GdCBr Structure: ABC_mC12_12_i_i_i-003

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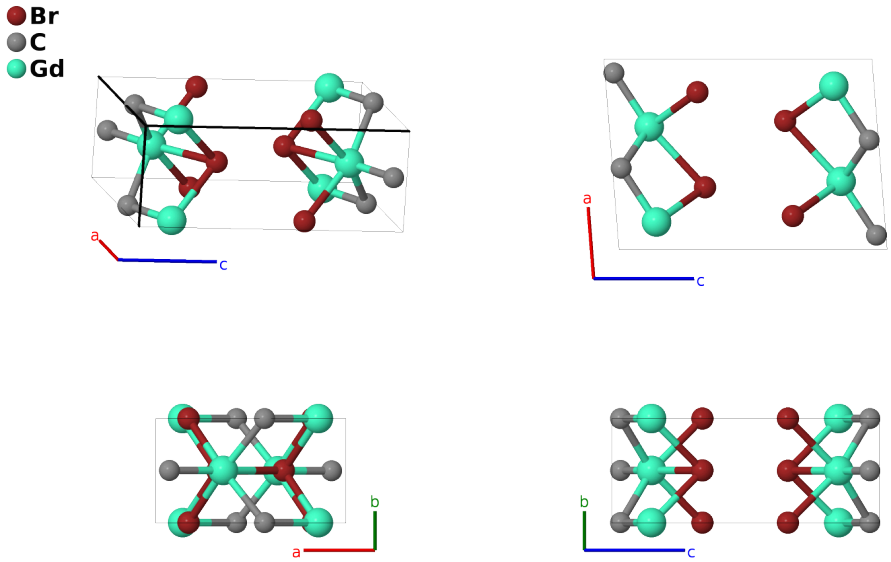
https://aflow.org/p/69PJ

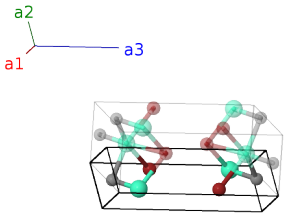
https://aflow.org/p/ABC_mC12_12_i_i_i-003



Prototype	BrCGd
AFLOW prototype label	ABC_mC12_12_i_i_i-003
ICSD	47225
Pearson symbol	mC12
Space group number	12
Space group symbol	$C2/m$
AFLOW prototype command	`aflow --proto=ABC_mC12_12_i_i_i-003 --params=`$a, b/a, c/a, \beta, x_1, z_1, x_2, z_2, x_3, z_3$

Other compounds with this structure
TbCBr, ThCN, YCBr, YCCl, YCI

Base-centered Monoclinic primitive vectors



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

Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(4i)	Br I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(4i)	Br I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	C I
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(4i)	C I
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Gd I
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(4i)	Gd I

References

[1] U. Schwanitz-Schüller and A. Simon, *New Gadolinium Carbide Bromides: $Gd_2C_2Br_2$ and Gd_2CBr_2*, Z. Naturforsch. B **40**, 710–716 (1985), doi:10.1515/znb-1985-0602.

Found in

[1] A. Simon, *Empty, Filled, and Condensed Metal Clusters*, J. Solid State Chem. **57**, 2–16 (1985), doi:10.1016/S0022-4596(85)80055-4.

[2] R. W. Henn, R. K. Kremer, and A. Simon, *Magnetic Susceptibility Investigations on the Layered Superconductors $Y_2C_2Br_2$:RE (RE = Gd, Dy, Er)*, J. Supercond. Nov. Magn. **13**, 471–477 (2000), doi:10.1023/A:1007771529474.