# Bromocarnallite ($E2_6$, KMg(H$_2$O)$_6$(Cl,Br)$_3$) Structure: A3B6CD_tP44_85_acg_3g_bc_d-001

This structure originally had the label `A3B6CD_tP44_85_bcg_3g_ac_e`. Calls to that address will be redirected here.

https://aflow.org/p/PV6C

https://aflow.org/p/A3B6CD_tP44_85_acg_3g_bc_d-001
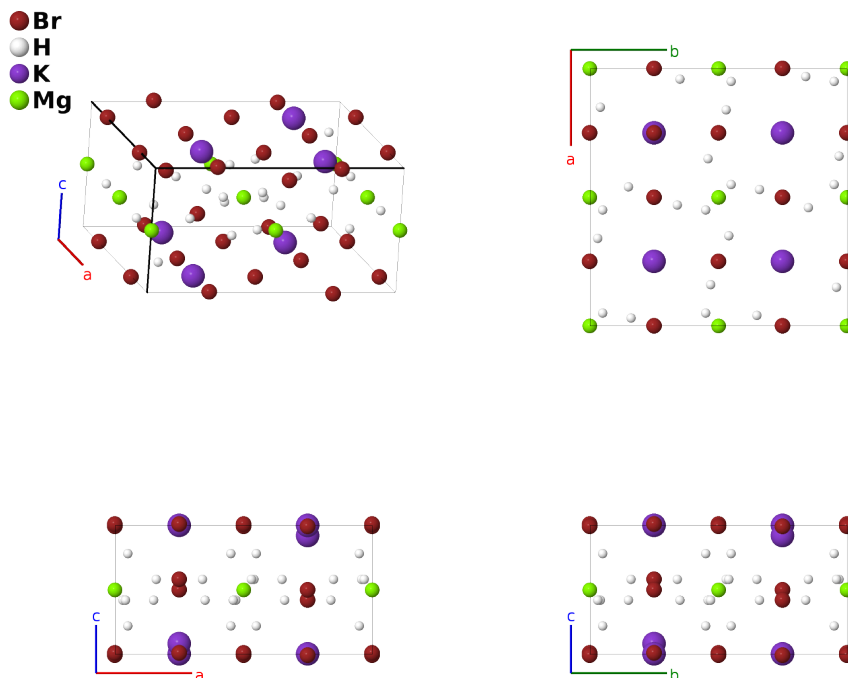


| Prototype | Br$_3$(H$_2$O)$_6$KMg |
|---|---|
| **AFLOW prototype label** | A3B6CD_tP44_85_acg_3g_bc_d-001 |
| ***Strukturbericht* designation** | $E2_6$ |
| **Mineral name** | bromocarnallite |
| **ICSD** | 30220 |
| **Pearson symbol** | tP44 |
| **Space group number** | 85 |
| **Space group symbol** | $P4/n$ |
| **AFLOW prototype command** | aflow --proto=A3B6CD_tP44_85_acg_3g_bc_d-001<br>        --params=$a, c/a, z_3, z_4, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9$ |

- (Andreß, 1939) first determined the structure of bromocarnallite, using a sample with 75% bromine on the halide site.

- They were unable to locate the hydrogen atoms, and placed the compound in space group $P4/n$ #85. The data was given by (Hermann, 1939) in setting 1 of this group, but we used FINDSYM to place it in the standard setting 2.

- (Hermann, 1939) assigned this compound the *Strukcturbericht* symbol $E2_6$.

- (Schlemper, 1985) re-examined the structure for the pure chlorine version, Carnalliite. They located the hydrogen atoms and placed the system in space group $Pnna$ #52. We present this structure in the Carnallite structure page.

