Cubic Perovskite ($CaTiO_3$, $E2_1$) Structure: AB3C_cP5_221_a_c_b-001

This structure previously used the label(s) `AB3C_cP5_221_a_c_b`. Calls to these addresses will be redirected here.

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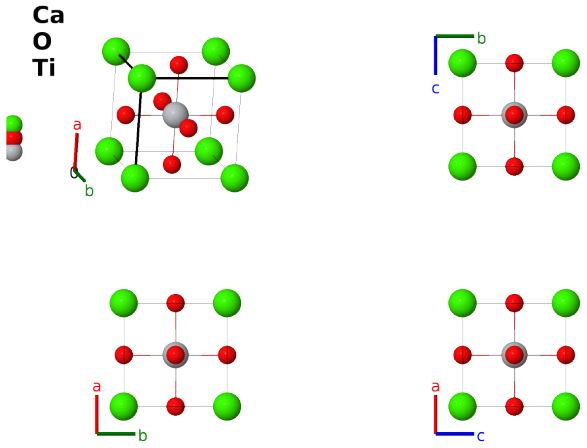
https://aflow.org/prototype-encyclopedia/QUKL

https://aflow.org/prototype-encyclopedia/AB3C_cP5_221_a_c_b-001



Prototype	$CaTiO_3$
AFLOW prototype label	AB3C_cP5_221_a_c_b-001
***Strukturbericht* designation**	$E2_1$
Mineral name	perovskite
ICSD	31865
CCDC	1605807
Pearson symbol	cP5
Space group number	221
Space group symbol	$Pm\bar{3}m$
AFLOW prototype command	`aflow --proto=AB3C_cP5_221_a_c_b-001 --params=`a

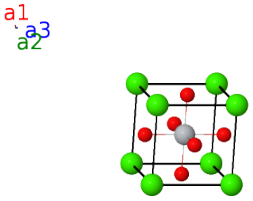
Other compounds with this structure

$AlCFe_3$, $AlCMn_3$, $AlCTi_3$, $AlNMn_3$, $AuOCs_3$, $BaCeO_3$, $BaCrO_3$, $BaLiH_3$, $BaPuO_3$, $BaSnO_3$, $BaTiO_3$, $BaZrO_3$, $BaZrS_3$, $BiFeO_3$, $CeCRu_3$, $CeCrO_3$, $CuNMn_3$, $EuTiO_3$, $GaCMn_3$, $GaNMn_3$, $GeCMn_3$, $InCTi_3$, $InNTi_3$, $KCoF_3$, $KFeF_3$, $KMgF_3$, $KMnF_3$, $KNiO_3$, $KTaO_3$, $KZnO_3$, $LaAlO_3$, $LaCoO_3$, $LaGaO_3$, $MgCNi_3$, $MgNaF_3$, $NiNFe_3$, $NiNMn_3$, $PbTiO_3$, $PbZrO_3$, $PdNFe_3$, $PrCoO_3$, $PtNFe_3$, $RbFeF_3$, $SmCoO_3$, $SmCrO_3$, $SnCFe_3$, $SnNFe_3$, $SrLiH_3$, $SrRuO_3$, $SrTiO_3$, $SrTlO_3$, $TlCTi_3$, $TlNTi_3$, $YAlO_3$, $ZnCMn_3$, Ba_3N_2, Ba_3P_2, Ba_3Sb_2

- Cubic perovskite is actually the high-temperature phase of the compounds listed here. The ground states of these compounds are distored perovskite structures. Many of these substances are ferroelectric.
- By removing one atom type we get various structures, all with space group $Pm\bar{3}m$ #221:
  - Removing the calcium atoms leads to the α-ReO_3 ($D0_9$) structure;
  - removing the titanium atoms leads to the Cu_3Au ($L1_2$) structure;
  - removing the oxygen atoms leads to the CsCl ($B2$) structure;
  - removing the calcium or titanium and the oxygen atoms leads to the simple cubic (A_h) structure.
- (Ewald, 1931) originally gave this compound the *Strukturbericht* Designation $G4$, but this was changed by (Gottfried, 1937) to $E2_1$.

Simple Cubic primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = a\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Ca I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(1b)	Ti I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(3c)	O I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{z}}$	(3c)	O I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}a\,\hat{\mathbf{y}}$	(3c)	O I

References

[1] T. Barth, *Die Kristallstruktur von Perowskit und verwandter Verbindungen*, Norsk. Geol. Tidssk. **8**, 201–216 (1925).

[2] P. P. Ewald and C. Hermann, eds., *Strukturbericht 1913-1928* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1931).

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

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