$CaTiO_3$ *Pnma* Perovskite Structure: AB3C_oP20_62_c_cd_a-001

This structure previously used the label(s) `AB3C_oP20_62_c_cd_a`. Calls to these addresses will be redirected here.

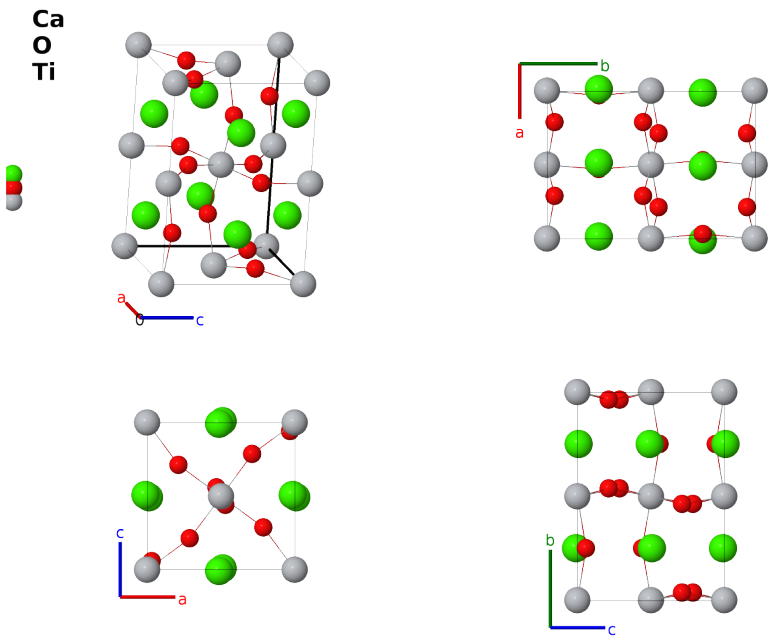
Cite this page as:

- 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/2KF1

https://aflow.org/prototype-encyclopedia/AB3C_oP20_62_c_cd_a-001



Prototype	CaO_3Ti
AFLOW prototype label	AB3C_oP20_62_c_cd_a-001
ICSD	94568
CCDC	1653994
Pearson symbol	oP20
Space group number	62
Space group symbol	*Pnma*
AFLOW prototype command	`aflow --proto=AB3C_oP20_62_c_cd_a-001 --params=`$a, b/a, c/a, x_2, z_2, x_3, z_3, x_4, y_4, z_4$

Other compounds with this structure

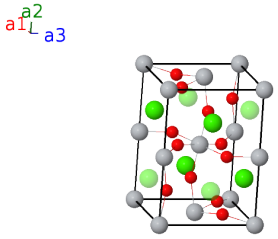
$AgKF_3$, $AlDyO_3$, $AlGdO_3$, $AlHoO_3$, $AlScO_3$, $AlSmO_3$, $AlTbO_3$, $AlTmO_3$, $AsNBa_3$, $AsNCa_3$, $BaCeO_3$, $BaHfS_3$, $BaPrO_3$, $BaPuO_3$, $BaTbO_3$, $BaThO_3$, $BaUS_3$, $BaUSe_3$, $BaZrS_3$, $BiCoO_3$, $BiCrO_3$, $BiFeO_3$, $BiInO_3$, $BiMnO_3$, $BiRhO_3$, $BiSrO_3$, $CaCoO_3$,

