$KAuBr_4 \cdot 2H_2O$ ($H4_{19}$) Structure: AB4C2D_mP32_14_e_4e_2e_e-001

This structure originally had the label `AB4C2D_mP32_14_e_4e_2e_e`. Calls to that address will be redirected here.

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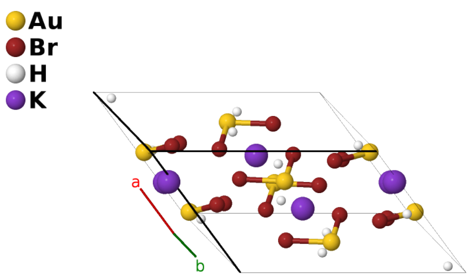
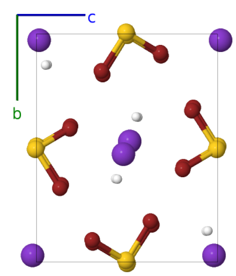
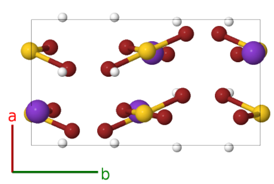
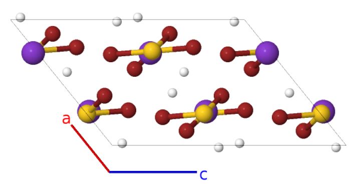
https://aflow.org/p/SAP5

https://aflow.org/p/AB4C2D_mP32_14_e_4e_2e_e-001







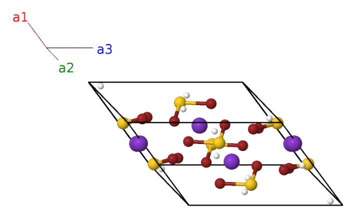


Prototype	$AuBr_4(H_2O)_2K$
AFLOW prototype label	AB4C2D_mP32_14_e_4e_2e_e-001
***Strukturbericht* designation**	$H4_{19}$
ICSD	61248
Pearson symbol	mP32
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	`aflow --proto=AB4C2D_mP32_14_e_4e_2e_e-001` `--params=`$a, b/a, c/a, \beta, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8$

- (Cox, 1936) determined lattice constants for $KAuBr_4{\cdot}H_2O$ which were very close to those later found by (Omarni, 1986). However, Cox *et al.* found that the (100) planes (in our orientation) with odd indices showed very weak diffraction spots. Neglecting these spots gives a unit cell which has a lattice constant a (in our orientation) which is half the size of that found by Omarni *et al*, and so Pearson symbol mP16. Fitting this cell into space group $P2_1/c$ #14 then required that the gold atom be at the (2a) Wyckoff position and the potassium atom at (2b), while the later paper found that these atoms are slightly displaced from those points.
- The results of (Omarni, 1986) are very close to those of (Cox, 1936) and can indeed reduce to the Cox *et al.* structure by allowing some uncertainty in the atomic positions. Given this, and the fact that the former reference actually found the correct unit cell, we will use the more modern work as our prototype for *Strukturbericht* symbol $H4_{19}$.
- The positions of the hydrogen atoms in the water molecules were not determined, so we only show the oxygen positions, labeled H_2O.
- (Omarni, 1986) gave the unit cell and Wyckoff positions in terms of setting $P2_1/n$ of space group #14. Changing this to the standard $P2_1/c$ setting required a rotation of the lattice and a significant rewriting of the primitive vectors.
- The anhydrous form of this compound can be seen at $KAuBr_4$ (AB4C_mP24_14_ab_4e_e).

Simple Monoclinic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\left(ax_1 + cz_1\cos\beta\right)\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(4e)	Au I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right)\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\mathbf{a}_3$	=	$-\left(ax_1 + c\left(z_1 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Au I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-\left(ax_1 + cz_1\cos\beta\right)\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(4e)	Au I
$\mathbf{B_4}$	=	$x_1\,\mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right)\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\mathbf{a}_3$	=	$\left(ax_1 + c\left(z_1 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Au I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\left(ax_2 + cz_2\cos\beta\right)\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	Br I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right)\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\mathbf{a}_3$	=	$-\left(ax_2 + c\left(z_2 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Br I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-\left(ax_2 + cz_2\cos\beta\right)\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	Br I
$\mathbf{B_8}$	=	$x_2\,\mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right)\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\mathbf{a}_3$	=	$\left(ax_2 + c\left(z_2 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Br I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\left(ax_3 + cz_3\cos\beta\right)\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	Br II
$\mathbf{B_{10}}$	=	$-x_3\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\mathbf{a}_3$	=	$-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Br II
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-\left(ax_3 + cz_3\cos\beta\right)\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	Br II
$\mathbf{B_{12}}$	=	$x_3\,\mathbf{a}_1 - \left(y_3 - \frac{1}{2}\right)\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\mathbf{a}_3$	=	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Br II
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\left(ax_4 + cz_4\cos\beta\right)\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	Br III

