

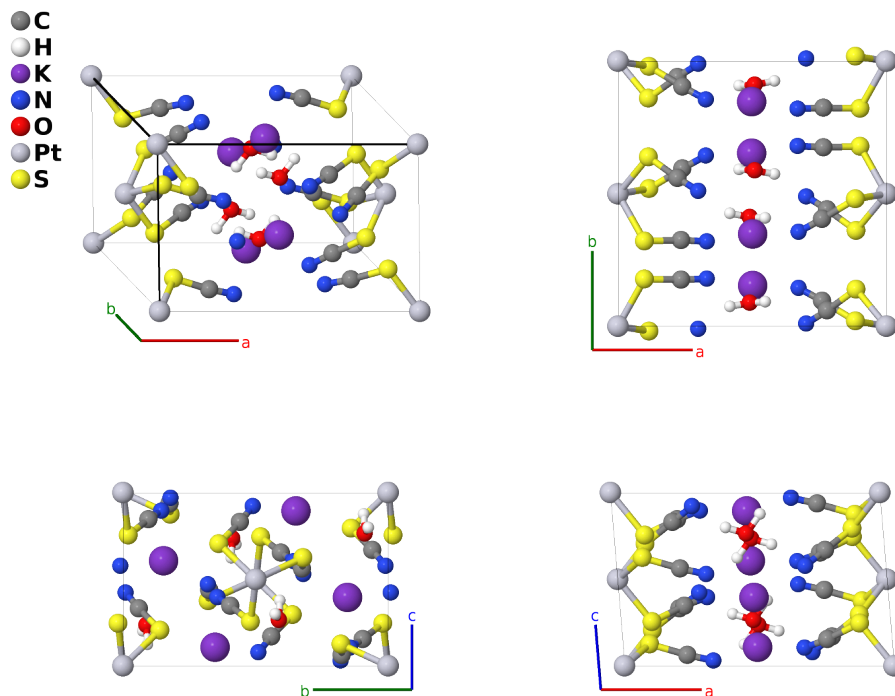
# $K_2Pt(SCN)_6 \cdot 2H_2O$ Structure: A6B4C2D6E2FG6\_mP54\_14\_3e\_2e\_e\_3e\_e\_a\_3e-001

This structure originally had the label A6B4C2D6E2FG6\_mP54\_14\_3e\_2e\_e\_3e\_e\_a\_3e. Calls to that address will be redirected here.

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<https://aflow.org/p/0UZV>

[https://aflow.org/p/A6B4C2D6E2FG6\\_mP54\\_14\\_3e\\_2e\\_e\\_3e\\_e\\_a\\_3e-001](https://aflow.org/p/A6B4C2D6E2FG6_mP54_14_3e_2e_e_3e_e_a_3e-001)



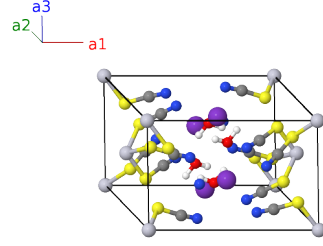
Prototype	$C_6H_4K_2N_6O_2PtS_6$
AFLOW prototype label	A6B4C2D6E2FG6_mP54_14_3e_2e_e_3e_e_a_3e-001
ICSD	74381
Pearson symbol	mP54
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	<pre>aflow --proto=A6B4C2D6E2FG6_mP54_14_3e_2e_e_3e_e_a_3e-001       --params=a, b/a, c/a, <math>\beta</math>, <math>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}</math></pre>

**Other compounds with this structure**  
 $Rb_2Pt(SCN)_6 \cdot 2H_2O$ ,  $NH_4Pt(SCN)_6 \cdot 2H_2O$

- This is the hydrated form. For the anhydrous structure, see the  $H6_3$  structure page.

### Simple Monoclinic primitive vectors

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



### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$0$	$=$	$0$	(2a)	Pt I
$\mathbf{B}_2$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \cos \beta \hat{\mathbf{x}} + \frac{1}{2} b \hat{\mathbf{y}} + \frac{1}{2} c \sin \beta \hat{\mathbf{z}}$	(2a)	Pt I
$\mathbf{B}_3$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4e)	C I
$\mathbf{B}_4$	$-x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_2 + c(z_2 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C I
$\mathbf{B}_5$	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4e)	C I
$\mathbf{B}_6$	$x_2 \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C I
$\mathbf{B}_7$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4e)	C II
$\mathbf{B}_8$	$-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C II
$\mathbf{B}_9$	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4e)	C II
$\mathbf{B}_{10}$	$x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C II
$\mathbf{B}_{11}$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4e)	C III
$\mathbf{B}_{12}$	$-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C III
$\mathbf{B}_{13}$	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4e)	C III
$\mathbf{B}_{14}$	$x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C III
$\mathbf{B}_{15}$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4e)	H I
$\mathbf{B}_{16}$	$-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_5 + c(z_5 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	H I
$\mathbf{B}_{17}$	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4e)	H I
$\mathbf{B}_{18}$	$x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	H I
$\mathbf{B}_{19}$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4e)	H II
$\mathbf{B}_{20}$	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-(ax_6 + c(z_6 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	H II
$\mathbf{B}_{21}$	$-x_6 \mathbf{a}_1 - y_6 \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(4e)	H II



$$\begin{aligned}
\mathbf{B}_{49} &= -x_{13} \mathbf{a}_1 - y_{13} \mathbf{a}_2 - z_{13} \mathbf{a}_3 &= & - (ax_{13} + cz_{13} \cos \beta) \hat{\mathbf{x}} - by_{13} \hat{\mathbf{y}} - & (4e) & \text{S II} \\
& & & & & & cz_{13} \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{50} &= x_{13} \mathbf{a}_1 - (y_{13} - \frac{1}{2}) \mathbf{a}_2 + &= & (ax_{13} + c(z_{13} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - & (4e) & \text{S II} \\
& & & & & & b(y_{13} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{13} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{51} &= x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3 &= & (ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} + by_{14} \hat{\mathbf{y}} + cz_{14} \sin \beta \hat{\mathbf{z}} & (4e) & \text{S III} \\
\mathbf{B}_{52} &= -x_{14} \mathbf{a}_1 + (y_{14} + \frac{1}{2}) \mathbf{a}_2 - &= & - (ax_{14} + c(z_{14} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + & (4e) & \text{S III} \\
& & & & & & b(y_{14} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{14} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{53} &= -x_{14} \mathbf{a}_1 - y_{14} \mathbf{a}_2 - z_{14} \mathbf{a}_3 &= & - (ax_{14} + cz_{14} \cos \beta) \hat{\mathbf{x}} - by_{14} \hat{\mathbf{y}} - & (4e) & \text{S III} \\
& & & & & & cz_{14} \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{54} &= x_{14} \mathbf{a}_1 - (y_{14} - \frac{1}{2}) \mathbf{a}_2 + &= & (ax_{14} + c(z_{14} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - & (4e) & \text{S III} \\
& & & & & & b(y_{14} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{14} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}
\end{aligned}$$

## References

- [1] J. Arpalatti, J. Hölsä, and R. Sillanpää, *Studies on Potassium Thiocyanatoplatinates. II. Crystal Structure of Potassium Hexathiocyanatoplatinate(IV) Dihydrate,  $K_2Pt(SCN)_6 \cdot 2H_2O$* , Acta Chem. Scand. **47**, 1078–1082 (1993), doi:10.3891/acta.chem.scand.47-1078.