$CaCrO_3$, $CaFeO_3$, $CaGeO_3$, $CaHfS_3$, $CaIrO_3$, $CaKF_3$, $CaMnO_3$, $CaMoO_3$, $CaNbO_3$, $CaOsO_3$, $CaPbO_3$, $CaRbCl_3$, $CaRbF_3$, $CaRhO_3$, $CaRuO_3$, $CaSnO_3$, $CaTcO_3$, $CaTiO_3$, $CaVO_3$, $CaZrO_3$, $CaZrS_3$, $CdGeO_3$, $CdKF_3$, $CdSnO_3$, $CdTcO_3$, $CdTiO_3$, $CdVO_3$, $CeCrO_3$, $CeGaO_3$, $CeScO_3$, $CeScS_3$, $CeSrO_3$, $CeVO_3$, $CoDyO_3$, $CoErO_3$, $CoEuO_3$, $CoHoO_3$, $CoInO_3$, $CoNaF_3$, $CoNdO_3$, $CoPrO_3$, $CoScO_3$, $CoSmO_3$, $CoTbO_3$, $CoTmO_3$, $CoYO_3$, $CoYbO_3$, $CrDyO_3$, $CrErO_3$, $CrEuO_3$, $CrGdO_3$, $CrHoO_3$, $CrInO_3$, $CrNdO_3$, $CrPrO_3$, $CrScO_3$, $CrTbO_3$, $CrThS_3$, $CrThSe_3$, $CrTlO_3$, $CrTmO_3$, $CrUS_3$, $CrUSe_3$, $CsDyI_3$, $CsEuBr_3$, $CsPbCl_3$, $CsPbI_3$, $CsPrBr_3$, $CsSnI_3$, $CsYbI_3$, $CuNdO_3$, $CuPrO_3$, $DyCrO_3$, $DyCsI_3$, $DyFeO_3$, $DyGaO_3$, $DyMnO_3$, $DyNiO_3$, $DyScO_3$, $DyVO_3$, $ErFeO_3$, $ErLaO_3$, $ErMnO_3$, $ErNiO_3$, $ErVO_3$, $EuFeO_3$, $EuHfS_3$, $EuInO_3$, $EuMnO_3$, $EuNiO_3$, $EuRhO_3$, $EuRuO_3$, $EuScO_3$, $EuTiO_3$, $EuZrO_3$, $EuZrS_3$, $FeGdO_3$, $FeHoO_3$, $FeLaO_3$, $FeLuO_3$, $FeNaF_3$, $FeNdO_3$, $FePrO_3$, $FeTbO_3$, $FeTlO_3$, $FeTmO_3$, $FeYO_3$, $FeYbO_3$, $GaGdO_3$, $GaHoO_3$, $GaLaO_3$, $GaNdO_3$, $GaPrO_3$, $GdAlO_3$, $GdCrO_3$, $GdFeO_3$, $GdMnO_3$, $GdNiO_3$, $GdScO_3$, $GdScS_3$, $GdTiO_3$, $GdVO_3$, $GeOBa_3$, H_3MgNa, $HfSrO_3$, $HfSrS_3$, $HgKF_3$, $HoCrO_3$, $HoLaO_3$, $HoMnO_3$, $HoNiO_3$, $HoScO_3$, $HoVO_3$, $INaO_3$, $InLaO_3$, $InPrO_3$, $InRhO_3$, $InSmO_3$, $IrSrO_3$, $KCaF_3$, $KMgCl_3$, $KMnCl_3$, $KMnF_3$, $KPdF_3$, $LaCrO_3$, $LaFeO_3$, $LaInO_3$, $LaLuO_3$, $LaMnO_3$, $LaPdO_3$, $LaRhO_3$, $LaRuO_3$, $LaScO_3$, $LaTiO_3$, $LaTmO_3$, $LaVO_3$, $LaYO_3$, $LaYbO_3$, $LaYbS_3$, $LiTaO_3$, $LuCrO_3$, $LuMnO_3$, $LuNiO_3$, $LuPrO_3$, $LuRhO_3$, $LuVO_3$, $MgNaD_3$, $MgNaF_3$, $MgSiO_3$, $MnNaF_3$, $MnNdO_3$, $MnPrO_3$, $MnSmO_3$, $MnTbO_3$, $MnTiO_3$, $MnTlCl_3$, $MnTmO_3$, $MnVO_3$, $MnYO_3$, $MnYbO_3$, $NaNbO_3$, $NaNiF_3$, $NaOsO_3$, $NaSbO_3$, $NaTaO_3$, $NaUO_3$, $NaZnF_3$, $NbSrO_3$, $NdFeO_3$, $NdNiO_3$, $NdRhO_3$, $NdRuO_3$, $NdScO_3$, $NdTiO_3$, $NdVO_3$, $NiPbO_3$, $NiPrO_3$, $NiSmO_3$, $NiTlO_3$, $NiTmO_3$, $NiUS_3$, $NiUSe_3$, $NiYO_3$, $NiYbO_3$, $OsSrO_3$, $PbCsBr_3$, $PbRbBr_3$, $PbSrO_3$, $PdUSe_3$, $PrCrO_3$, $PrCsBr_3$, $PrFeO_3$, $PrGaO_3$, $PrRhO_3$, $PrRuO_3$, $PrScO_3$, $PrSrO_3$, $PrVO_3$, $RbSrCl_3$, $RbYbBr_3$, $RhSmO_3$, $RhSrO_3$, $RhTbO_3$, $RhUS_3$, $RuSrO_3$, $RuUS_3$, $ScSmO_3$, $ScTbO_3$, $ScVO_3$, $ScYO_3$, $SiOBa_3$, $SmCrO_3$, $SmFeO_3$, $SmRhO_3$, $SmTiO_3$, $SmVO_3$, $SnSrO_3$, $SrIrO_3$, $SrSnO_3$, $SrTbO_3$, $SrTcO_3$, $SrVO_3$, $SrZrO_3$, $SrZrSe_3$, $TbVO_3$, $ThRhO_3$, $TiYO_3$, $TmVO_3$, $UVSe_3$, VYO_3, $VYbO_3$, $YAlO_3$, $YCrO_3$, $YCrbO_3$, $YFeO_3$, $YbAlO_3$, $YbCrO_3$

