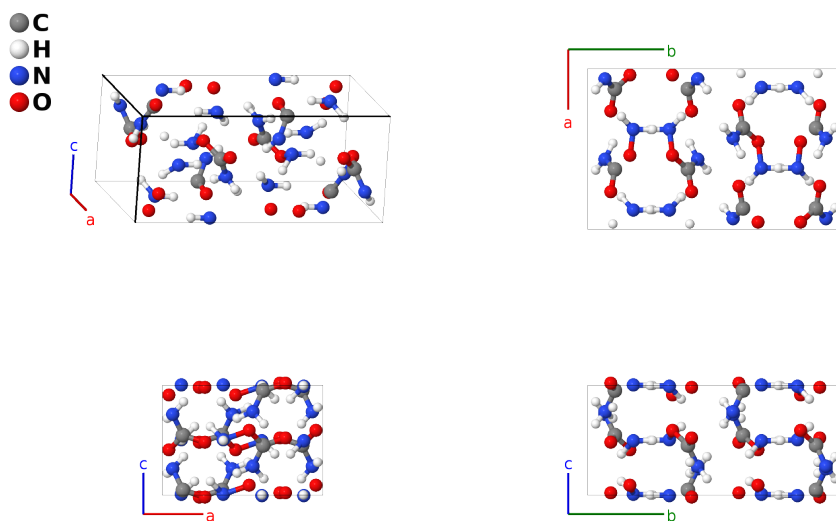


O-Carbamoylhydroxylamine ($\text{CH}_4\text{N}_2\text{O}_2$) Structure: AB4C2D2_oP72_61_c_4c_2c_2c-001

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<https://aflow.org/p/K3UE>

https://aflow.org/p/AB4C2D2_oP72_61_c_4c_2c_2c-001

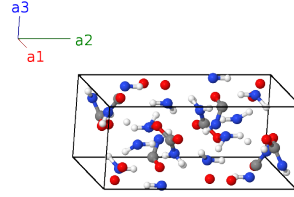


| | |
|--------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Prototype | $\text{CH}_4\text{N}_2\text{O}_2$ |
| AFLOW prototype label | AB4C2D2_oP72_61_c_4c_2c_2c-001 |
| Mineral name | O-carbamoylhydroxylamine |
| CCDC | 1119388 |
| Pearson symbol | oP72 |
| Space group number | 61 |
| Space group symbol | $Pbca$ |
| AFLOW prototype command | <pre>aflow --proto=AB4C2D2_oP72_61_c_4c_2c_2c-001 --params=a,b/a,c/a,x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,x5,y5,z5,x6,y6,z6,x7, y7,z7,x8,y8,z8,x9,y9,z9</pre> |

- $\text{CH}_4\text{N}_2\text{O}_2$ is found in two isomers: monoclinic N-hydroxyurea ($\text{H}_2\text{NCONHOH}$), and
- orthorhombic O-hydroxyurea ($\text{C}(\text{NH}_2)\text{ONH}_2$) (this structure).

Simple Orthorhombic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= a \hat{\mathbf{x}} \\ \mathbf{a}_2 &= b \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$



