Cinnabar (HgS, $B9$) Structure: AB_hP6_154_a_b-001

This structure previously used the label(s) `AB_hP6_154_a_b`. Calls to these addresses will be redirected here.

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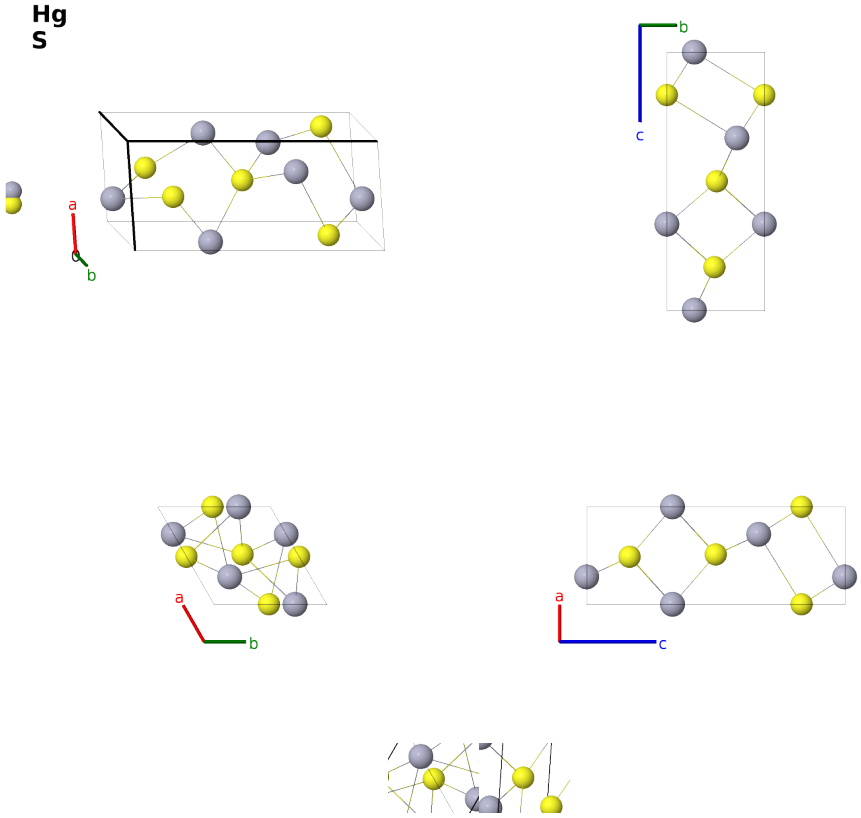
https://aflow.org/prototype-encyclopedia/A3TK

https://aflow.org/prototype-encyclopedia/AB_hP6_154_a_b-001



Prototype	HgS
AFLOW prototype label	AB_hP6_154_a_b-001
***Strukturbericht* designation**	$B9$
Mineral name	cinnabar
ICSD	70054
CCDC	1631878
Pearson symbol	hP6
Space group number	154

Space group symbol $P3_221$

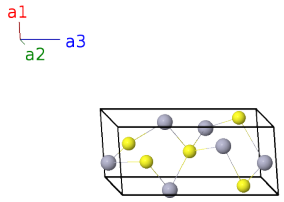
AFLOW prototype command `aflow --proto=AB_hP6_154_a_b-001 --params=`$a, c/a, x_1, x_2$

Other compounds with this structure
HgO

- As space group $P3_121$ #152 is enantiomorphic to $P3_221$ #154, it should be possible to find HgS in that space group as well.

Trigonal (Hexagonal) primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_1\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \frac{2}{3}c\,\hat{\mathbf{z}}$	(3a)	Hg I
$\mathbf{B_2}$	=	$x_1\,\mathbf{a}_2 + \frac{1}{3}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_1\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_1\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$	(3a)	Hg I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2$	=	$-ax_1\,\hat{\mathbf{x}}$	(3a)	Hg I
$\mathbf{B_4}$	=	$x_2\,\mathbf{a}_1 + \frac{1}{6}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_2\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{1}{6}c\,\hat{\mathbf{z}}$	(3b)	S I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_2 + \frac{5}{6}\,\mathbf{a}_3$	=	$\frac{1}{2}ax_2\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{5}{6}c\,\hat{\mathbf{z}}$	(3b)	S I
$\mathbf{B_6}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(3b)	S I

References

[1] P. Auvray and F. Genet, *Affinement de la structure cristalline du cinabre α-HgS*, Bull. Soc. fr. Minéral. Crystallogr. **96**, 218–219 (1973).

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

M. J. Mehl, D. Hicks, C. Toher, O. Levy, R. M. Hanson, G. L. W. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 1*, Comput. Mater. Sci. **136**, S1-828 (2017). doi: 10.1016/j.commatsci.2017.01.017