Ca_2UO_5 Structure: A2B5C_mP32_14_2e_5e_ab-001
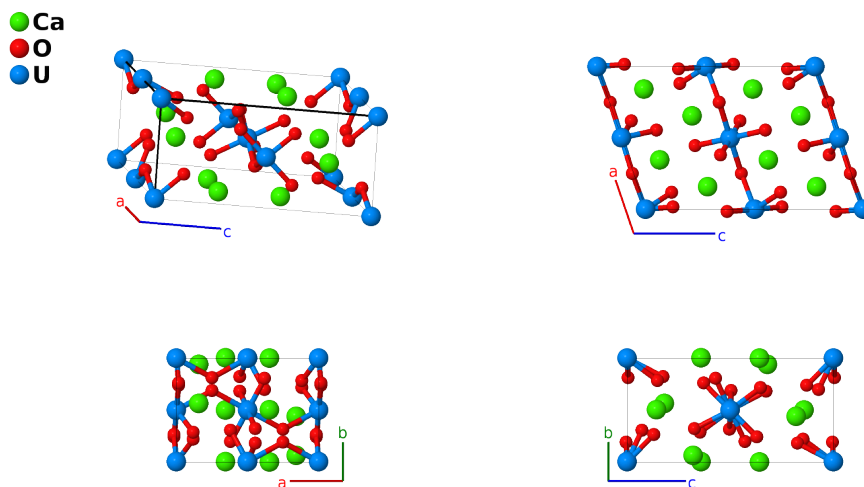
This structure originally had the label `A2B5C_mP32_14_2e_5e_ab`. Calls to that address will be redirected here.

https://aflow.org/p/E7S8

https://aflow.org/p/A2B5C_mP32_14_2e_5e_ab-001

Prototype	Ca_2O_5U
AFLOW prototype label	A2B5C_mP32_14_2e_5e_ab-001
ICSD	23198
Pearson symbol	mP32
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	aflow --proto=A2B5C_mP32_14_2e_5e_ab-001 --params=$a, b/a, c/a, \beta, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9$

