Lucabindiite (KAs_4O_6Cl) Structure: A4BCD6_hP12_191_h_a_b_i-001

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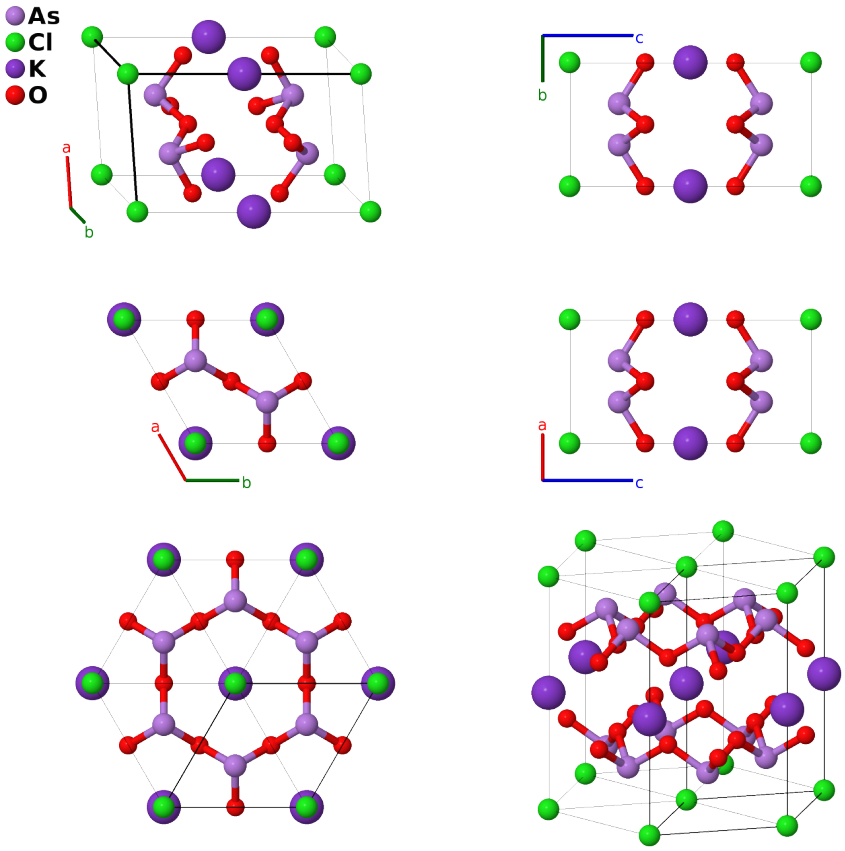
https://aflow.org/p/4NVE

https://aflow.org/p/A4BCD6_hP12_191_h_a_b_i-001



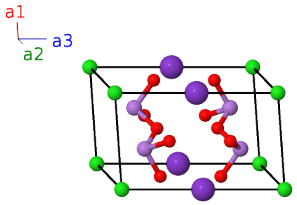
Prototype	As_4ClKO_6
AFLOW prototype label	A4BCD6_hP12_191_h_a_b_i-001
Mineral name	lucabindiite
ICSD	65205
Pearson symbol	hP12
Space group number	191
Space group symbol	$P6/mmm$
AFLOW prototype command	`aflow --proto=A4BCD6_hP12_191_h_a_b_i-001 --params=`$a, c/a, z_3, z_4$

Other compounds with this structure
KAs_4O_6Br, KAs_4O_6I, $NH_4As_4O_6Br$, $NH_4As_4O_6I$

- (Pertlik, 1988) puts this in the non-centrosymmetric space group $P622$ #177. The only Wyckoff position in this space group which is not centrosymmetric is the general point, (12n). All the other Wyckoff positions have counterparts in the centrosymmetric space group $P6/mmm$ #191, as shown here.

Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\ \mathbf{a_3} &= c\,\hat{\mathbf{z}}\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Cl I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	K I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4h)	As I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4h)	As I
$\mathbf{B_5}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4h)	As I
$\mathbf{B_6}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(4h)	As I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 + z_4\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(6i)	O I
$\mathbf{B_8}$	=	$\frac{1}{2}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(6i)	O I
$\mathbf{B_9}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + cz_4\,\hat{\mathbf{z}}$	(6i)	O I
$\mathbf{B_{10}}$	=	$\frac{1}{2}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(6i)	O I
$\mathbf{B_{11}}$	=	$\frac{1}{2}\,\mathbf{a}_1 - z_4\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{4}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(6i)	O I
$\mathbf{B_{12}}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - cz_4\,\hat{\mathbf{z}}$	(6i)	O I

References

[1] F. Pertlik, *The compounds KAs_4O_6X (X=Cl, Br, I) and $NH_4As_4O_6X$ (X=Br, I): Hydrothermal syntheses and structure determinations*, Monat. Chemie **119**, 451–456 (1988), doi:10.1007/BF00810425.

Found in

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