Post-perovskite ($MgSiO_3$) Structure: AB3C_oC20_63_c_cf_a-001

This structure originally had the label `AB3C_oC20_63_c_cf_a`. Calls to that address will be redirected here.

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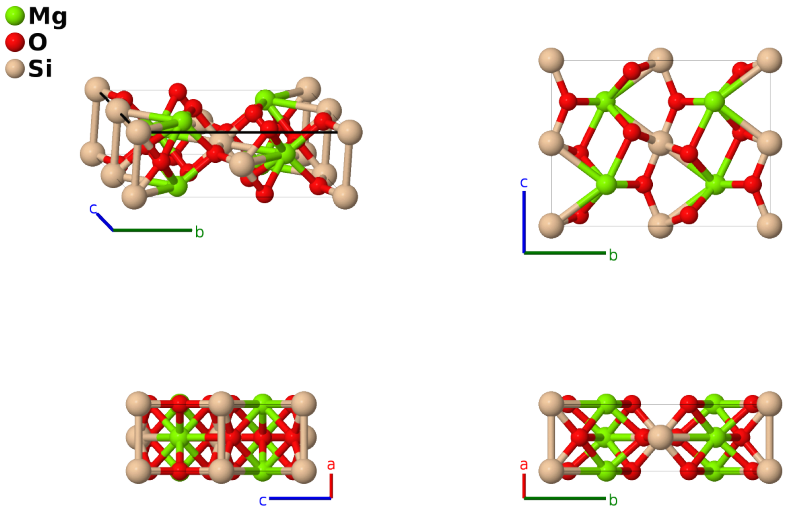
https://aflow.org/p/BCSA

https://aflow.org/p/AB3C_oC20_63_c_cf_a-001



Prototype	MgO_3Si
AFLOW prototype label	AB3C_oC20_63_c_cf_a-001
ICSD	158959
Pearson symbol	oC20
Space group number	63
Space group symbol	*Cmcm*
AFLOW prototype command	`aflow --proto=AB3C_oC20_63_c_cf_a-001 --params=`$a, b/a, c/a, y_2, y_3, y_4, z_4$

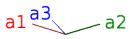
Other compounds with this structure

$AlNHf_3$, $AlNTi_3$, $AlNZr_3$, $AsCCr_3$, $AsCV_3$, $CaBrIn_3$, $CaIrO_3$, $CaPtO_3$, $CaRhO_3$, $CeYbSe_3$, $FeNaF_3$, $GeCV_3$, $GeNV_3$, $LaYbS_3$, $LaYbSe_3$, $LuNdSe_3$, $LuPrSe_3$, $MgGeO_3$, $NaIrO_3$, $NaMgF_3$, $NaNiF_3$, $NdYbSe_3$, $NiOZr_3$, PCV_3, $PNCr_3$, PNV_3, $POZr_3$, $PbTlI_3$, $PrYbSe_3$, $ScUS_3$

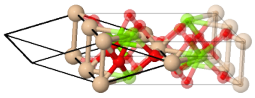
- This structure was determined by a combination of x-ray diffraction measurements and atomistic simulations of $MgSiO_3$ at a pressure of 121 GPa and a temperature of 300 K. This approximates the conditions at the Earth's core-mantle boundary.

- An earlier version of this page (Hicks, 2021) inadvertently switched the positions of the silicon and magnesium atoms, producing an incorrect structure with the AFLOW label AB3C_oC20_63_a_cf_c. Searches for that structure will redirect here. We apologize for the error.
- The ground state structure of $MgSiO_3$ is enstatite ($S4_3$).

Base-centered Orthorhombic primitive vectors



$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(4a)	Si I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	Si I
$\mathbf{B_3}$	=	$-y_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	Mg I
$\mathbf{B_4}$	=	$y_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	Mg I
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_6}$	=	$y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(4c)	O I
$\mathbf{B_7}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_8}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_9}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{10}}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8f)	O II

References

[1] M. Murakami, K. Hirose, K. Kawamura, N. Sata, and Y. Ohishi, *Post-Perovskite Phase Transition in $MgSiO_3$*, Science **304**, 855–858 (2005), doi:10.1126/science.1095932.

[2] 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.