Juangodoyite [Na$_2$Cu(CO$_3$)$_2$] Structure: A2BC2D6_mP22_14_e_a_e_3e-001

https://aflow.org/p/DUCH

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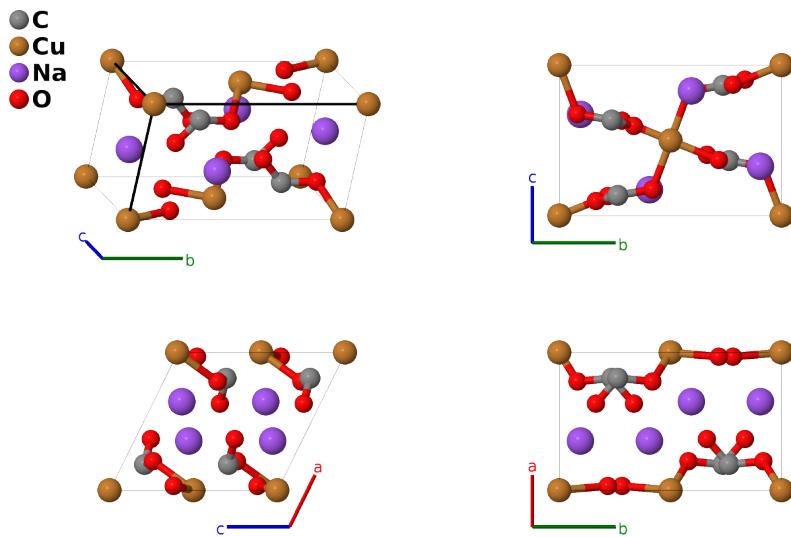
Prototype	C$_2$CuNa$_2$O$_6$
AFLOW prototype label	A2BC2D6_mP22_14_e_a_e_3e-001
Mineral name	juangodoyite
ICSD	60858
Pearson symbol	mP22
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	aflow --proto=A2BC2D6_mP22_14_e_a_e_3e-001 --params=$a, b/a, c/a, \beta, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

## Other compounds with this structure

Sr$_2$Cu(BO$_3$)$_2$

- (Maslen, 1986) give the structure in the $P2_1/a$ setting of space group #14. We used FINDSYM to transform this to the standard $P2_1/c$ setting.

Simple Monoclinic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$

$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$

$$\mathbf{a_3} = c\cos\beta\,\hat{\mathbf{x}} + c\sin\beta\,\hat{\mathbf{z}}$$
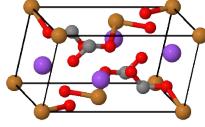
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	0	$=$	0	(2a)	Cu I
$\mathbf{B_2}$	$=$	$\frac{1}{2}\mathbf{a_2} + \frac{1}{2}\mathbf{a_3}$	$=$	$\frac{1}{2}c\cos\beta\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2a)	Cu I
$\mathbf{B_3}$	$=$	$x_2\mathbf{a_1} + y_2\mathbf{a_2} + z_2\mathbf{a_3}$	$=$	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	C I
$\mathbf{B_4}$	$=$	$-x_2\mathbf{a_1} + \left(y_2 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_2 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_2 + c\left(z_2 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	C I
$\mathbf{B_5}$	$=$	$-x_2\mathbf{a_1} - y_2\mathbf{a_2} - z_2\mathbf{a_3}$	$=$	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4e)	C 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)	C I
$\mathbf{B_7}$	$=$	$x_3\mathbf{a_1} + y_3\mathbf{a_2} + z_3\mathbf{a_3}$	$=$	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	Na I
$\mathbf{B_8}$	$=$	$-x_3\mathbf{a_1} + \left(y_3 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_3 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Na I
$\mathbf{B_9}$	$=$	$-x_3\mathbf{a_1} - y_3\mathbf{a_2} - z_3\mathbf{a_3}$	$=$	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	Na I
$\mathbf{B_{10}}$	$=$	$x_3\mathbf{a_1} - \left(y_3 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_3 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_3 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Na I
$\mathbf{B_{11}}$	$=$	$x_4\mathbf{a_1} + y_4\mathbf{a_2} + z_4\mathbf{a_3}$	$=$	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_{12}}$	$=$	$-x_4\mathbf{a_1} + \left(y_4 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_4 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_{13}}$	$=$	$-x_4\mathbf{a_1} - y_4\mathbf{a_2} - z_4\mathbf{a_3}$	$=$	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_{14}}$	$=$	$x_4\mathbf{a_1} - \left(y_4 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_4 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_{15}}$	$=$	$x_5\mathbf{a_1} + y_5\mathbf{a_2} + z_5\mathbf{a_3}$	$=$	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{16}}$	$=$	$-x_5\mathbf{a_1} + \left(y_5 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_5 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_5 + c\left(z_5 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{17}}$	$=$	$-x_5\mathbf{a_1} - y_5\mathbf{a_2} - z_5\mathbf{a_3}$	$=$	$-(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} - by_5\,\hat{\mathbf{y}} - cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{18}}$	$=$	$x_5\mathbf{a_1} - \left(y_5 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_5 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_5 + c\left(z_5 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{19}}$	$=$	$x_6\mathbf{a_1} + y_6\mathbf{a_2} + z_6\mathbf{a_3}$	$=$	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_{20}}$	$=$	$-x_6\mathbf{a_1} + \left(y_6 + \frac{1}{2}\right)\mathbf{a_2} - \left(z_6 - \frac{1}{2}\right)\mathbf{a_3}$	$=$	$-\left(ax_6 + c\left(z_6 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_{21}}$	$=$	$-x_6\mathbf{a_1} - y_6\mathbf{a_2} - z_6\mathbf{a_3}$	$=$	$-(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} - by_6\,\hat{\mathbf{y}} - cz_6\sin\beta\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_{22}}$	$=$	$x_6\mathbf{a_1} - \left(y_6 - \frac{1}{2}\right)\mathbf{a_2} + \left(z_6 + \frac{1}{2}\right)\mathbf{a_3}$	$=$	$\left(ax_6 + c\left(z_6 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O III

References

[1] E. N. Maslen, N. Spadaccini, K. J. Watson, and A. H. White, *Electron density in non-ideal metal complexes. II. Sodium bis(carbonato)cuprate(II)*, Acta Crystallogr. Sect. B **42**, 430–436 (1986), doi:10.1107/S0108768186097926.

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