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**Simple Tetragonal primitive vectors**



$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$

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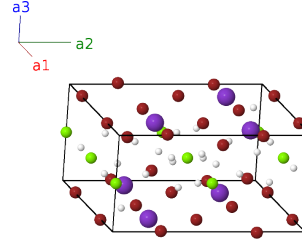
**Basis vectors**

| | | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|---|---|---|---|---|---|---|
| $\mathbf{B_1}$ | $=$ | $\frac{1}{4}\mathbf{a_1} + \frac{3}{4}\mathbf{a_2}$ | $=$ | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}}$ | (2a) | Br I |
| $\mathbf{B_2}$ | $=$ | $\frac{3}{4}\mathbf{a_1} + \frac{1}{4}\mathbf{a_2}$ | $=$ | $\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$ | (2a) | Br I |
| $\mathbf{B_3}$ | $=$ | $\frac{1}{4}\mathbf{a_1} + \frac{3}{4}\mathbf{a_2} + \frac{1}{2}\mathbf{a_3}$ | $=$ | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (2b) | K I |
| $\mathbf{B_4}$ | $=$ | $\frac{3}{4}\mathbf{a_1} + \frac{1}{4}\mathbf{a_2} + \frac{1}{2}\mathbf{a_3}$ | $=$ | $\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$ | (2b) | K I |
| $\mathbf{B_5}$ | $=$ | $\frac{1}{4}\mathbf{a_1} + \frac{1}{4}\mathbf{a_2} + z_3\,\mathbf{a_3}$ | $=$ | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$ | (2c) | Br II |
| $\mathbf{B_6}$ | $=$ | $\frac{3}{4}\mathbf{a_1} + \frac{3}{4}\mathbf{a_2} - z_3\,\mathbf{a_3}$ | $=$ | $\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$ | (2c) | Br II |
| $\mathbf{B_7}$ | $=$ | $\frac{1}{4}\mathbf{a_1} + \frac{1}{4}\mathbf{a_2} + z_4\,\mathbf{a_3}$ | $=$ | $\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$ | (2c) | K II |
| $\mathbf{B_8}$ | $=$ | $\frac{3}{4}\mathbf{a_1} + \frac{3}{4}\mathbf{a_2} - z_4\,\mathbf{a_3}$ | $=$ | $\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$ | (2c) | K II |
| $\mathbf{B_9}$ | $=$ | $0$ | $=$ | $0$ | (4d) | Mg I |
| $\mathbf{B_{10}}$ | $=$ | $\frac{1}{2}\mathbf{a_1} + \frac{1}{2}\mathbf{a_2}$ | $=$ | $\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$ | (4d) | Mg I |
| $\mathbf{B_{11}}$ | $=$ | $\frac{1}{2}\mathbf{a_1}$ | $=$ | $\frac{1}{2}a\,\hat{\mathbf{x}}$ | (4d) | Mg I |
| $\mathbf{B_{12}}$ | $=$ | $\frac{1}{2}\mathbf{a_2}$ | $=$ | $\frac{1}{2}a\,\hat{\mathbf{y}}$ | (4d) | Mg I |
| $\mathbf{B_{13}}$ | $=$ | $x_6\,\mathbf{a_1} + y_6\,\mathbf{a_2} + z_6\,\mathbf{a_3}$ | $=$ | $ax_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (8g) | Br III |
| $\mathbf{B_{14}}$ | $=$ | $-\left(x_6 - \frac{1}{2}\right)\mathbf{a_1} - \left(y_6 - \frac{1}{2}\right)\mathbf{a_2} + z_6\,\mathbf{a_3}$ | $=$ | $-a\left(x_6 - \frac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_6 - \frac{1}{2}\right)\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (8g) | Br III |
| $\mathbf{B_{15}}$ | $=$ | $-\left(y_6 - \frac{1}{2}\right)\mathbf{a_1} + x_6\,\mathbf{a_2} + z_6\,\mathbf{a_3}$ | $=$ | $-a\left(y_6 - \frac{1}{2}\right)\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (8g) | Br III |
| $\mathbf{B_{16}}$ | $=$ | $y_6\,\mathbf{a_1} - \left(x_6 - \frac{1}{2}\right)\mathbf{a_2} + z_6\,\mathbf{a_3}$ | $=$ | $ay_6\,\hat{\mathbf{x}} - a\left(x_6 - \frac{1}{2}\right)\hat{\mathbf{y}} + cz_6\,\hat{\mathbf{z}}$ | (8g) | Br III |
| $\mathbf{B_{17}}$ | $=$ | $-x_6\,\mathbf{a_1} - y_6\,\mathbf{a_2} - z_6\,\mathbf{a_3}$ | $=$ | $-ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$ | (8g) | Br III |
| $\mathbf{B_{18}}$ | $=$ | $\left(x_6 + \frac{1}{2}\right)\mathbf{a_1} + \left(y_6 + \frac{1}{2}\right)\mathbf{a_2} - z_6\,\mathbf{a_3}$ | $=$ | $a\left(x_6 + \frac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_6 + \frac{1}{2}\right)\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$ | (8g) | Br III |
| $\mathbf{B_{19}}$ | $=$ | $\left(y_6 + \frac{1}{2}\right)\mathbf{a_1} - x_6\,\mathbf{a_2} - z_6\,\mathbf{a_3}$ | $=$ | $a\left(y_6 + \frac{1}{2}\right)\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$ | (8g) | Br III |
| $\mathbf{B_{20}}$ | $=$ | $-y_6\,\mathbf{a_1} + \left(x_6 + \frac{1}{2}\right)\mathbf{a_2} - z_6\,\mathbf{a_3}$ | $=$ | $-ay_6\,\hat{\mathbf{x}} + a\left(x_6 + \frac{1}{2}\right)\hat{\mathbf{y}} - cz_6\,\hat{\mathbf{z}}$ | (8g) | Br III |
| $\mathbf{B_{21}}$ | $=$ | $x_7\,\mathbf{a_1} + y_7\,\mathbf{a_2} + z_7\,\mathbf{a_3}$ | $=$ | $ax_7\,\hat{\mathbf{x}} + ay_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$ | (8g) | H I |
| $\mathbf{B_{22}}$ | $=$ | $-\left(x_7 - \frac{1}{2}\right)\mathbf{a_1} - \left(y_7 - \frac{1}{2}\right)\mathbf{a_2} + z_7\,\mathbf{a_3}$ | $=$ | $-a\left(x_7 - \frac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_7 - \frac{1}{2}\right)\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$ | (8g) | H I |

