High-Temperature UP_2 Structure: A2B_tP6_129_ac_c-002

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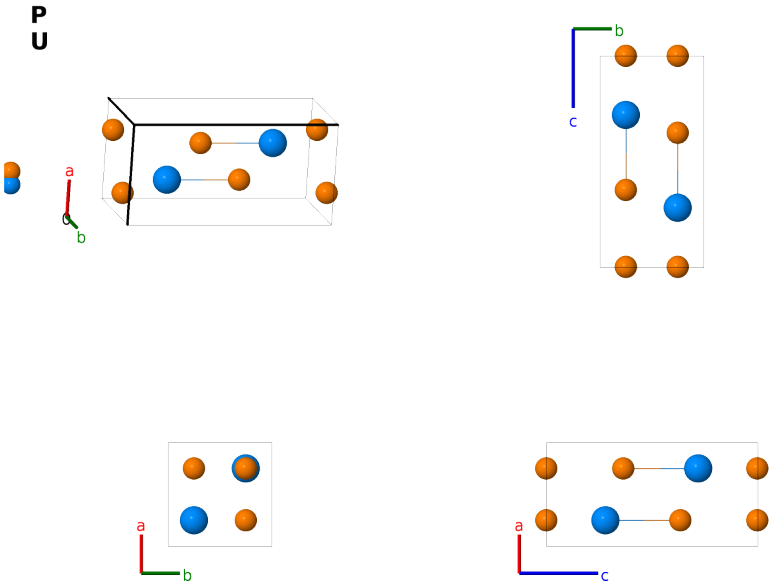
https://aflow.org/prototype-encyclopedia/1R27

https://aflow.org/prototype-encyclopedia/A2B_tP6_129_ac_c-002



Prototype	P_2U
AFLOW prototype label	A2B_tP6_129_ac_c-002
ICSD	648244
CCDC	2138750
Pearson symbol	tP6
Space group number	129
Space group symbol	$P4/nmm$
AFLOW prototype command	`aflow --proto=A2B_tP6_129_ac_c-002 --params=`$a, c/a, z_2, z_3$

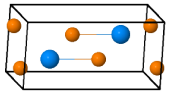
Other compounds with this structure

AmS_2, $AmSe_2$, $AmTe_2$, CeS_2, $CeSe_2$, $CeTe_2$, CmS_2, $CmSe_2$, $CmTe_2$, DyS_2, $DySe_2$, $DyTe_2$, ErS_2, $ErSe_2$, $ErTe_2$, GdS_2, $GdSe_2$, $GdTe_2$, $HfSb_2$, HoS_2, $HoSe_2$, $HoTe_2$, LaS_2, $LaSe_2$, $LaTe_2$, LuS_2, $LuSe_2$, $LuTe_2$, $NdSe_2$, $NdTe_2$, $NpAs_2$, $NpTe_2$, $PaAs_2$, PaP_2, $PaSb_2$, $PrSe_2$, $PrTe_2$, PuS_2, $PuSe_2$, $PuTe_2$, $SmSe_2$, $SmTe_2$, TbS_2, $TbTe_2$, $ThAs_2$, $ThBi_2$, $ThSb_2$, TmS_2, $TmSe_2$, $TmTe_2$, UAs_2, UBi_2, UP_2, USb_2, UTe_2, YbS_2, $YbSe_2$, $YbTe_2$, YS_2, YSe_2, YTe_2

- At temperatures below 83°C UP_2 transforms into its low-temperature structure (Gerward, 1990).
- The atomic positions are not explicitly given in (Gerward, 1990), so we take them from the ICSD entry.
- Cu_2Sb ($C38$), UP_2, and $LaSe_{1.85}$ have similar AFLOW prototype labels, A2B_tP6_129_ac_c for the first two and AB2_tP6_129_c_ac for the third. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- We consider all of these to be binary forms of Matlockite ($E0_1$)/PrOI.
- We somewhat arbitrarily assign
  - Structures with c/a < 2 to the Cu_2Sb prototype,
  - Structures with $2 <$ c/a < 3 to the UP_2 prototype, and
  - Structures with c/a ≈ 4 to the $LaSe_{1.85}$ prototype.
- The ICSD distinction between Cu_2Sb and UP_2 is not the same as ours, and they often assign binary compounds to the ternary prototypes.

Simple Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(2a)	P I
$\mathbf{B_2}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}}$	(2a)	P I
$\mathbf{B_3}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2c)	P II
$\mathbf{B_4}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2c)	P II
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2c)	U I
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2c)	U I

References

[1] L. Gerward, J. S. Olsen, U. Benedict, S. Dabos-Seignon, and H. Luo, *Crystal structures of UP_2, UAs_2, UAsS and UAsSe in the pressure range up to 60 GPa*, High T - High P **22**, 523–532 (1990).

Found in

[1] *Inorganic Crystal Structure Database*. Entry 648244 (UP_2).

First cited in

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