$C26_a$ (NO_2) (*Obsolete*) Structure: AB2_cI36_199_b_c-001

This structure originally had the label `AB2_cI36_199_b_c`. Calls to that address will be redirected here.

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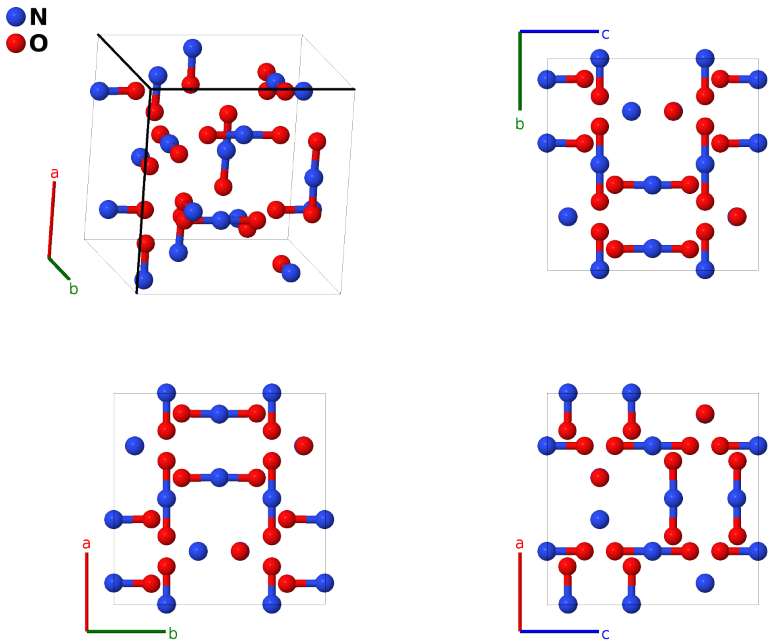
https://aflow.org/p/VGMG

https://aflow.org/p/AB2_cI36_199_b_c-001



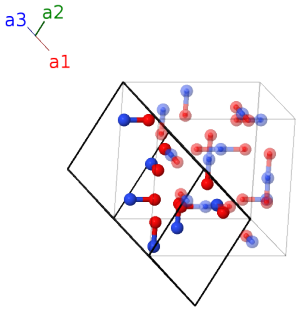
Prototype	NO_2
AFLOW prototype label	AB2_cI36_199_b_c-001
***Strukturbericht* designation**	$C26_a$
ICSD	31175
Pearson symbol	cI36
Space group number	199
Space group symbol	$I2_13$
AFLOW prototype command	`aflow --proto=AB2_cI36_199_b_c-001 --params=`a, x_1, x_2, y_2, z_2

- (Hermann, 1937) listed two possible structures for the low temperature solid cubic phase of NO_2, which were given *Strukturbericht* designations $C26_a$ and $C26_b$, the only structures with Roman subscripts in the original series.
- $C26_a$ (AB2_cI36_199_b_c) was set in space group $I2_13$ #199. Hermann noted that this structure has a very short distance (1.88Å) between oxygen atoms on different NO_2 molecules, and that this structure does not form the $(NO_2)_2$ aggregate molecule found in the $C26_b$ structure, making "making this proposed structure very unlikely."

- Recognizing this, (Hendricks, 1931) suggested that NO_2 was actually in space group $I23$ #197. (Hermann, 1997) gave this structure the $C26_b$ designation, but noted that based on Hendricks's atomic positions the space group was actually $Im\overline{3}$ #204.
- The modern accepted structure for NO_2, AB2_cI36_204_d_g, is set in space group $Im\overline{3}$, confirming Hendricks.