- This is the true ground state of $CaTiO_3$. The cubic perovskite structure ($E2_1$) is the high-temperature phase.
- The ICSD uses $GdFeO_3$ as the prototype for this phase.

Simple Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Ti I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	Ti I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}b\,\hat{\mathbf{y}}$	(4a)	Ti I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	Ti I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	Ca I
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Ca I
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4c)	Ca I
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Ca I
$\mathbf{B_9}$	=	$x_3\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(4c)	O I

$\mathbf{B_{10}}$	=	$-\left(x_3-\frac{1}{2}\right)\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_3-\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{3}{4}b\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1+\frac{3}{4}\,\mathbf{a}_2-z_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}+\frac{3}{4}b\,\hat{\mathbf{y}}-cz_3\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{12}}$	=	$\left(x_3+\frac{1}{2}\right)\,\mathbf{a}_1+\frac{1}{4}\,\mathbf{a}_2-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_3+\frac{1}{2}\right)\,\hat{\mathbf{x}}+\frac{1}{4}b\,\hat{\mathbf{y}}-c\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_{13}}$	=	$x_4\,\mathbf{a}_1+y_4\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{14}}$	=	$-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1-y_4\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{15}}$	=	$-x_4\,\mathbf{a}_1+\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}+b\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{16}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1-\left(y_4-\frac{1}{2}\right)\,\mathbf{a}_2-\left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}-b\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{17}}$	=	$-x_4\,\mathbf{a}_1-y_4\,\mathbf{a}_2-z_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}-by_4\,\hat{\mathbf{y}}-cz_4\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{18}}$	=	$\left(x_4+\frac{1}{2}\right)\,\mathbf{a}_1+y_4\,\mathbf{a}_2-\left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_4+\frac{1}{2}\right)\,\hat{\mathbf{x}}+by_4\,\hat{\mathbf{y}}-c\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{19}}$	=	$x_4\,\mathbf{a}_1-\left(y_4-\frac{1}{2}\right)\,\mathbf{a}_2+z_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}-b\left(y_4-\frac{1}{2}\right)\,\hat{\mathbf{y}}+cz_4\,\hat{\mathbf{z}}$	(8d)	O II
$\mathbf{B_{20}}$	=	$-\left(x_4-\frac{1}{2}\right)\,\mathbf{a}_1+\left(y_4+\frac{1}{2}\right)\,\mathbf{a}_2+\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_4-\frac{1}{2}\right)\,\hat{\mathbf{x}}+b\left(y_4+\frac{1}{2}\right)\,\hat{\mathbf{y}}+c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8d)	O II

References

[1] T. Yamanaka, N. Hirai, and Y. Komatsu, *Structure change of $Ca_{1-x}Sr_xTiO_3$ perovskite with composition and pressure*, Am. Mineral. **87**, 1183–1189 (2002), doi:10.2138/am-2002-8-917.

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