

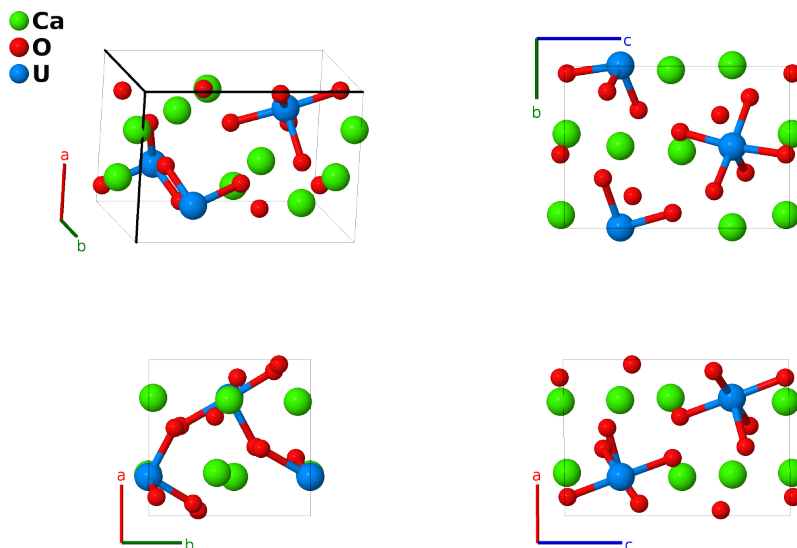
# Ca<sub>3</sub>UO<sub>6</sub> Structure: A3B6C\_mP20\_4\_3a\_6a\_a-001

This structure originally had the label `A3B6C_mP20_4_3a_6a_a`. Calls to that address will be redirected here.

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<https://afLOW.org/p/T9UP>

[https://afLOW.org/p/A3B6C\\_mP20\\_4\\_3a\\_6a\\_a-001](https://afLOW.org/p/A3B6C_mP20_4_3a_6a_a-001)



Prototype	Ca <sub>3</sub> O <sub>6</sub> U
AFLOW prototype label	A3B6C_mP20_4_3a_6a_a-001
ICSD	23200
Pearson symbol	mP20
Space group number	4
Space group symbol	$P2_1$
AFLOW prototype command	<pre>afLOW --proto=A3B6C_mP20_4_3a_6a_a-001 --params=a, b/a, c/a, <math>\beta</math>, x<sub>1</sub>, y<sub>1</sub>, z<sub>1</sub>, x<sub>2</sub>, y<sub>2</sub>, z<sub>2</sub>, x<sub>3</sub>, y<sub>3</sub>, z<sub>3</sub>, x<sub>4</sub>, y<sub>4</sub>, z<sub>4</sub>, x<sub>5</sub>, y<sub>5</sub>, z<sub>5</sub>, x<sub>6</sub>, y<sub>6</sub>, z<sub>6</sub>, x<sub>7</sub>, y<sub>7</sub>, z<sub>7</sub>, x<sub>8</sub>, y<sub>8</sub>, z<sub>8</sub>, x<sub>9</sub>, y<sub>9</sub>, z<sub>9</sub>, x<sub>10</sub>, y<sub>10</sub>, z<sub>10</sub></pre>

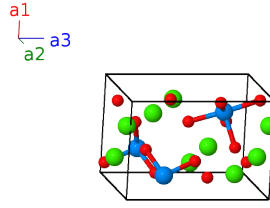
## Other compounds with this structure

Sr<sub>3</sub>UO<sub>6</sub>

- Space group  $P2_1$  #4 allows the  $y$  coordinates to have an arbitrary origin. Here this freedom is used to set  $y_{10} = 0$  for the Uranium position.

## Simple Monoclinic primitive vectors

$$\begin{aligned}
\mathbf{a}_1 &= a \hat{\mathbf{x}} \\
\mathbf{a}_2 &= b \hat{\mathbf{y}} \\
\mathbf{a}_3 &= c \cos \beta \hat{\mathbf{x}} + c \sin \beta \hat{\mathbf{z}}
\end{aligned}$$



## Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(2a)	Ca I
$\mathbf{B}_2$	$-x_1 \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(2a)	Ca I
$\mathbf{B}_3$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(2a)	Ca II
$\mathbf{B}_4$	$-x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(2a)	Ca II
$\mathbf{B}_5$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(2a)	Ca III
$\mathbf{B}_6$	$-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(2a)	Ca III
$\mathbf{B}_7$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_8$	$-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(2a)	O I
$\mathbf{B}_9$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B}_{10}$	$-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(2a)	O II
$\mathbf{B}_{11}$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(2a)	O III
$\mathbf{B}_{12}$	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	=	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(2a)	O III
$\mathbf{B}_{13}$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	=	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(2a)	O IV
$\mathbf{B}_{14}$	$-x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	=	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(2a)	O IV
$\mathbf{B}_{15}$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	=	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(2a)	O V
$\mathbf{B}_{16}$	$-x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3$	=	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(2a)	O V
$\mathbf{B}_{17}$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	=	$(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \sin \beta \hat{\mathbf{z}}$	(2a)	O VI
$\mathbf{B}_{18}$	$-x_9 \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 - z_9 \mathbf{a}_3$	=	$-(ax_9 + cz_9 \cos \beta) \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - cz_9 \sin \beta \hat{\mathbf{z}}$	(2a)	O VI
$\mathbf{B}_{19}$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	=	$(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \sin \beta \hat{\mathbf{z}}$	(2a)	U I
$\mathbf{B}_{20}$	$-x_{10} \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 - z_{10} \mathbf{a}_3$	=	$-(ax_{10} + cz_{10} \cos \beta) \hat{\mathbf{x}} + b(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} - cz_{10} \sin \beta \hat{\mathbf{z}}$	(2a)	U I

## 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.