Modern $C26$ (NO_2) Structure: AB2_cI36_204_d_g-001

This structure previously used the label(s) `AB2_cI36_204_d_g`. Calls to these addresses will be redirected here.

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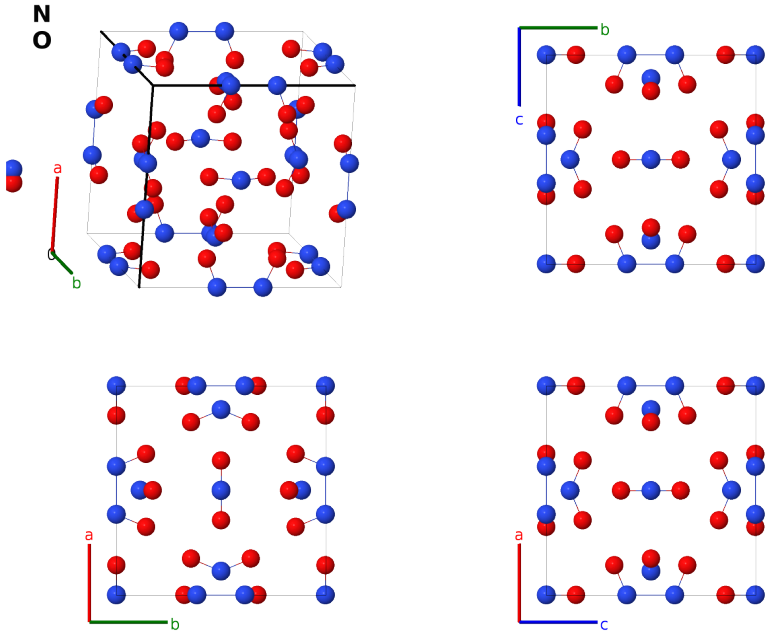
https://aflow.org/prototype-encyclopedia/XJC7

https://aflow.org/prototype-encyclopedia/AB2_cI36_204_d_g-001

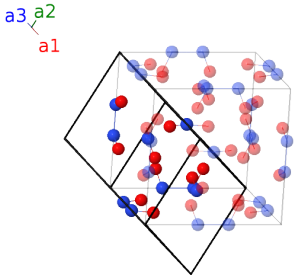


Prototype	NO_2
AFLOW prototype label	AB2_cI36_204_d_g-001
***Strukturbericht* designation**	$C26$
ICSD	201140
CCDC	1705882
Pearson symbol	cI36
Space group number	204
Space group symbol	$Im\bar{3}$
AFLOW prototype command	`aflow --proto=AB2_cI36_204_d_g-001 --params=`a, x_1, y_2, z_2

- (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 $Im\bar{3}$ #204.
- The modern accepted structure for No_2, AB2_cI36_204_d_g, is set in space group $Im\bar{3}$, confirming Hendricks. We follow (Villars, 2005) and give this the $C26$ designation, depreciating the $C26_b$ label.
- We used the experimental data for this phase collected at 20K.

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_2 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}}$	(12d)	N I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_2 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}}$	(12d)	N I
$\mathbf{B_3}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{y}}$	(12d)	N I
$\mathbf{B_4}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{y}}$	(12d)	N I
$\mathbf{B_5}$	=	$x_1\,\mathbf{a}_1 + x_1\,\mathbf{a}_2$	=	$ax_1\,\hat{\mathbf{z}}$	(12d)	N I
$\mathbf{B_6}$	=	$-x_1\,\mathbf{a}_1 - x_1\,\mathbf{a}_2$	=	$-ax_1\,\hat{\mathbf{z}}$	(12d)	N I
$\mathbf{B_7}$	=	$(y_2 + z_2)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 + y_2\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{y}} + az_2\,\hat{\mathbf{z}}$	(24g)	O I
$\mathbf{B_8}$	=	$-(y_2 - z_2)\,\mathbf{a}_1 + z_2\,\mathbf{a}_2 - y_2\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{y}} + az_2\,\hat{\mathbf{z}}$	(24g)	O I
$\mathbf{B_9}$	=	$(y_2 - z_2)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 + y_2\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{y}} - az_2\,\hat{\mathbf{z}}$	(24g)	O I
$\mathbf{B_{10}}$	=	$-(y_2 + z_2)\,\mathbf{a}_1 - z_2\,\mathbf{a}_2 - y_2\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{y}} - az_2\,\hat{\mathbf{z}}$	(24g)	O I
$\mathbf{B_{11}}$	=	$y_2\,\mathbf{a}_1 + (y_2 + z_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$az_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{z}}$	(24g)	O I
$\mathbf{B_{12}}$	=	$-y_2\,\mathbf{a}_1 - (y_2 - z_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$az_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{z}}$	(24g)	O I
$\mathbf{B_{13}}$	=	$y_2\,\mathbf{a}_1 + (y_2 - z_2)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-az_2\,\hat{\mathbf{x}} + ay_2\,\hat{\mathbf{z}}$	(24g)	O I
$\mathbf{B_{14}}$	=	$-y_2\,\mathbf{a}_1 - (y_2 + z_2)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-az_2\,\hat{\mathbf{x}} - ay_2\,\hat{\mathbf{z}}$	(24g)	O I
$\mathbf{B_{15}}$	=	$z_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + (y_2 + z_2)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} + az_2\,\hat{\mathbf{y}}$	(24g)	O I
$\mathbf{B_{16}}$	=	$z_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - (y_2 - z_2)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} + az_2\,\hat{\mathbf{y}}$	(24g)	O I
$\mathbf{B_{17}}$	=	$-z_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + (y_2 - z_2)\,\mathbf{a}_3$	=	$ay_2\,\hat{\mathbf{x}} - az_2\,\hat{\mathbf{y}}$	(24g)	O I
$\mathbf{B_{18}}$	=	$-z_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - (y_2 + z_2)\,\mathbf{a}_3$	=	$-ay_2\,\hat{\mathbf{x}} - az_2\,\hat{\mathbf{y}}$	(24g)	O I

References

[1] A. Kvick, R. K. McMullan, and M. D. Newton, *The structure of dinitrogen tetroxide N_2O_4: Neutron diffraction study at 100, 60 and 20 K and* ab initio *theoretical calculations*, J. Chem. Phys. **76**, 3754–3761 (1982), doi:10.1063/1.443414.

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

[3] S. B. Hendricks, *Die Kristallstruktur von N_2O_4*, Z. Physik **70**, 699–700 (1931), doi:10.1007/BF01340758.

Found in

[1] P. Villars and K. Cenzual, eds., *Crystal Structure Data of Inorganic Compounds* (Springer-Verlag, Berlin, Heidelberg, 2005). Landolt-Bornstein Volume III 43A2.

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