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

This structure originally had the label `AB2_cI36_204_d_g`. Calls to that address will be redirected here.

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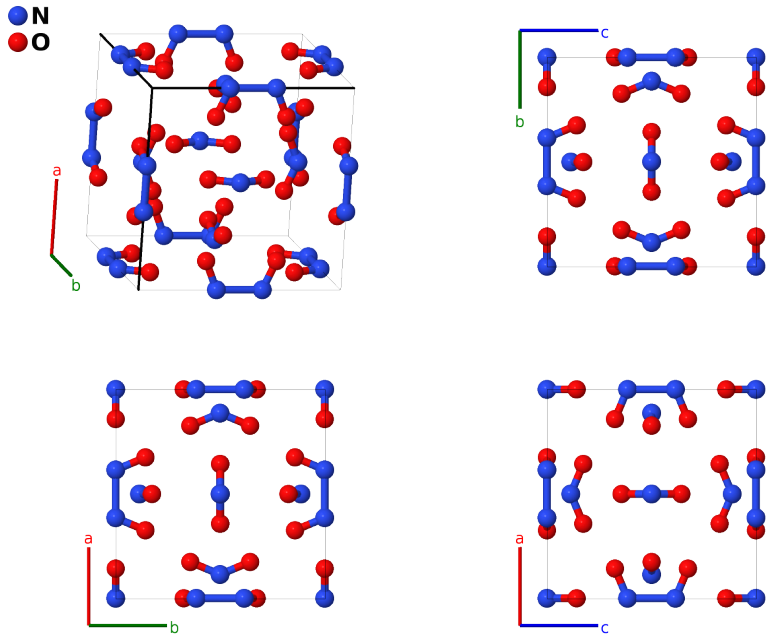
https://aflow.org/p/XJC7

https://aflow.org/p/AB2_cI36_204_d_g-001




| | |
|---|---|
| **Prototype** | $NO_2$ |
| **AFLOW prototype label** | AB2_cI36_204_d_g-001 |
| ***Strukturbericht* designation** | $C26$ |
| **ICSD** | 201140 |
| **Pearson symbol** | cI36 |
| **Space group number** | 204 |
| **Space group symbol** | $Im\overline{3}$ |
| **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 $Im\overline{3}$ #204.
- The modern accepted structure for $No_2$, AB2_cI36_204_d_g, is set in space group $Im\overline{3}$, confirming Hendricks. 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.

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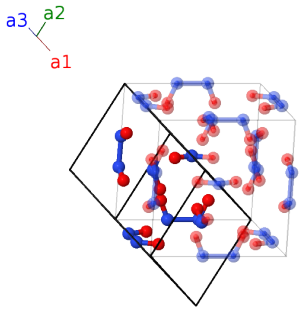
**Body-centered Cubic primitive vectors**

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

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**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.