$$\mathbf{B_{23}} = -\left(y_7 - \tfrac{1}{2}\right)\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = -a\left(y_7 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H I}$$

$$\mathbf{B_{24}} = y_7\,\mathbf{a}_1 - \left(x_7 - \tfrac{1}{2}\right)\mathbf{a}_2 + z_7\,\mathbf{a}_3 = ay_7\,\hat{\mathbf{x}} - a\left(x_7 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H I}$$

$$\mathbf{B_{25}} = -x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 = -ax_7\,\hat{\mathbf{x}} - ay_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H I}$$

$$\mathbf{B_{26}} = \left(x_7 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_7 + \tfrac{1}{2}\right)\mathbf{a}_2 - z_7\,\mathbf{a}_3 = a\left(x_7 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_7 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H I}$$

$$\mathbf{B_{27}} = \left(y_7 + \tfrac{1}{2}\right)\mathbf{a}_1 - x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 = a\left(y_7 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H I}$$

$$\mathbf{B_{28}} = -y_7\,\mathbf{a}_1 + \left(x_7 + \tfrac{1}{2}\right)\mathbf{a}_2 - z_7\,\mathbf{a}_3 = -ay_7\,\hat{\mathbf{x}} + a\left(x_7 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H I}$$

$$\mathbf{B_{29}} = x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = ax_8\,\hat{\mathbf{x}} + ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H II}$$

$$\mathbf{B_{30}} = -\left(x_8 - \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_8 - \tfrac{1}{2}\right)\mathbf{a}_2 + z_8\,\mathbf{a}_3 = -a\left(x_8 - \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_8 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H II}$$

