

S₃U₄ Structure:

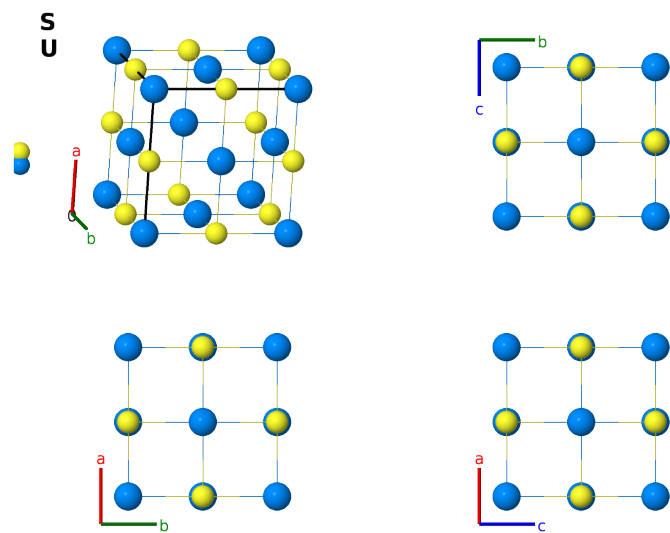
A3B4_cP7_221_d_ac-001

Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- D. Hicks, M. J. Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi: 10.1016/j.commatsci.2021.110450.

<https://aflow.org/prototype-encyclopedia/62DR>

https://aflow.org/prototype-encyclopedia/A3B4_cP7_221_d_ac-001



Prototype	S ₃ U ₄
AFLOW prototype label	A3B4_cP7_221_d_ac-001
ICSD	38354
CCDC	1609002
Pearson symbol	cP7
Space group number	221
Space group symbol	$Pm\bar{3}m$
AFLOW prototype command	<code>aflow --proto=A3B4_cP7_221_d_ac-001 --params=a</code>

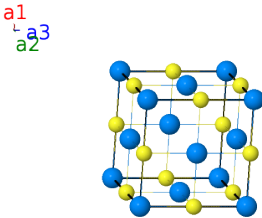
Other compounds with this structure

NbC

- This is the rock salt (*B1*) structure with the central atom removed in each cube.
- The ICSD entry for this structure uses $a = 5.505\text{\AA}$, but (Zumbush, 1940) states that the correct value is $5.49\text{\AA}$. As this is consistent with the S-S and S-U distances given in the paper we use this value.

Simple Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= a \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$=$	0	$=$	0	$(1a)$ U I
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_2 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{y}} + \frac{1}{2} a \hat{\mathbf{z}}$	$(3c)$ U II
$\mathbf{B}_3$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{z}}$	$(3c)$ U II
$\mathbf{B}_4$	$=$	$\frac{1}{2} \mathbf{a}_1 + \frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{1}{2} a \hat{\mathbf{y}}$	$(3c)$ U II
$\mathbf{B}_5$	$=$	$\frac{1}{2} \mathbf{a}_1$	$=$	$\frac{1}{2} a \hat{\mathbf{x}}$	$(3d)$ S I
$\mathbf{B}_6$	$=$	$\frac{1}{2} \mathbf{a}_2$	$=$	$\frac{1}{2} a \hat{\mathbf{y}}$	$(3d)$ S I
$\mathbf{B}_7$	$=$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{z}}$	$(3d)$ S I

References

[1] M. Zumbusch, *Über die Strukturen des Uransubsulfids und der Subphosphide des Iridiums und Rhodiums*, Z. Anorganische und Allgemeine Chemie **243**, 322–329 (1940), doi:10.1002/zaac.19402430403.

Found in

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

First cited in

H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.