Gd_2CuO_4 Structure: AB2C4_oC28_64_a_d_ef-001

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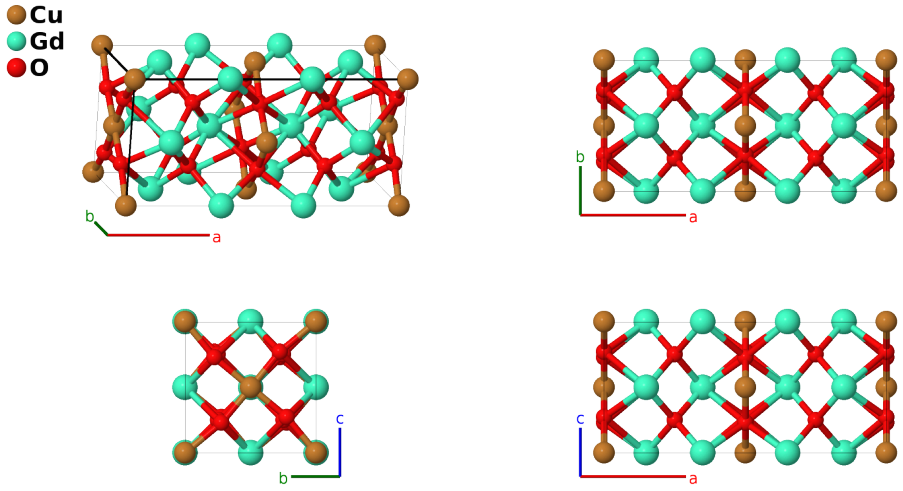


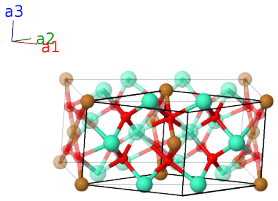
Prototype	$CuGd_2O_4$
AFLOW prototype label	AB2C4_oC28_64_a_d_ef-001
ICSD	75425
Pearson symbol	oC28
Space group number	64
Space group symbol	*Cmce*
AFLOW prototype command	`aflow --proto=AB2C4_oC28_64_a_d_ef-001 --params=`$a, b/a, c/a, x_2, y_3, y_4, z_4$

Other compounds with this structure
Eu_2CuO_4

- This is a slight orthorhombic distortion of the Nd_2CuO_4 structure, and there is some evidence that both Gd_2CuO_4 and Eu_2CuO_4 transform to the Nd_2CuO_4 structure at higher temperatures.
- We did not find an ICSD from (Luo, 1999), so we use the one from the earlier work of (Braden, 1994).

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)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4a)	Cu I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2$	=	$ax_2\,\hat{\mathbf{x}}$	(8d)	Gd I
$\mathbf{B_4}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8d)	Gd I
$\mathbf{B_5}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2$	=	$-ax_2\,\hat{\mathbf{x}}$	(8d)	Gd I
$\mathbf{B_6}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(8d)	Gd I
$\mathbf{B_7}$	=	$-\left(y_3 - \frac{1}{4}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B_8}$	=	$\left(y_3 + \frac{1}{4}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{1}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B_9}$	=	$\left(y_3 + \frac{3}{4}\right)\,\mathbf{a}_1 - \left(y_3 - \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B_{10}}$	=	$-\left(y_3 - \frac{3}{4}\right)\,\mathbf{a}_1 + \left(y_3 + \frac{3}{4}\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(8e)	O I
$\mathbf{B_{11}}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$by_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{12}}$	=	$\left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{13}}$	=	$-\left(y_4 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(y_4 + \frac{1}{2}\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(8f)	O II
$\mathbf{B_{14}}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-by_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(8f)	O II

References

[1] H. M. Luo, Y. Y. Hsu, B. N. Lin, Y. P. Chi, T. J. Lee, and H. C. Ku, *Correlation between weak ferromagnetism and crystal symmetry in Gd_2CuO_4-type cuprates*, Phys. Rev. B **60**, 13119–13124 (1999), doi:10.1103/PhysRevB.60.13119.

[2] M. Braden, W. Paulus, A. C. P. Vigoureux, G. Heger, A. Goukassov, P. Bourges, and D. Petitgrand, *Structure analysis of Gd_2CuO_4: a new modification of the T' phase*, EPL-Europhys. Lett. **25**, 625–630 (1994), doi:10.1209/0295-5075/25/8/011.

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