# $KCa_2Fe_4As_4F_2$ Structure (12442-type superconductor): A4B2C2D4E_tI26_139_2e_e_d_g_a-001

Cite this page as:


- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.


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https://aflow.org/prototype-encyclopedia/YU5Q

https://aflow.org/prototype-encyclopedia/A4B2C2D4E_tI26_139_2e_e_d_g_a-001

| | |
|---|---|
| **Prototype** | $As_4Ca_2F_2Fe_4K$ |
| **AFLOW prototype label** | A4B2C2D4E_tI26_139_2e_e_d_g_a-001 |
| **ICSD** | 239952 |
| **CCDC** | 1925452 |
| **Pearson symbol** | tI26 |
| **Space group number** | 139 |
| **Space group symbol** | $I4/mmm$ |
| **AFLOW prototype command** | `aflow --proto=A4B2C2D4E_tI26_139_2e_e_d_g_a-001 --params=`$a, c/a, z_3, z_4, z_5, z_6$ |

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**Other compounds with this structure**

$CsCa_2Fe_4As_4F_2$, $CsCa_2Fe_4As_4O_2$, $CsDy_2Fe_4As_4F_2$, $CsDy_2Fe_4As_4O_2$, $CsGd_2Fe_4As_4F_2$, $CsGd_2Fe_4As_4O_2$, $CsHo_2Fe_4As_4F_2$, $CsHo_2Fe_4As$
$CsNd_2Fe_4As_4F_2$, $CsNd_2Fe_4As_4O_2$, $CsSm_2Fe_4As_4F_2$, $CsSm_2Fe_4As_4O_2$, $CsTb_2Fe_4As_4F_2$, $CsTb_2Fe_4As_4O_2$, $KCa_2Fe_4As_4O_2$, $KDy_2Fe_4As_4$
$KDy_2Fe_4As_4O_2$, $KGd_2Fe_4As_4F_2$, $KGd_2Fe_4As_4O_2$, $KHo_2Fe_4As_4F_2$, $KHo_2Fe_4As_4O_2$, $KNd_2Fe_4As_4F_2$, $KNd_2Fe_4As_4O_2$, $KSm_2Fe_4As_4F_2$,
$KSm_2Fe_4As_4O_2$, $KTb_2Fe_4As_4F_2$, $KTb_2Fe_4As_4O_2$, $RbCa_2Fe_4As_4F_2$, $RbCa_2Fe_4As_4O_2$, $RbDy_2Fe_4As_4F_2$, $RbDy_2Fe_4As_4O_2$, $RbGd_2Fe_4As$
$RbGd_2Fe_4As_4O_2$, $RbHo_2Fe_4As_4F_2$, $RbHo_2Fe_4As_4O_2$, $RbNd_2Fe_4As_4F_2$, $RbNd_2Fe_4As_4O_2$, $RbSm_2Fe_4As_4F_2$, $RbSm_2Fe_4As_4O_2$,
$RbTb_2Fe_4As_4F_2$, $RbTb_2Fe_4As_4O_2$

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- $KCa_2Fe_4As_4F_2$ is superconducting below 33K.
- The Wyckoff coordinates in Table I of (Wang, 2016) do not agree with the coordinates in the CIF in their supplementary material. The positions in the CIF agree with the positions shown in their Figure 1, so we use the CIF to generate the coordinates.

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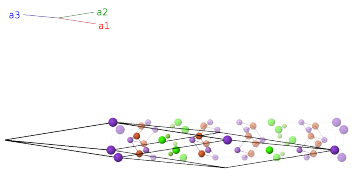
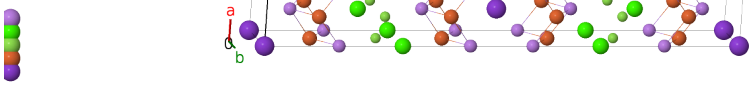
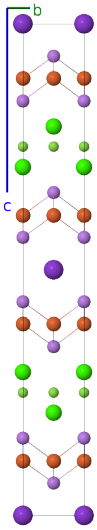
**Body-centered Tetragonal primitive vectors**

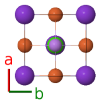
$$\mathbf{a_1} = -\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}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

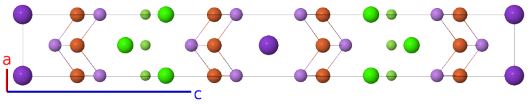


**As**
**Ca**
**F**
**Fe**
**K**



**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (2a) | K I |
| $\mathbf{B_2}$ | = | $\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (4d) | F I |
| $\mathbf{B_3}$ | = | $\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (4d) | F I |
| $\mathbf{B_4}$ | = | $z_3\,\mathbf{a}_1 + z_3\,\mathbf{a}_2$ | = | $cz_3\,\hat{\mathbf{z}}$ | (4e) | As I |
| $\mathbf{B_5}$ | = | $-z_3\,\mathbf{a}_1 - z_3\,\mathbf{a}_2$ | = | $-cz_3\,\hat{\mathbf{z}}$ | (4e) | As I |
| $\mathbf{B_6}$ | = | $z_4\,\mathbf{a}_1 + z_4\,\mathbf{a}_2$ | = | $cz_4\,\hat{\mathbf{z}}$ | (4e) | As II |
| $\mathbf{B_7}$ | = | $-z_4\,\mathbf{a}_1 - z_4\,\mathbf{a}_2$ | = | $-cz_4\,\hat{\mathbf{z}}$ | (4e) | As II |
| $\mathbf{B_8}$ | = | $z_5\,\mathbf{a}_1 + z_5\,\mathbf{a}_2$ | = | $cz_5\,\hat{\mathbf{z}}$ | (4e) | Ca I |
| $\mathbf{B_9}$ | = | $-z_5\,\mathbf{a}_1 - z_5\,\mathbf{a}_2$ | = | $-cz_5\,\hat{\mathbf{z}}$ | (4e) | Ca I |
| $\mathbf{B_{10}}$ | = | $\left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (8g) | Fe I |
| $\mathbf{B_{11}}$ | = | $z_6\,\mathbf{a}_1 + \left(z_6 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} + cz_6\,\hat{\mathbf{z}}$ | (8g) | Fe I |
| $\mathbf{B_{12}}$ | = | $-\left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_1 - z_6\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$ | (8g) | Fe I |
| $\mathbf{B_{13}}$ | = | $-z_6\,\mathbf{a}_1 - \left(z_6 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}a\,\hat{\mathbf{x}} - cz_6\,\hat{\mathbf{z}}$ | (8g) | Fe I |

**References**


[1] Z.-C. Wang, C.-Y. He, S.-Q. Wu, Z.-T. Tang, Y. Liu, A. Ablimit, C.-M. Feng, and G.-H. Cao, *Superconductivity in $KCa_2Fe_4As_4F_2$ with Separate Double $Fe_2As_2$ Layers*, J. Am. Chem. Soc. **138**, 7856–7859 (2016), doi:10.1021/jacs.6b04538.


**Found in**


[1] Z.-C. Wang, C.-Y. He, S.-Q. Wu, Z.-T. Tang, Y. Liu, and G.-H. Cao, *Synthesis, Crystal Structure and Superconductivity in $RbLn_2Fe_4As_4O_2$ (Ln = Sm, Tb, Dy, and Ho)*, Chem. Mater. **29**, 1805–1812 (2017), doi:10.1021/acs.chemmater.6b05458.


**First cited in**


H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.