Other compounds with this structure

Sr_2UO_5

Simple Monoclinic primitive vectors

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

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

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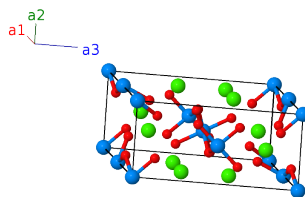
Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	$=$	0	$=$	0	(2a)	U 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)	U I
$\mathbf{B_3}$	$=$	$\frac{1}{2}\,\mathbf{a}_1$	$=$	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(2b)	U II
$\mathbf{B_4}$	$=$	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	$=$	$\frac{1}{2}\left(a + c\cos\beta\right)\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\sin\beta\,\hat{\mathbf{z}}$	(2b)	U II
$\mathbf{B_5}$	$=$	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	$=$	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4e)	Ca I
$\mathbf{B_6}$	$=$	$-x_3\,\mathbf{a}_1 + \left(y_3 + \frac{1}{2}\right)\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_3 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Ca 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)	Ca 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)	Ca I
$\mathbf{B_9}$	$=$	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	$=$	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	Ca II
$\mathbf{B_{10}}$	$=$	$-x_4\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_4 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Ca II
$\mathbf{B_{11}}$	$=$	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	$=$	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(4e)	Ca II
$\mathbf{B_{12}}$	$=$	$x_4\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_4 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	Ca II
$\mathbf{B_{13}}$	$=$	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	$=$	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_{14}}$	$=$	$-x_5\,\mathbf{a}_1 + \left(y_5 + \frac{1}{2}\right)\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-\left(ax_5 + c\left(z_5 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_5 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_5 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O 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 I
$\mathbf{B_{16}}$	$=$	$x_5\,\mathbf{a}_1 - \left(y_5 - \frac{1}{2}\right)\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$\left(ax_5 + c\left(z_5 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_5 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_5 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O I
$\mathbf{B_{17}}$	$=$	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	$=$	$(ax_6 + cz_6\cos\beta)\,\hat{\mathbf{x}} + by_6\,\hat{\mathbf{y}} + cz_6\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{18}}$	$=$	$-x_6\,\mathbf{a}_1 + \left(y_6 + \frac{1}{2}\right)\mathbf{a}_2 - \left(z_6 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-\left(ax_6 + c\left(z_6 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_6 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_6 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O 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 II
$\mathbf{B_{20}}$	$=$	$x_6\,\mathbf{a}_1 - \left(y_6 - \frac{1}{2}\right)\mathbf{a}_2 + \left(z_6 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$\left(ax_6 + c\left(z_6 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_6 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_6 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O II
$\mathbf{B_{21}}$	$=$	$x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	$=$	$(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\sin\beta\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_{22}}$	$=$	$-x_7\,\mathbf{a}_1 + \left(y_7 + \frac{1}{2}\right)\mathbf{a}_2 - \left(z_7 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-\left(ax_7 + c\left(z_7 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_7 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_7 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_{23}}$	$=$	$-x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	$=$	$-(ax_7 + cz_7\cos\beta)\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\sin\beta\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_{24}}$	$=$	$x_7\,\mathbf{a}_1 - \left(y_7 - \frac{1}{2}\right)\mathbf{a}_2 + \left(z_7 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$\left(ax_7 + c\left(z_7 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_7 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_7 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O III
$\mathbf{B_{25}}$	$=$	$x_8\,\mathbf{a}_1 + y_8\,\mathbf{a}_2 + z_8\,\mathbf{a}_3$	$=$	$(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\sin\beta\,\hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B_{26}}$	$=$	$-x_8\,\mathbf{a}_1 + \left(y_8 + \frac{1}{2}\right)\mathbf{a}_2 - \left(z_8 - \frac{1}{2}\right)\mathbf{a}_3$	$=$	$-\left(ax_8 + c\left(z_8 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + b\left(y_8 + \frac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_8 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B_{27}}$	$=$	$-x_8\,\mathbf{a}_1 - y_8\,\mathbf{a}_2 - z_8\,\mathbf{a}_3$	$=$	$-(ax_8 + cz_8\cos\beta)\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\sin\beta\,\hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B_{28}}$	$=$	$x_8\,\mathbf{a}_1 - \left(y_8 - \frac{1}{2}\right)\mathbf{a}_2 + \left(z_8 + \frac{1}{2}\right)\mathbf{a}_3$	$=$	$\left(ax_8 + c\left(z_8 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - b\left(y_8 - \frac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_8 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(4e)	O IV
$\mathbf{B_{29}}$	$=$	$x_9\,\mathbf{a}_1 + y_9\,\mathbf{a}_2 + z_9\,\mathbf{a}_3$	$=$	$(ax_9 + cz_9\cos\beta)\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\sin\beta\,\hat{\mathbf{z}}$	(4e)	O V

$$\mathbf{B_{30}} = \begin{aligned} &-x_9\,\mathbf{a}_1 + \left(y_9 + \tfrac{1}{2}\right)\mathbf{a}_2 - \\ &\left(z_9 - \tfrac{1}{2}\right)\mathbf{a}_3 \end{aligned} = \begin{aligned} &-\left(ax_9 + c\left(z_9 - \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + \\ &b\left(y_9 + \tfrac{1}{2}\right)\hat{\mathbf{y}} - c\left(z_9 - \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \end{aligned} \qquad \text{(4e)} \qquad \text{O V}$$

$$\mathbf{B_{31}} = -x_9\,\mathbf{a}_1 - y_9\,\mathbf{a}_2 - z_9\,\mathbf{a}_3 = -\left(ax_9 + cz_9\cos\beta\right)\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} - cz_9\sin\beta\,\hat{\mathbf{z}} \qquad \text{(4e)} \qquad \text{O V}$$

$$\mathbf{B_{32}} = x_9\,\mathbf{a}_1 - \left(y_9 - \tfrac{1}{2}\right)\mathbf{a}_2 + \left(z_9 + \tfrac{1}{2}\right)\mathbf{a}_3 = \begin{aligned} &\left(ax_9 + c\left(z_9 + \tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - \\ &b\left(y_9 - \tfrac{1}{2}\right)\hat{\mathbf{y}} + c\left(z_9 + \tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \end{aligned} \qquad \text{(4e)} \qquad \text{O V}$$

References

[1] B. O. Loopstra and H. M. Rietveld, *The structure of some alkaline-earth metal uranates*, Acta Crystallogr. Sect. B **25**, 787–791 (1969), doi:10.1107/S0567740869002974.