CoW_2B_2 Structure: A2BC2_oI10_71_e_c_g-001

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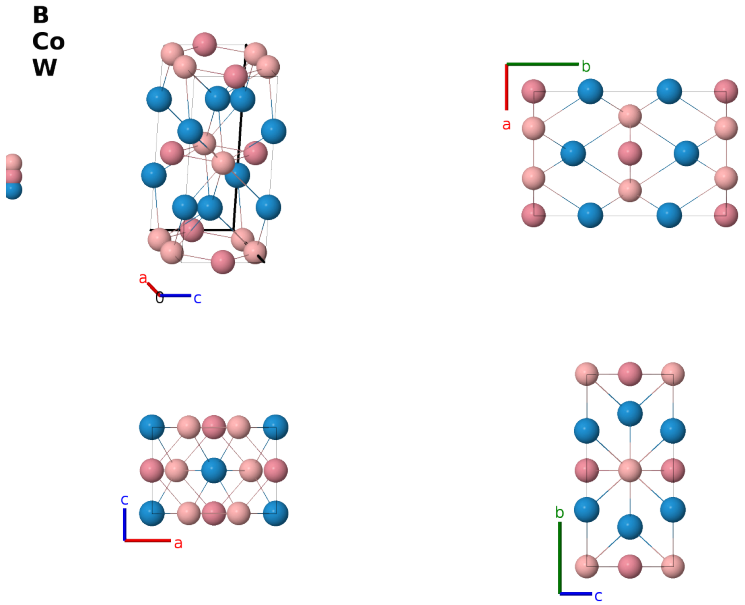
https://aflow.org/prototype-encyclopedia/PF2H

https://aflow.org/prototype-encyclopedia/A2BC2_oI10_71_e_c_g-001



Prototype	B_2CoW_2
AFLOW prototype label	A2BC2_oI10_71_e_c_g-001
ICSD	16776
CCDC	1597325
Pearson symbol	oI10
Space group number	71
Space group symbol	$Immm$
AFLOW prototype command	`aflow --proto=A2BC2_oI10_71_e_c_g-001 --params=`$a, b/a, c/a, x_2, y_3$

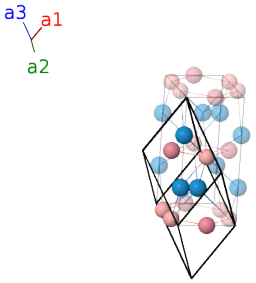
Other compounds with this structure

Ca_2AgPd_2, Ca_2CdPd_2, Ca_2CdPt_2, Ca_2GaCu_2, Ca_2MgPd_2, Ca_2MgPt_2, Ce_2SnNi_2, Ce_2ZnNi_2, Co_2AlGd_2, Dy_2AlCo_2, Dy_2AlNi_2, Er_2AlCo_2, Er_2AlNi_2, Er_2AlSi_2, Er_2GaNi_2, Gd_2AlCo_2, Gd_2AlNi_2, Ho_2AlCo_2, Ho_2AlNi_2, Ho_2AlSi_2, Ho_2GaNi_2, La_2AlNi_2, La_2ZnNi_2, Lu_2AlNi_2, Lu_2AlSi_2, Lu_2GaNi_2, Mo_2CoB_2, Mo_2NiB_2, Nd_2AlCo_2, Nd_2AlNi_2, Ni_2ZnTb_2, Pr_2AlCo_2, Pr_2AlNi_2, Pr_2SnNi_2, Sm_2SnNi_2, Sr_2CdPt_2, Tb_2AlCo_2, Tb_2AlNi_2, Tb_2GaCo_2, Tb_2GaNi_2, Tm_2AlCo_2, Tm_2AlNi_2, Tm_2AlSi_2, Tm_2GaNi_2, W_2FeB_2, W_2NiB_2, Y_2AlNi_2, Y_2AlSi_2, Y_2SnNi_2

- The AFLOW prototype label protocol rotates the crystal by 90° about the z-axis, interchanging the a and b lattice constants. It also shifts the origin, moving the cobalt atom from the (2a) site to the (2c) site.
- We apologize to (Zhang, 2025). At the time this entry was posted their full publication information was not available. We hope that the DOI is correct.

Body-centered Orthorhombic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	Co I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}}$	(4e)	B I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}}$	(4e)	B I
$\mathbf{B_4}$	=	$y_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_3$	=	$by_3\,\hat{\mathbf{y}}$	(4g)	W I
$\mathbf{B_5}$	=	$-y_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_3$	=	$-by_3\,\hat{\mathbf{y}}$	(4g)	W I

References

[1] W. Rieger, H. Nowotny, and F. Benesovsky, *Die Kristallstruktur von W_2CoB_2 und isotypen Phasen*, Monatsh. Chem. **97**, 378–382 (1966), doi:10.1007/BF00905254.

Found in

[1] Z. Zhang, E. H. Gamage, G. Amobi, S. Pradhan, A. Kutepov, K. D. Belashchenko, Y. Sun, K. Kovnir, and V. Antropov, *Discovery and Synthesis of a Family of Boride Altermagnets*, J. Am. Chem. Soc. **XXX**, XXX (2025), doi:10.1021/jacs.5c07874.

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