S_3U_4 Structure: A3B4_cP7_221_d_ac-001

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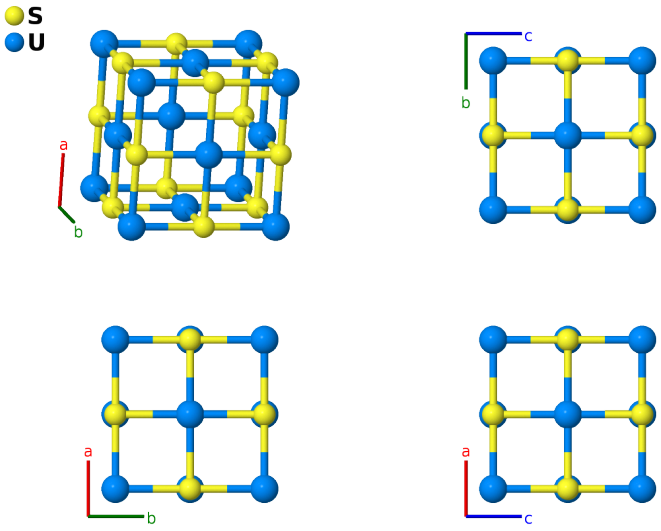
https://aflow.org/p/62DR

https://aflow.org/p/A3B4_cP7_221_d_ac-001



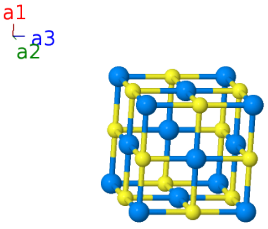
Prototype	S_3U_4
AFLOW prototype label	A3B4_cP7_221_d_ac-001
ICSD	38354
Pearson symbol	cP7
Space group number	221
Space group symbol	$Pm\bar{3}m$
AFLOW prototype command	`aflow --proto=A3B4_cP7_221_d_ac-001 --params=`a

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 = 5.505Å, but (Zumbush, 1940) states that the correct value is 5.49Å. As this is consistent with the S-S and S-U distances given in the paper we use this value.

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



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).