# $MgSO_4$ Structure: ABC4_oC24_63_c_a_fg-001

This structure originally had the label `AB4C_oC24_63_a_fg_c`. Calls to that address will be redirected here.

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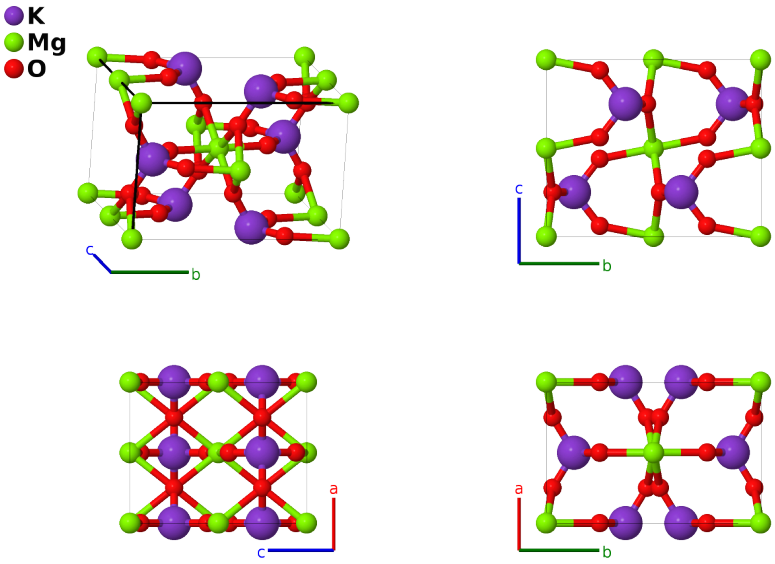
https://aflow.org/p/FNXT

https://aflow.org/p/ABC4_oC24_63_c_a_fg-001




| | |
|---|---|
| **Prototype** | $MgO_4S$ |
| **AFLOW prototype label** | ABC4_oC24_63_c_a_fg-001 |
| **ICSD** | 16759 |
| **Pearson symbol** | oC24 |
| **Space group number** | 63 |
| **Space group symbol** | $Cmcm$ |
| **AFLOW prototype command** | `aflow --proto=ABC4_oC24_63_c_a_fg-001 --params=`$a, b/a, c/a, y_2, y_3, z_3, x_4, y_4$ |

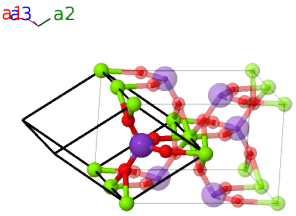
**Other compounds with this structure**

$CdCrO_4$, $CoCrO_4$, $CuCrO_4$, $MgCrO_4$, $MnCrO_4$, $NiCrO_4$, $ZnCrO_4$, $AlPO_4$, $\beta$-$CrPO_4$, $FePO_4$, $InPO_4$, $TlPO_4$, $TlPO_4$, $VPO_4$, $CdSO_4$, $CoSO_4$, $CuSO_4$, $FeSO_4$, $NiSO_4$, $ZnSO_4$, $CoSeO_4$, $CuSeO_4$, $MnSeO_4$, $ZnSeO_4$, $CrVO_4$, $FeVO_4$, $InVO_4$, $TlVO_4$

- (Baran, 1998) gives $CrVO_4$ or $\beta$-$CrPO_4$ as the prototype for this structure.

**Base-centered Orthorhombic primitive vectors**

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

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**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | = | $0$ | = | $0$ | (4a) | Mg I |
| $\mathbf{B_2}$ | = | $\frac{1}{2}\,\mathbf{a}_3$ | = | $\frac{1}{2}c\,\hat{\mathbf{z}}$ | (4a) | Mg I |
| $\mathbf{B_3}$ | = | $-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (4c) | K I |
| $\mathbf{B_4}$ | = | $y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $-by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (4c) | K I |
| $\mathbf{B_5}$ | = | $-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$ | = | $by_3\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (8f) | O I |
| $\mathbf{B_6}$ | = | $y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $-by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (8f) | O I |
| $\mathbf{B_7}$ | = | $-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\,\mathbf{a}_3$ | = | $by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$ | (8f) | O I |
| $\mathbf{B_8}$ | = | $y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$ | = | $-by_3\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$ | (8f) | O I |
| $\mathbf{B_9}$ | = | $(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (8g) | O II |
| $\mathbf{B_{10}}$ | = | $-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $-ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (8g) | O II |
| $\mathbf{B_{11}}$ | = | $-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$ | = | $-ax_4\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$ | (8g) | O II |
| $\mathbf{B_{12}}$ | = | $(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$ | = | $ax_4\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$ | (8g) | O II |

**References**


[1] P. J. Rentzeperis and C. T. Soldatos, *The crystal structure of the anhydrous magnesium sulphate*, Acta Cryst. **11**, 686–688 (1958), doi:10.1107/S0365110X58001857.

[2] E. J. Baran, *Review: Materials belonging to the $CrVO_4$ structure type: preparation, crystal chemistry and physicochemical properties*, J. Mater. Sci. **33**, 2479–2497 (1998), doi:10.1023/A:1004380530309.


**Found in**


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