}$	S	$\vec{b}_9 = x_S a\hat{x} + y_S a\hat{y} + z_S c\hat{z}$
Pd-I	$\vec{b}_2 = \frac{1}{2}a\hat{x} + \frac{1}{2}c\hat{z}$	S	$\vec{b}_{10} = -x_S a\hat{x} - y_S a\hat{y} + z_S c\hat{z}$
Pd-II	$\vec{b}_3 = \frac{1}{4}c\hat{z}$	S	$\vec{b}_{11} = x_S a\hat{x} - y_S a\hat{y} - z_S c\hat{z}$
Pd-II	$\vec{b}_4 = \frac{3}{4}c\hat{z}$	S	$\vec{b}_{12} = x_S a\hat{x} + y_S a\hat{y} - z_S c\hat{z}$
Pd-III	$\vec{b}_5 = x_{Pd} a\hat{x} + y_{Pd} a\hat{y}$	S	$\vec{b}_{13} = -y_S a\hat{x} + x_S a\hat{y} + (\frac{1}{2} + z_S)c\hat{z}$
Pd-III	$\vec{b}_6 = -x_{Pd} a\hat{x} - y_{Pd} a\hat{y}$	S	$\vec{b}_{14} = +y_S a\hat{x} - x_S a\hat{y} + (\frac{1}{2} + z_S)c\hat{z}$
Pd-III	$\vec{b}_7 = -y_{Pd} a\hat{x} - x_{Pd} a\hat{y} + \frac{1}{2}c\hat{z}$	S	$\vec{b}_{15} = -y_S a\hat{x} - x_S a\hat{y} + (\frac{1}{2} - z_S)c\hat{z}$
Pd-III	$\vec{b}_8 = -y_{Pd} a\hat{x} - x_{Pd} a\hat{y} + \frac{1}{2}c\hat{z}$	S	$\vec{b}_{16} = +y_S a\hat{x} + x_S a\hat{y} + (\frac{1}{2} - z_S)c\hat{z}$

PdS is in space group #84 $P4_2/m$: The long name is $P\,4_2/m$ (tetragonal)
$4_2/m$ - 4-fold screw axis along the c-axis and a mirror plane perpendicular to c-axis

Screw Axis Operators: oriented along the c-axis

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \frac{1}{2} \end{bmatrix} = \begin{bmatrix} -y \\ x \\ z+\frac{1}{2} \end{bmatrix} \qquad \begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \frac{1}{2} \end{bmatrix} = \begin{bmatrix} y \\ -x \\ z+\frac{1}{2} \end{bmatrix}$$

Mirror Plane Operator: about the x-y plane

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} x \\ y \\ -z \end{bmatrix}$$