# $K_2PtCl_6$ ($J1_1$) Structure: A6B2C_cF36_225_e_c_a-001

This structure originally had the label `A6B2C_cF36_225_e_c_a`. Calls to that address will be redirected here.

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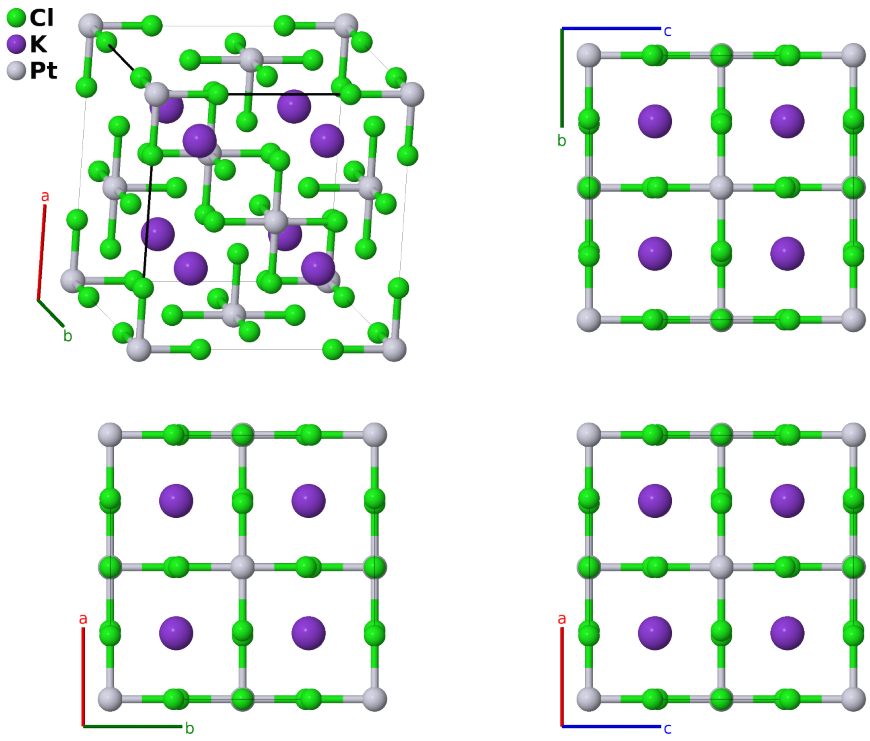
https://aflow.org/p/L6LF

https://aflow.org/p/A6B2C_cF36_225_e_c_a-001

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|---|---|
| **Prototype** | $Cl_6K_2Pt$ |
| **AFLOW prototype label** | A6B2C_cF36_225_e_c_a-001 |
| ***Strukturbericht* designation** | $J1_1$ |
| **ICSD** | 31114 |
| **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**

$Ba_2RuH_6$, $Ca_2FeH_6$, $Ca_2OsH_6$, $Ca_2RuH_6$, $Cs_2CoF_6$, $Cs_2CsF_6$, $Cs_2GeCl_6$, $Cs_2GeF_6$, $Cs_2MnCl_6$, $Cs_2NbI_6$, $Cs_2PbCl_6$, $Cs_2PdBr_6$, $Cs_2PtCl_6$, $Cs_2SnBr_6$, $Cs_2SnCl_6$, $Cs_2SnI_6$, $Cs_2TeCl_6$, $Cs_2TiCl_6$, $Cs_2TlCl_6$, $Cs_2ZrCl_6$, $Gd_2MnGa_6$, $K_2MnCl_6$, $K_2OsBr_2$, $K_2OsCl_6$,

$K_2PtCl_6$, $K_2PtCl_6$, $K_2ReCl_6$, $K_2SnBr_6$, $K_2SnCl_6$, $K_2SnI_6$, $K_2TeBr_6$, $Mg_2FeH_6$, $Mg_2OsH_6$, $Mg_2RuH_6$, $Rb_2MnCl_6$, $Rb_2PbCl_6$, $Rb_2PdCl_6$, $Rb_2PtCl_6$, $Rb_2SeCl_6$, $Rb_2SnBr_6$, $Rb_2SnCl_6$, $Rb_2SnI_6$, $Rb_2TaBr_6$, $Rb_2TeCl_6$, $Rb_2ZrCl_6$, $Sr_2FeH_6$, $Sr_2OsH_6$, $Sr_2RuH_6$, $Tl_2SnCl_6$, $(NH_4)_2PbCl_6$, $(NH_4)_2PtCl_6$, $(NH_4)_2SbCl_6$, $(NH_4)_2SiF_6$, $(NH_4)_2SnCl_6$, $Br_2Ni(NH_3)_6$, $Cl_2Co(NH_3)_6$, $Cs_2Ni(NH_3)_6$, $I_2Co(NH_3)_6$, $I_2Ni(NH_3)_6$

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- (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. An ammonium ion ($NH_4^+$) can also substitute for the alkali.

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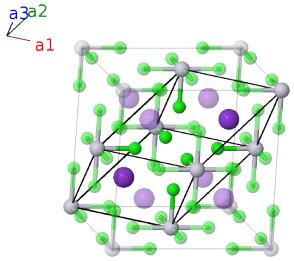
**Face-centered Cubic primitive vectors**

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

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**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 |

**References**


[1] G. Engel, *The Crystal Structure of Potassium Chloroplatinate*, Z. Krystallogr. **68**, 223–230 (1928), doi:10.1524/zkri.1928.68.1.223.

[2] G. Engel, *Die Kristallstrukturen einiger Hexachlorokomplexsalze*, Z. Krystallogr. **90**, 341–373 (1935), doi:10.1524/zkri.1935.90.1.341.

[3] B. Douglas and S.-M. Ho, *Structure and Chemistry of Crystalline Solids* (Springer, 2006).

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

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**Found in**

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).