$$\mathbf{B_{14}} = -x_4\,\mathbf{a}_1 + \left(y_4+\tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\left(ax_4 + c\left(z_4-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_4+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_4-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{Br III}$$

$$\mathbf{B_{15}} = -x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3 = -\left(ax_4 + cz_4\cos\beta\right)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{Br III}$$

$$\mathbf{B_{16}} = x_4\,\mathbf{a}_1 - \left(y_4-\tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \left(ax_4 + c\left(z_4+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_4-\tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_4+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{Br III}$$

$$\mathbf{B_{17}} = x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3 = \left(ax_5 + cz_5\cos\beta\right)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{Br IV}$$

$$\mathbf{B_{18}} = -x_5\,\mathbf{a}_1 + \left(y_5+\tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_5-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\left(ax_5 + c\left(z_5-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_5+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_5-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{Br IV}$$

$$\mathbf{B_{19}} = -x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3 = -\left(ax_5 + cz_5\cos\beta\right)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{Br IV}$$

$$\mathbf{B_{20}} = x_5\,\mathbf{a}_1 - \left(y_5-\tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_5+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \left(ax_5 + c\left(z_5+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_5-\tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_5+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{Br IV}$$

$$\mathbf{B_{21}} = x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3 = \left(ax_6 + cz_6\cos\beta\right)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{H I}$$

$$\mathbf{B_{22}} = -x_6\,\mathbf{a}_1 + \left(y_6+\tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_6-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\left(ax_6 + c\left(z_6-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_6+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_6-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{H I}$$

$$\mathbf{B_{23}} = -x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3 = -\left(ax_6 + cz_6\cos\beta\right)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{H I}$$

$$\mathbf{B_{24}} = x_6\,\mathbf{a}_1 - \left(y_6-\tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_6+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \left(ax_6 + c\left(z_6+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_6-\tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_6+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{H I}$$

$$\mathbf{B_{25}} = x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3 = \left(ax_7 + cz_7\cos\beta\right)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{H II}$$

$$\mathbf{B_{26}} = -x_7\,\mathbf{a}_1 + \left(y_7+\tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_7-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\left(ax_7 + c\left(z_7-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_7+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_7-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{H II}$$

$$\mathbf{B_{27}} = -x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3 = -\left(ax_7 + cz_7\cos\beta\right)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{H II}$$

$$\mathbf{B_{28}} = x_7\,\mathbf{a}_1 - \left(y_7-\tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_7+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \left(ax_7 + c\left(z_7+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_7-\tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_7+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{H II}$$

$$\mathbf{B_{29}} = x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3 = \left(ax_8 + cz_8\cos\beta\right)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{K I}$$

$$\mathbf{B_{30}} = -x_8\,\mathbf{a}_1 + \left(y_8+\tfrac{1}{2}\right)\,\mathbf{a}_2 - \left(z_8-\tfrac{1}{2}\right)\,\mathbf{a}_3 = -\left(ax_8 + c\left(z_8-\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} + b\left(y_8+\tfrac{1}{2}\right)\,\hat{\mathbf{y}} - c\left(z_8-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{K I}$$

$$\mathbf{B_{31}} = -x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3 = -\left(ax_8 + cz_8\cos\beta\right)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\sin\beta\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{K I}$$

$$\mathbf{B_{32}} = x_8\,\mathbf{a}_1 - \left(y_8-\tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(z_8+\tfrac{1}{2}\right)\,\mathbf{a}_3 = \left(ax_8 + c\left(z_8+\tfrac{1}{2}\right)\cos\beta\right)\,\hat{\mathbf{x}} - b\left(y_8-\tfrac{1}{2}\right)\,\hat{\mathbf{y}} + c\left(z_8+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad \text{(4e)} \quad \text{K I}$$

References

[1] H. Omrani, F. Théobald, and H. Vivier, *Structure of potassium tetrabromoaurate(III) dihydrate*, Acta Crystallogr. Sect. C **24**, 1091–1092 (1986), doi:10.1107/S0108270186093344.

[2] E. G. Cox and K. C. Webster, *The stereochemistry of quadricovalent atoms : tervalent gold*, J. Chem. Soc. London pp. 1635–1637 (1936), doi:10.1039/JR9360001635.

Found in

[1] R. Welter, H. Omrani, and R. Vangelisti, *Sodium tetrabromoaurate(III) dihydrate*, Acta Crystallogr. Sect. E **57**, i8–i9 (2001), doi:10.1107/S1600536800021140.