K_2PtCl_6 ($J1_1$) Structure: A6B2C_cF36_225_e_c_a-001

This structure previously used the label(s) `A6B2C_cF36_225_e_c_a`. Calls to these addresses will be redirected here.

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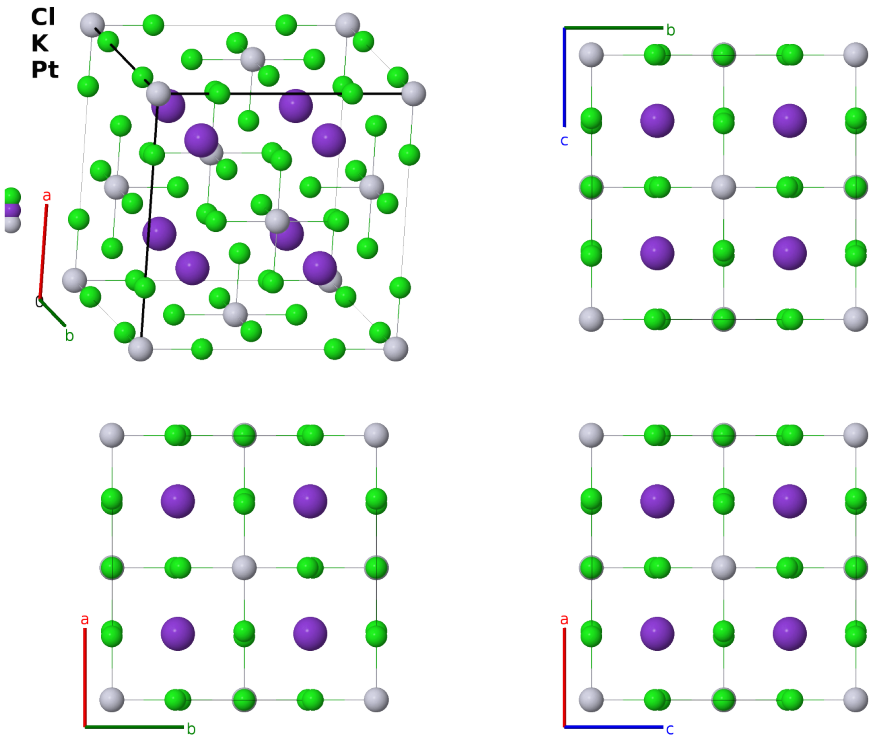
https://aflow.org/prototype-encyclopedia/L6LF

https://aflow.org/prototype-encyclopedia/A6B2C_cF36_225_e_c_a-001



Prototype	Cl_6K_2Pt
AFLOW prototype label	A6B2C_cF36_225_e_c_a-001
***Strukturbericht* designation**	$J1_1$
ICSD	31114
CCDC	1605276
Pearson symbol	cF36
Space group number	225
Space group symbol	$Fm\bar{3}m$
AFLOW prototype command	`aflow --proto=A6B2C_cF36_225_e_c_a-001 --params=`a, x_3

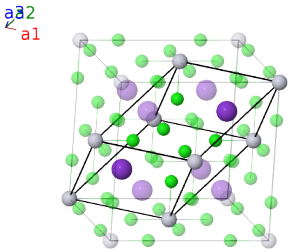
Other compounds with this structure

Ba_2RuH_6, Ca_2FeH_6, Ca_2OsH_6, Ca_2RuH_6, Cs_2CoF_6, Cs_2CsF_6, Cs_2GeCl_6, Cs_2GeF_6, Cs_2MnCl_6, Cs_2NbI_6, Cs_2PbCl_6, Cs_2PdBr_6, Cs_2PtCl_6, Cs_2SnBr_6, Cs_2SnCl_6, Cs_2SnI_6, Cs_2TeCl_6, Cs_2TiCl_6, Cs_2TlCl_6, Cs_2ZrCl_6, Gd_2MnGa_6, K_2MnCl_6, K_2OsBr_2, K_2OsCl_6, K_2PtCl_6, K_2PtCl_6, K_2ReCl_6, K_2SnBr_6, K_2SnCl_6, K_2SnI_6, K_2TeBr_6, Mg_2FeH_6, Mg_2OsH_6, Mg_2RuH_6, Rb_2MnCl_6, Rb_2PbCl_6, Rb_2PdCl_6, Rb_2PtCl_6, Rb_2SeCl_6, Rb_2SnBr_6, Rb_2SnCl_6, Rb_2SnI_6, Rb_2TaBr_6, Rb_2TeCl_6, Rb_2ZrCl_6, Sr_2FeH_6, Sr_2OsH_6, Sr_2RuH_6, Tl_2SnCl_6, $(NH_4)_2PbCl_6$, $(NH_4)_2PtCl_6$, $(NH_4)_2SbCl_6$, $(NH_4)_2SiF_6$, $(NH_4)_2SnCl_6$, $Br_2Ni(NH_3)_6$, $Cl_2Co(NH_3)_6$, $Cs_2Ni(NH_3)_6$, $I_2Co(NH_3)_6$, $I_2Ni(NH_3)_6$

- (Ewald, 1931) originally listed this as *Strukturbericht* $H61$ ($H6_1$ in later notation). (Hermann, 1937) changed this to $I1_1$, and (Gottfried, 1937) changed it to $J1_1$.
- (Douglas, 2006), Table 6.6, provides an extensive list of compounds with this structure. Most have the formula A_2MX_6, where A is an alkali metal, M is a metal, and X is a halide. One can think of this as the fluorite ($C1$) structure with the MX_6 radical replacing the atom on the calcium site. An ammonium ion (NH_4^+) can also substitute for the alkali.
- (Dolui, 2023) used computations to predict that Mg_2IrH_6 can forms in this structure and becomes a superconductor at temperatures less than $T_c = 160$K.

Face-centered Cubic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Pt I
$\mathbf{B_2}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	K I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{3}{4}a\,\hat{\mathbf{z}}$	(8c)	K I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}$	(24e)	Cl I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}$	(24e)	Cl I
$\mathbf{B_6}$	=	$x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{y}}$	(24e)	Cl I
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{y}}$	(24e)	Cl I
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{z}}$	(24e)	Cl I
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{z}}$	(24e)	Cl I

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Found in

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