$K_2Pt(SCN)_6$ ($H6_3$) Structure: A2BC6_hP9_164_d_a_i-001

This structure previously used the label(s) `A2BC6_hP9_164_d_a_i`. Calls to these addresses will be redirected here.

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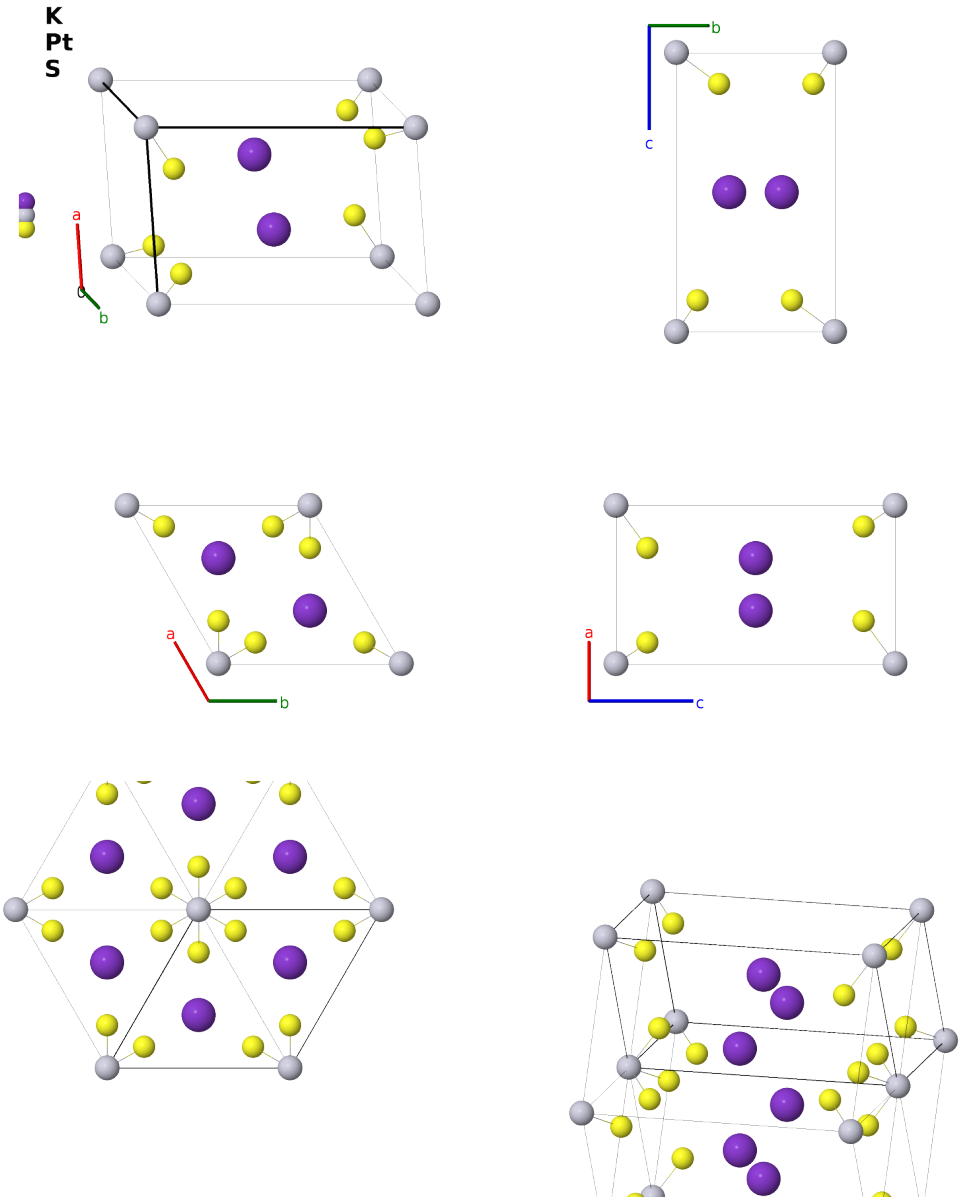
https://aflow.org/prototype-encyclopedia/F3SY

https://aflow.org/prototype-encyclopedia/A2BC6_hP9_164_d_a_i-001



Prototype $K_2Pt(SCN)_6$

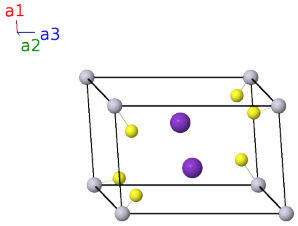
AFLOW prototype label	A2BC6_hP9_164_d_a_i-001
***Strukturbericht* designation**	$H6_3$
ICSD	35511
CCDC	1607608
Pearson symbol	hP9
Space group number	164
Space group symbol	$P\bar{3}m1$
AFLOW prototype command	`aflow --proto=A2BC6_hP9_164_d_a_i-001 --params=`$a, c/a, z_2, x_3, z_3$

Other compounds with this structure
$(NH_4)_2Pt(SCN)_6$, $Rb_2Pt(SCN)_6$

- The structure here must be regarded at tentative. Even the "official" labeling of the structure is uncertain:
- (Hendricks, 1928) made the only structural study of this compound that we have been able to find. Unfortunately, they were not able to determine the positions of the carbon and silicon atoms. Presumably $(SCN)^-$ forms a straight-line ionic system making a roughly 105° angle with the Pt-S line, as it does in the hydrated form $K_2Pt(SCN)_6 \cdot 2H_2O$.
- (Hendricks, 1928) were also uncertain about the space group, giving two possibilities: $P\bar{3}1m$ #162 and $P\bar{3}m1$ #164. They prefer the later, so we present this as a $P\bar{3}m1$.
- The positions of the potassium and sulfur ions are not well determined. (Hendricks, 1928) give $z_2 \approx 0.5$, $x_3 = 0.10 - 0.17$, and $z_3 = 0.09 - 0.135$. We used the average values for the S-III coordinates, so our structure differs slightly from the ICSD.
- While (Ewald, 1931) gave this the *Strukturbericht* designation $H6_3$, (Hermann, 1937) lists it as $I1_3$, "previously $H6_3$." However, they then go on to describe structures of the form $SrCl_2(H_2O)_6$, with a very different c/a ratio.
- (Ewald, 1931) originally used the $H6$ *Strukturbericht* category for compounds of the form $B(X)_6$, but (Herman, 1937) and following volumes use both I and J for $B(X)_6$, sometimes changing a previous $H6$ designation to $I1$ or $J1$. In general we will follow this change in notation, but given the striking difference in structures between $K_2Pt(SCN)_6$ and $CaCl_2(H_2O)_6$ we will continue to uses $H6_3$ for $K_2Pt(SCN)_6$ and $I1_3$ for $CaCl_2(H_2O)_6$.

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Pt I

$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2d)	K I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2d)	K I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-\sqrt{3}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6i)	S I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + 2x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6i)	S I
$\mathbf{B_6}$	=	$-2x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_3\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(6i)	S I
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\sqrt{3}ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(6i)	S I
$\mathbf{B_8}$	=	$2x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{3}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(6i)	S I
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_1 - 2x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-\frac{3}{2}ax_3\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(6i)	S I

References

[1] S. B. Hendricks and H. E. Merwin, *The atomic arrangement in crystals of alkali platini-thiocyanates*, Am. J. Science **15**, 487–494 (1928), doi:10.2475/ajs.s5-15.90.487.

[2] P. P. Ewald and C. Hermann, eds., *Strukturbericht 1913-1928* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1931).

[3] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).

Found in

[1] P. P. Ewald and C. Hermann, eds., *Strukturbericht 1913-1928* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1931).

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