Body-centered Cubic primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}a\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\tfrac{1}{4}\,\mathbf{a}_1 + \left(x_1 + \tfrac{1}{4}\right)\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \tfrac{1}{4}a\,\hat{\mathbf{z}}$	(12b)	N I
$\mathbf{B_2}$	=	$\tfrac{3}{4}\,\mathbf{a}_1 - \left(x_1 - \tfrac{1}{4}\right)\,\mathbf{a}_2 - \left(x_1 - \tfrac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{4}a\,\hat{\mathbf{z}}$	(12b)	N I
$\mathbf{B_3}$	=	$x_1\,\mathbf{a}_1 + \tfrac{1}{4}\,\mathbf{a}_2 + \left(x_1 + \tfrac{1}{4}\right)\,\mathbf{a}_3$	=	$\tfrac{1}{4}a\,\hat{\mathbf{x}} + ax_1\,\hat{\mathbf{y}}$	(12b)	N I
$\mathbf{B_4}$	=	$-\left(x_1 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + \tfrac{3}{4}\,\mathbf{a}_2 - \left(x_1 - \tfrac{1}{4}\right)\,\mathbf{a}_3$	=	$\tfrac{1}{4}a\,\hat{\mathbf{x}} - ax_1\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}}$	(12b)	N I
$\mathbf{B_5}$	=	$\left(x_1 + \tfrac{1}{4}\right)\,\mathbf{a}_1 + x_1\,\mathbf{a}_2 + \tfrac{1}{4}\,\mathbf{a}_3$	=	$\tfrac{1}{4}a\,\hat{\mathbf{y}} + ax_1\,\hat{\mathbf{z}}$	(12b)	N I
$\mathbf{B_6}$	=	$-\left(x_1 - \tfrac{1}{4}\right)\,\mathbf{a}_1 - \left(x_1 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \tfrac{3}{4}\,\mathbf{a}_3$	=	$\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{4}a\,\hat{\mathbf{y}} - ax_1\,\hat{\mathbf{z}}$	(12b)	N I
$\mathbf{B_7}$	=	$(y_2 + z_2)\,\mathbf{a}_1 + (x_2 + z_2)\,\mathbf{a}_2 + (x_2 + y_2)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}} + az_2\,\hat{\mathbf{z}}$	(24c)	O I
$\mathbf{B_8}$	=	$\left(-y_2 + z_2 + \tfrac{1}{2}\right)\,\mathbf{a}_1 - (x_2 - z_2)\,\mathbf{a}_2 - \left(x_2 + y_2 - \tfrac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} - a\left(y_2 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + az_2\,\hat{\mathbf{z}}$	(24c)	O I
$\mathbf{B_9}$	=	$(y_2 - z_2)\,\mathbf{a}_1 - \left(x_2 + z_2 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(-x_2 + y_2 + \tfrac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{y}} - az_2\,\hat{\mathbf{z}}$	(24c)	O I
$\mathbf{B_{10}}$	=	$-\left(y_2 + z_2 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(x_2 - z_2 + \tfrac{1}{2}\right)\,\mathbf{a}_2 + (x_2 - y_2)\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{y}} - a\left(z_2 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$	(24c)	O I
$\mathbf{B_{11}}$	=	$(x_2 + y_2)\,\mathbf{a}_1 + (y_2 + z_2)\,\mathbf{a}_2 + (x_2 + z_2)\,\mathbf{a}_3$	=	$az_2\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} + ay_2\,\hat{\mathbf{z}}$	(24c)	O I
$\mathbf{B_{12}}$	=	$-\left(x_2 + y_2 - \tfrac{1}{2}\right)\,\mathbf{a}_1 + \left(-y_2 + z_2 + \tfrac{1}{2}\right)\,\mathbf{a}_2 - (x_2 - z_2)\,\mathbf{a}_3$	=	$az_2\,\hat{\mathbf{x}} - ax_2\,\hat{\mathbf{y}} - a\left(y_2 - \tfrac{1}{2}\right)\,\hat{\mathbf{z}}$	(24c)	O I
$\mathbf{B_{13}}$	=	$\left(-x_2 + y_2 + \tfrac{1}{2}\right)\,\mathbf{a}_1 + (y_2 - z_2)\,\mathbf{a}_2 - \left(x_2 + z_2 - \tfrac{1}{2}\right)\,\mathbf{a}_3$	=	$-az_2\,\hat{\mathbf{x}} - a\left(x_2 - \tfrac{1}{2}\right)\,\hat{\mathbf{y}} + ay_2\,\hat{\mathbf{z}}$	(24c)	O I
$\mathbf{B_{14}}$	=	$(x_2 - y_2)\,\mathbf{a}_1 - \left(y_2 + z_2 - \tfrac{1}{2}\right)\,\mathbf{a}_2 + \left(x_2 - z_2 + \tfrac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(z_2 - \tfrac{1}{2}\right)\,\hat{\mathbf{x}} + ax_2\,\hat{\mathbf{y}} - ay_2\,\hat{\mathbf{z}}$	(24c)	O I
$\mathbf{B_{15}}$	=	$(x_2 + z_2)\,\mathbf{a}_1 + (x_2 + y_2)\,\mathbf{a}_2 + (y_2 + z_2)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} + az_2\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(24c)	O I

$\mathbf{B_{16}}$	=	$-(x_2 - z_2)\,\mathbf{a}_1 - \left(x_2 + y_2 - \frac{1}{2}\right)\,\mathbf{a}_2 + \left(-y_2 + z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(y_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + az_2\,\hat{\mathbf{y}} - ax_2\,\hat{\mathbf{z}}$	(24c)	O I
$\mathbf{B_{17}}$	=	$-\left(x_2 + z_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \left(-x_2 + y_2 + \frac{1}{2}\right)\,\mathbf{a}_2 + (y_2 - z_2)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} - az_2\,\hat{\mathbf{y}} - a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(24c)	O I
$\mathbf{B_{18}}$	=	$\left(x_2 - z_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + (x_2 - y_2)\,\mathbf{a}_2 - \left(y_2 + z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} - a\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + ax_2\,\hat{\mathbf{z}}$	(24c)	O I

References

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[2] P. Villars and K. Cenzual, eds., *Crystal Structure Data of Inorganic Compounds*, vol. III (Springer-Verlag, Berlin, Heidelberg, 2005).

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Found in

[1] C. Hermann, O. Lohrmann, and H. Philipp, eds., *Strukturbericht Band II 1928-1932* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1937).