Basis vectors

| | Lattice coordinates | | Cartesian coordinates | Wyckoff position | Atom type |
|-------------------|---------------------------------------------------------------------------------------------|-----|----------------------------------------------------------------------------------------------------------|------------------|-----------|
| \mathbf{B}_1 | $= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$ | $=$ | $ax_1 \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$ | (8c) | C I |
| \mathbf{B}_2 | $= -(x_1 - \frac{1}{2}) \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | C I |
| \mathbf{B}_3 | $= -x_1 \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ax_1 \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | C I |
| \mathbf{B}_4 | $= (x_1 + \frac{1}{2}) \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 - z_1 \mathbf{a}_3$ | $=$ | $a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$ | (8c) | C I |
| \mathbf{B}_5 | $= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$ | $=$ | $-ax_1 \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$ | (8c) | C I |
| \mathbf{B}_6 | $= (x_1 + \frac{1}{2}) \mathbf{a}_1 + y_1 \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | C I |
| \mathbf{B}_7 | $= x_1 \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $ax_1 \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | C I |
| \mathbf{B}_8 | $= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 + z_1 \mathbf{a}_3$ | $=$ | $-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$ | (8c) | C I |
| \mathbf{B}_9 | $= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$ | $=$ | $ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$ | (8c) | H I |
| \mathbf{B}_{10} | $= -(x_2 - \frac{1}{2}) \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | H I |
| \mathbf{B}_{11} | $= -x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ax_2 \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | H I |
| \mathbf{B}_{12} | $= (x_2 + \frac{1}{2}) \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 - z_2 \mathbf{a}_3$ | $=$ | $a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$ | (8c) | H I |
| \mathbf{B}_{13} | $= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$ | $=$ | $-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$ | (8c) | H I |
| \mathbf{B}_{14} | $= (x_2 + \frac{1}{2}) \mathbf{a}_1 + y_2 \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | H I |
| \mathbf{B}_{15} | $= x_2 \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $ax_2 \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | H I |
| \mathbf{B}_{16} | $= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 + z_2 \mathbf{a}_3$ | $=$ | $-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$ | (8c) | H I |
| \mathbf{B}_{17} | $= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$ | $=$ | $ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$ | (8c) | H II |
| \mathbf{B}_{18} | $= -(x_3 - \frac{1}{2}) \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | H II |
| \mathbf{B}_{19} | $= -x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $-ax_3 \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | H II |
| \mathbf{B}_{20} | $= (x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$ | $=$ | $a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$ | (8c) | H II |
| \mathbf{B}_{21} | $= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$ | $=$ | $-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$ | (8c) | H II |
| \mathbf{B}_{22} | $= (x_3 + \frac{1}{2}) \mathbf{a}_1 + y_3 \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$ | $=$ | $a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | H II |
| \mathbf{B}_{23} | $= x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$ | $=$ | $ax_3 \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$ | (8c) | H II |
| \mathbf{B}_{24} | $= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 + z_3 \mathbf{a}_3$ | $=$ | $-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$ | (8c) | H II |
| \mathbf{B}_{25} | $= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$ | $=$ | $ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$ | (8c) | H III |

$$\begin{aligned}
\mathbf{B}_{58} &= \begin{matrix} -(x_8 - \frac{1}{2}) \mathbf{a}_1 - y_8 \mathbf{a}_2 + \\ (z_8 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}} & (8c) & \text{O I} \\
\mathbf{B}_{59} &= \begin{matrix} -x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - \\ (z_8 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ax_8 \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}} & (8c) & \text{O I} \\
\mathbf{B}_{60} &= (x_8 + \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3 = a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (8c) & \text{O I} \\
\mathbf{B}_{61} &= \begin{matrix} -x_8 \mathbf{a}_1 - y_8 \mathbf{a}_2 - z_8 \mathbf{a}_3 \end{matrix} = -ax_8 \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}} & (8c) & \text{O I} \\
\mathbf{B}_{62} &= (x_8 + \frac{1}{2}) \mathbf{a}_1 + y_8 \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3 = a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}} & (8c) & \text{O I} \\
\mathbf{B}_{63} &= x_8 \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3 = ax_8 \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}} & (8c) & \text{O I} \\
\mathbf{B}_{64} &= \begin{matrix} -(x_8 - \frac{1}{2}) \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 + \\ z_8 \mathbf{a}_3 \end{matrix} = -a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}} & (8c) & \text{O I} \\
\mathbf{B}_{65} &= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3 = ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (8c) & \text{O II} \\
\mathbf{B}_{66} &= \begin{matrix} -(x_9 - \frac{1}{2}) \mathbf{a}_1 - y_9 \mathbf{a}_2 + \\ (z_9 + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}} & (8c) & \text{O II} \\
\mathbf{B}_{67} &= \begin{matrix} -x_9 \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 - \\ (z_9 - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ax_9 \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}} & (8c) & \text{O II} \\
\mathbf{B}_{68} &= (x_9 + \frac{1}{2}) \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 - z_9 \mathbf{a}_3 = a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (8c) & \text{O II} \\
\mathbf{B}_{69} &= \begin{matrix} -x_9 \mathbf{a}_1 - y_9 \mathbf{a}_2 - z_9 \mathbf{a}_3 \end{matrix} = -ax_9 \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}} & (8c) & \text{O II} \\
\mathbf{B}_{70} &= (x_9 + \frac{1}{2}) \mathbf{a}_1 + y_9 \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3 = a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}} & (8c) & \text{O II} \\
\mathbf{B}_{71} &= x_9 \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3 = ax_9 \hat{\mathbf{x}} - b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}} & (8c) & \text{O II} \\
\mathbf{B}_{72} &= \begin{matrix} -(x_9 - \frac{1}{2}) \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 + \\ z_9 \mathbf{a}_3 \end{matrix} = -a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}} & (8c) & \text{O II}
\end{aligned}$$

References

- [1] I. K. Larsen, *The Crystal and Molecular Structure of O-Carbamoylhydroxylamine, an Isomer of Hydroxyurea*, Acta Chem. Scand. **22**, 843–853 (1968), doi:10.3891/acta.chem.scand.22-0843.