La_2O_3 ($D5_2$) Structure: A2B3_hP5_164_d_ad-001

This structure originally had the label `A2B3_hP5_164_d_ad`. Calls to that address will be redirected here.

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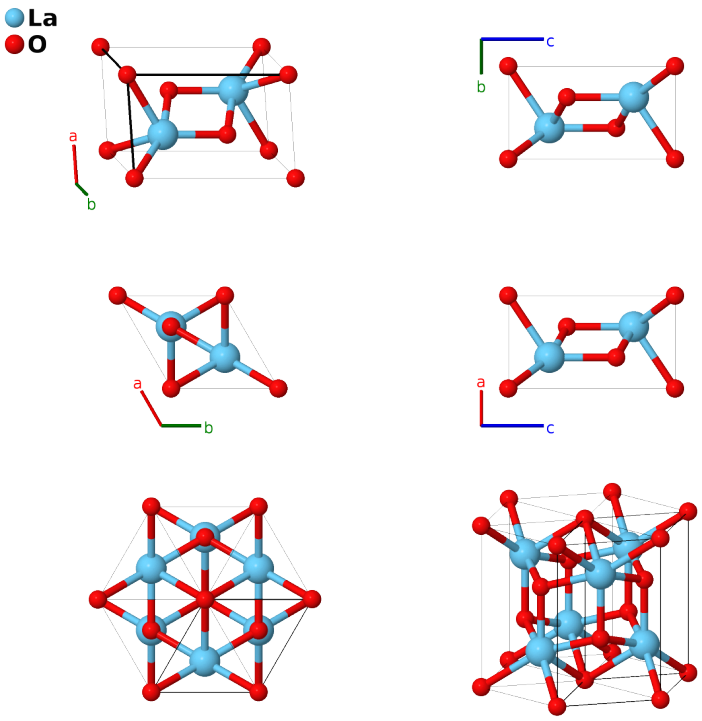
https://aflow.org/p/D3QE

https://aflow.org/p/A2B3_hP5_164_d_ad-001



Prototype	La_2O_3
AFLOW prototype label	A2B3_hP5_164_d_ad-001
***Strukturbericht* designation**	$D5_2$
ICSD	100204
Pearson symbol	hP5
Space group number	164
Space group symbol	$P\bar{3}m1$
AFLOW prototype command	`aflow --proto=A2B3_hP5_164_d_ad-001 --params=`$a, c/a, z_2, z_3$

Other compounds with this structure

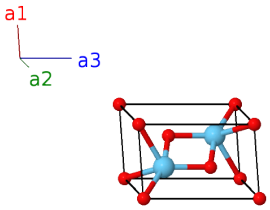
α-Bi_2Mg_3, α-Sb_2Mg_3, Ac_2O_3, As_2Mg_3, Ce_2O_3, Gd_2O_3, Nd_2O_3, Pr_2O_3, Pu_2O_3, Th_2N_3, Th_2N_2O, U_2N_3

- This structure has proved rather controversial:

- (Zachariasen 1926, 1929) originally proposed that the crystal structure of La_2O_3 and other lanthanide series oxides belong to trigonal space group $P\bar{3}21$ #150.
- This was immediately criticized by (Pauling, 1929), who suggested the trigonal space group ($P\bar{3}m1$ #164) later confirmed by (Koehler, 1953).
- Much later, (Aldebert, 1979) stated that the structure was hexagonal, space group $P6_3/mmc$ #194. This would represent a doubling of the $P\bar{3}m1$ unit cell in the z-direction, however they give structural parameters, also used by us and by (Villars, 1991, 2016), which have a density consistent with the $P\bar{3}m1$ structure, and are in reasonable agreement with lattice parameters given in (Pearson, 1958) and (Koehler, 1953). We agree with (Villars, 1991, 2016) that these are close to the correct values for the structure.
- This structure is very similar to Al_3Ni_2 ($D5_{13}$, A3B2_hP5_164_ad_d). We follow (Pearson, 1958) and assign the intermetallics as $D5_{13}$, keeping $D5_2$ for oxides and related compounds.
- The ternary Ce_2O_2S structure, *aka* $CaAl_2Si_2$, is related to this structure, the sulfur atom replacing the oxygen on the (1a) site.

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)	O 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)	La 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)	La 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 II
$\mathbf{B_5}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2d)	O II

References

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Found in

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