K_2PtCl_4 ($H1_5$) Structure: A4B2C_tP7_123_j_e_a-001

This structure originally had the label `A4B2C_tP7_123_j_e_a`. Calls to that address will be redirected here.

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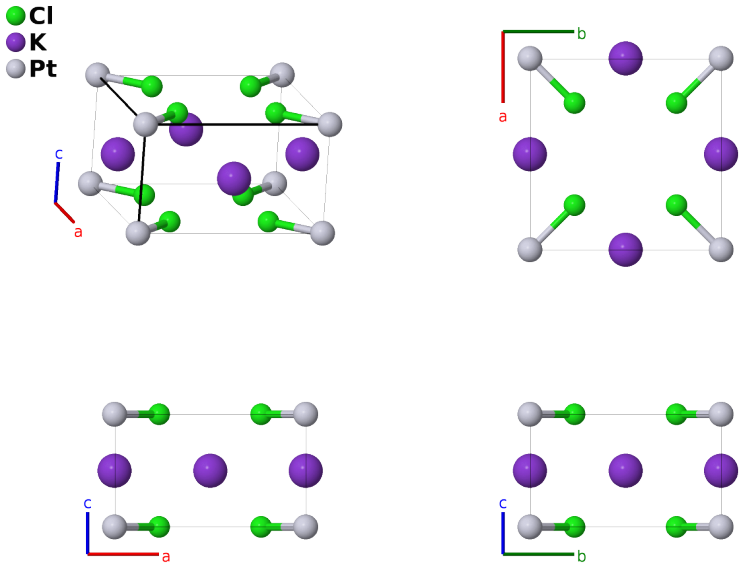
https://aflow.org/p/3SRH

https://aflow.org/p/A4B2C_tP7_123_j_e_a-001

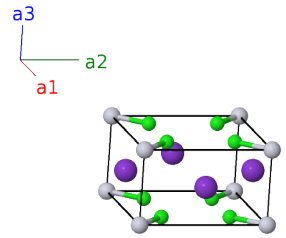


Prototype	Cl_4K_2Pt
AFLOW prototype label	A4B2C_tP7_123_j_e_a-001
***Strukturbericht* designation**	$H1_5$
ICSD	2722
Pearson symbol	tP7
Space group number	123
Space group symbol	$P4/mmm$
AFLOW prototype command	`aflow --proto=A4B2C_tP7_123_j_e_a-001 --params=`$a, c/a, x_3$

Other compounds with this structure
K_2PdCl_4

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
$\mathbf{B_1}$	=	0	=	0	(1a)	Pt I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2e)	K I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2e)	K I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(4j)	Cl I
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(4j)	Cl I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(4j)	Cl I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(4j)	Cl I

References

[1] R. H. B. Mais, P. G. Owston, and A. Wood, *The crystal structure of K_2PtCl_4 and K_2PdCl_4 with estimates of the factors affecting accuracy*, Acta Crystallogr. Sect. B **28**, 393–399 (1972), doi:10.1107/S0567740872002468.