Caswellsilverite ($CrNaS_2$, $F5_1$) Structure: ABC2_hR4_166_a_b_c-001

This structure previously used the label(s) `ABC2_hR4_166_a_b_c`. Calls to these addresses will be redirected here.

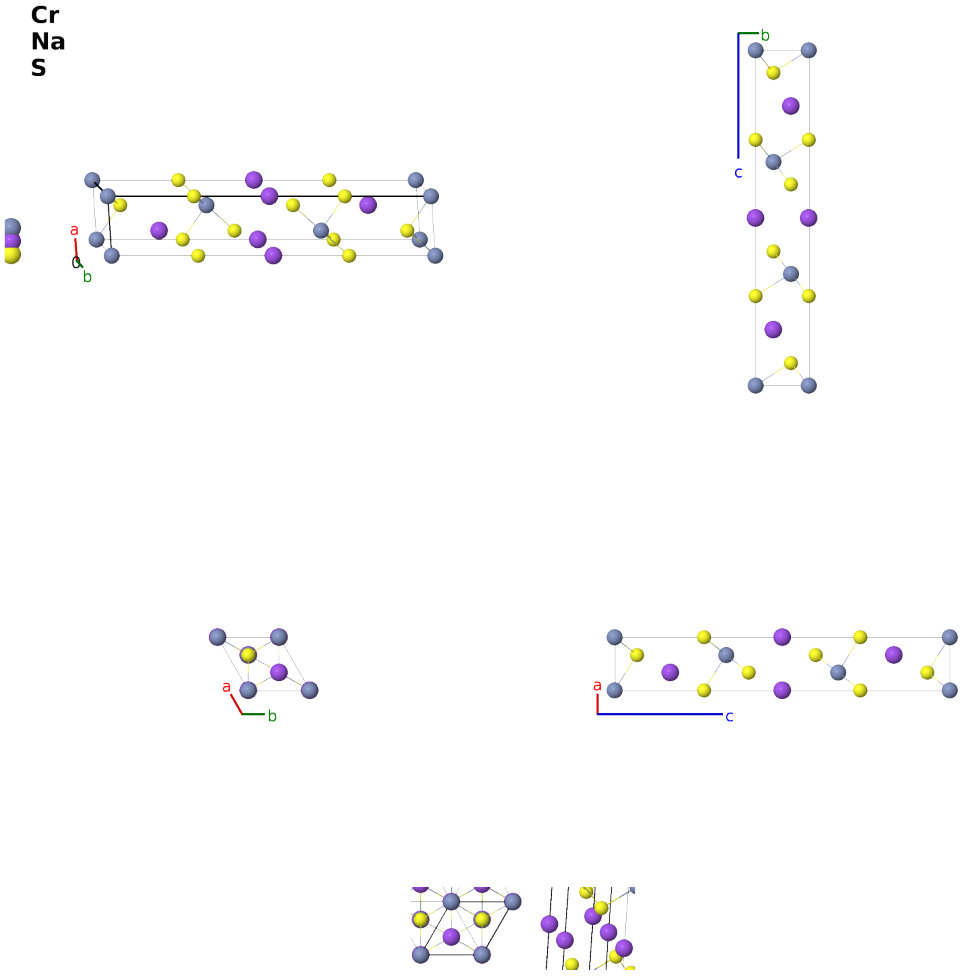
Cite this page as:

- H. Eckert, S. Divilov, M. J. Mehl, D. Hicks, A. C. Zettel, M. Esters, X. Campilongo, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*, Comput. Mater. Sci. **240**, 112988 (2024), doi: 10.1016/j.commatsci.2024.112988.
- 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.

---

https://aflow.org/prototype-encyclopedia/J6ND

https://aflow.org/prototype-encyclopedia/ABC2_hR4_166_a_b_c-001



Prototype	$CrNaS_2$
AFLOW prototype label	ABC2_hR4_166_a_b_c-001
***Strukturbericht* designation**	$F5_1$
Mineral name	caswellsilverite
ICSD	42389
CCDC	1612056

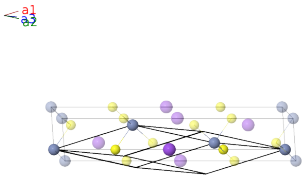
Pearson symbol	hR4
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=ABC2_hR4_166_a_b_c-001 --params=`$a, c/a, x_3$

Other compounds with this structure
$AgBiSe_2$, $AgBiTe_2$, $AlCV_2$, $BiTlSe_2$, $BiTlTe_2$, $CrNaSe_2$, $CrRbS_2$, $CrRbSe_2$, $CsICl_2$, $FeNiO_2$, $HNaF_2$, $HoTlS_2$, $InNaS_2$, $InNaSe_2$, $NaHF_2$, $SbTlTe_2$, $TlYTe_2$, TlS (HP), TlSe (HP)

- The name caswellsilverite was not used until natural samples of the mineral were found. (Okada, 1982).
- α-$NaFeO_2$, rhombohedral delafossite, $CuFeO_2$, caswellsilverite ($F5_1$), $LiNiO_2$ and $Li_2Mn_3O_7$ have the same prototype label, ABC2_hR4_166_a_b_c.
- The difference in the internal parameter z_3 between $CuFeO_2$ and $CrNaS_2$ causes a large change in the bonding of the two crystals, so we present them as different structures.
- The structures 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)	Cr 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)	Na I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	S I
$\mathbf{B_4}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	S I

References

[1] F. Engelsman, G. Wiegers, F. Jellinek, and B. V. Laar, *Crystal structures and magnetic structures of some metal(I) chromium(III) sulfides and selenides*, J. Solid State Chem. **6**, 574–582 (1973), doi:10.1016/S0022-4596(73)80018-0.

[2] A. Okada and K. Keil, *Caswellsilverite, $NaCrS_2$: a new mineral in the Norton County enstatite achondrite*, Am. Mineral. **67**, 132–136 (1982).

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