KSH ($B22$) Structure: AB_hR2_166_a_b-003

This structure originally had the label `AB_hR2_166_a_b.KSH`. Calls to that address will be redirected here.

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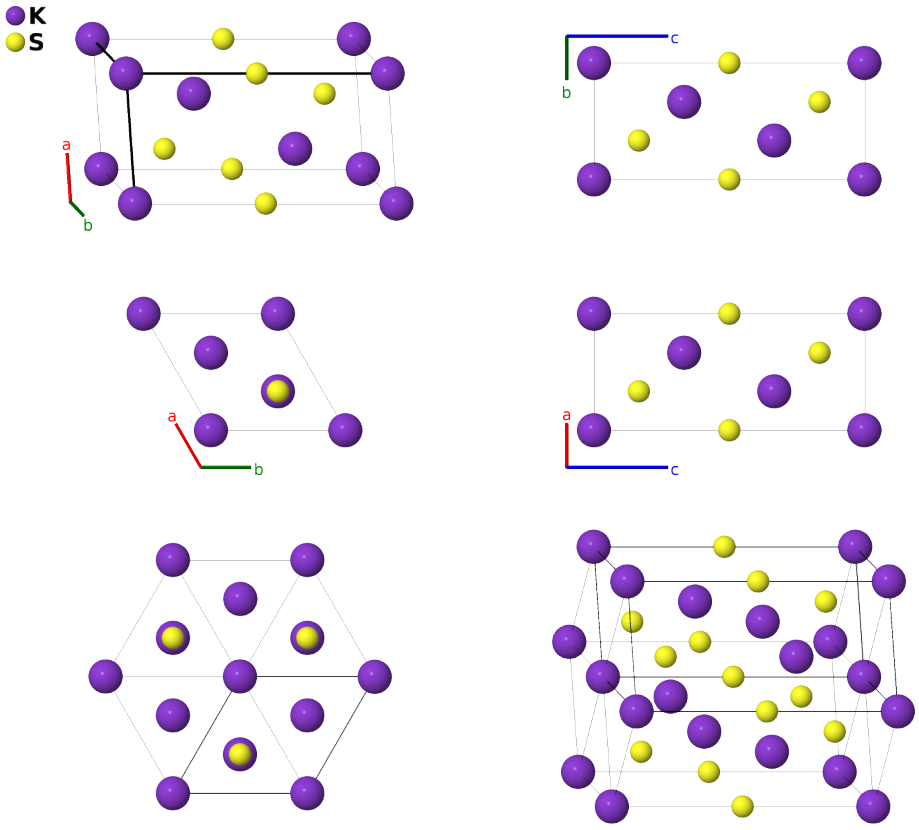
https://aflow.org/p/HA1H

https://aflow.org/p/AB_hR2_166_a_b-003



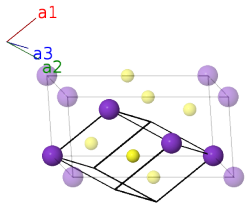
Prototype	HKS
AFLOW prototype label	AB_hR2_166_a_b-003
***Strukturbericht* designation**	$B22$
ICSD	27820
Pearson symbol	hR2
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=AB_hR2_166_a_b-003 --params=`$a, c/a$

Other compounds with this structure
NaSH, RbSH, CsSH, LiPb (LT)

- This is the room-temperature structure of KSH. The S and H atoms form an SH^- ion, and so are listed together at the (1b) Wyckoff postition, leading to the listing of this compound in the *B Strukturbericht* category.
- Our original presentation of this structure (Hicks, 2021) inadvertantly used a "face-centered" version of this structure. Here we use original orientation used by (West, 1934).
- CuPt ($L1_1$) and KSH have the same AFLOW prototype label, AB_hR2_166_a_b. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

Rhombohedral primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	K I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	S I

References

[1] C. D. West, *The Crystal Structures of Some Alkali Hydrosulfides and Monosulfides*, Z. Krystallogr. **88**, 97–115 (1934), doi:10.1524/zkri.1934.88.1.97.

[2] 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.

Found in

[1] C. Gottfried and F. Schossberger, eds., *Strukturbericht Band III 1933-1935* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).