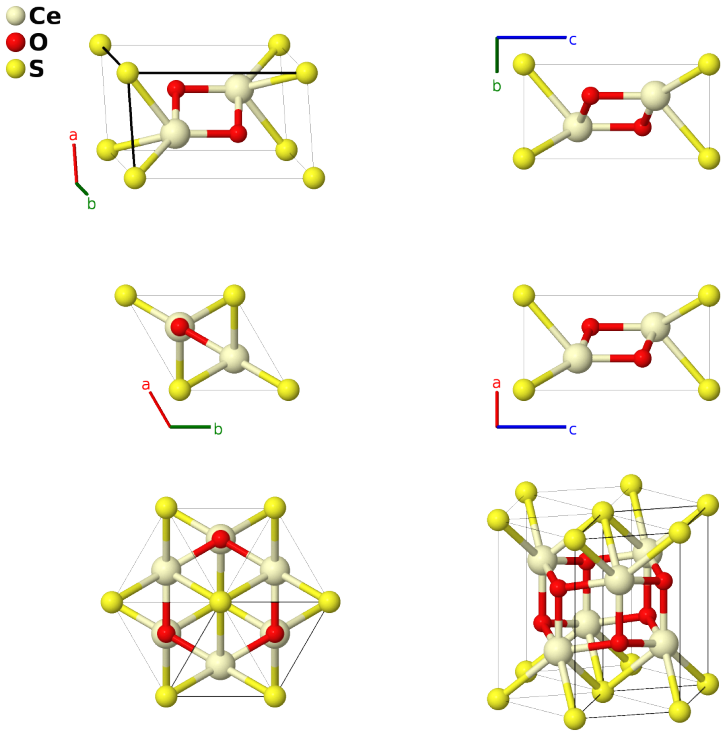
Ce_2O_2S Structure: A2B2C_hP5_164_d_d_a-002

This structure originally had the label `A2B2C_hP5_164_d_d_a`. Calls to that address will be redirected here.

Cite this page as: 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/p/FG79

https://aflow.org/p/A2B2C_hP5_164_d_d_a-002



Prototype	Ce_2O_2S
AFLOW prototype label	A2B2C_hP5_164_d_d_a-002
ICSD	31639
Pearson symbol	hP5
Space group number	164
Space group symbol	$P\bar{3}m1$
AFLOW prototype command	`aflow --proto=A2B2C_hP5_164_d_d_a-002 --params=`$a, c/a, z_2, z_3$

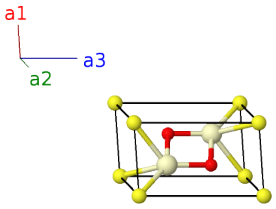
Other compounds with this structure

$BaCd_2As_2$, $CaAl_2Si_2$, $CaAs_2Bi_2$, $CaAs_2Mn_2$, $CaAs_2P_2$, $CaAs_2Sb_2$, $CaBi_2Mg_2$, $CaBi_2Mn_2$, $CaCd_2As_2$, $CaCd_2P_2$, $CaMg_2Bi_2$, $CaMg_2Sb_2$, $CaZn_2As_2$, $CaZn_2P_2$, $CaZn_2Sb_2$, $CeCuZnP_2$, $DyCuZnP_2$, $ErCuZnP_2$, $EuAs_2Cd_2$, $EuBi_2Mg_2$, $EuCd_2P_2$, $GdCuZnP_2$, $HoCuZnP_2$, $LaCuZnP_2$, $LuCuZnP_2$, $NdCuZnP_2$, $PrCuZnP_2$, SCe_2O_2, SCe_2Se_2, SLa_2O_2, SO_2Pu_2, $ScCuZnP_2$, $SmCuZnP_2$, $SrAs_2Mn_2$, $SrAs_2P_2$, $SrAs_2Sb_2$, $SrCd_2As_2$, $SrCd_2P_2$, $TbCuZnP_2$, $TmCuZnP_2$, $YCuZnP_2$, $YbCuZnP_2$, $YbMg_2Bi_2$, $YbMnCuP_2$

- This is the ternary form of the $D5_2$ La_2O_3 and the $D5_{13}$ Al_3Ni_2 structures. We have separated it from the parents because of the large number of compounds involved.
- Authors after (Zachariasen, 1949) often use $CaAl_2Si_2$ as the prototype for this structure.

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
$\mathbf{B_1}$	=	0	=	0	(1a)	S I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(2d)	Ce I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(2d)	Ce I
$\mathbf{B_4}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2d)	O I
$\mathbf{B_5}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2d)	O I

References

[1] W. H. Zachariasen, *Crystal chemical studies of the 5f-series of elements. VII. The crystal structure of Ce_2O_2S, La_2O_2S and Pu_2O_2S*, Acta Cryst. **2**, 60–62 (1949), doi:10.1107/S0365110X49000138.