$$\mathbf{B_{31}} = -\left(y_8 - \tfrac{1}{2}\right)\mathbf{a}_1 + x_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = -a\left(y_8 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H II}$$

$$\mathbf{B_{32}} = y_8\,\mathbf{a}_1 - \left(x_8 - \tfrac{1}{2}\right)\mathbf{a}_2 + z_8\,\mathbf{a}_3 = ay_8\,\hat{\mathbf{x}} - a\left(x_8 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H II}$$

$$\mathbf{B_{33}} = -x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 = -ax_8\,\hat{\mathbf{x}} - ay_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H II}$$

$$\mathbf{B_{34}} = \left(x_8 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_8 + \tfrac{1}{2}\right)\mathbf{a}_2 - z_8\,\mathbf{a}_3 = a\left(x_8 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_8 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H II}$$

$$\mathbf{B_{35}} = \left(y_8 + \tfrac{1}{2}\right)\mathbf{a}_1 - x_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 = a\left(y_8 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H II}$$

$$\mathbf{B_{36}} = -y_8\,\mathbf{a}_1 + \left(x_8 + \tfrac{1}{2}\right)\mathbf{a}_2 - z_8\,\mathbf{a}_3 = -ay_8\,\hat{\mathbf{x}} + a\left(x_8 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H II}$$

$$\mathbf{B_{37}} = x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 = ax_9\,\hat{\mathbf{x}} + ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H III}$$

$$\mathbf{B_{38}} = -\left(x_9 - \tfrac{1}{2}\right)\mathbf{a}_1 - \left(y_9 - \tfrac{1}{2}\right)\mathbf{a}_2 + z_9\,\mathbf{a}_3 = -a\left(x_9 - \tfrac{1}{2}\right)\hat{\mathbf{x}} - a\left(y_9 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H III}$$

$$\mathbf{B_{39}} = -\left(y_9 - \tfrac{1}{2}\right)\mathbf{a}_1 + x_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3 = -a\left(y_9 - \tfrac{1}{2}\right)\hat{\mathbf{x}} + ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H III}$$

$$\mathbf{B_{40}} = y_9\,\mathbf{a}_1 - \left(x_9 - \tfrac{1}{2}\right)\mathbf{a}_2 + z_9\,\mathbf{a}_3 = ay_9\,\hat{\mathbf{x}} - a\left(x_9 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H III}$$

$$\mathbf{B_{41}} = -x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3 = -ax_9\,\hat{\mathbf{x}} - ay_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H III}$$

$$\mathbf{B_{42}} = \left(x_9 + \tfrac{1}{2}\right)\mathbf{a}_1 + \left(y_9 + \tfrac{1}{2}\right)\mathbf{a}_2 - z_9\,\mathbf{a}_3 = a\left(x_9 + \tfrac{1}{2}\right)\hat{\mathbf{x}} + a\left(y_9 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H III}$$

$$\mathbf{B_{43}} = \left(y_9 + \tfrac{1}{2}\right)\mathbf{a}_1 - x_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3 = a\left(y_9 + \tfrac{1}{2}\right)\hat{\mathbf{x}} - ax_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H III}$$

$$\mathbf{B_{44}} = -y_9\,\mathbf{a}_1 + \left(x_9 + \tfrac{1}{2}\right)\mathbf{a}_2 - z_9\,\mathbf{a}_3 = -ay_9\,\hat{\mathbf{x}} + a\left(x_9 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \qquad (8g) \qquad \text{H III}$$

## References

[1] K. R. Andreß and O. Saffe, *Röntgenographische Untersuchung der Mischkristallreihe Karnallit-Bromkarnallit*, Z. Kristallogr. **101**, 451–469 (1939), doi:10.1524/zkri.1939.101.1.451.

[2] E. O. Schlemper, P. K. S. Gupta, and T. Zoltai, *Refinement of the structure of carnallite, $Mg(H_2O)_6KCl_3$*, Am. Mineral. **70**, 1309–1313 (1985).

## Found in

[1] K. Herrmann, ed., *Strukturbericht Band VII 1939* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1943).