Rhodan Hydrate ($H_2C_2N_2S_2O$) Structure: A2B2C2DE2_mC72_15_2f_2f_2f_f_2f-001

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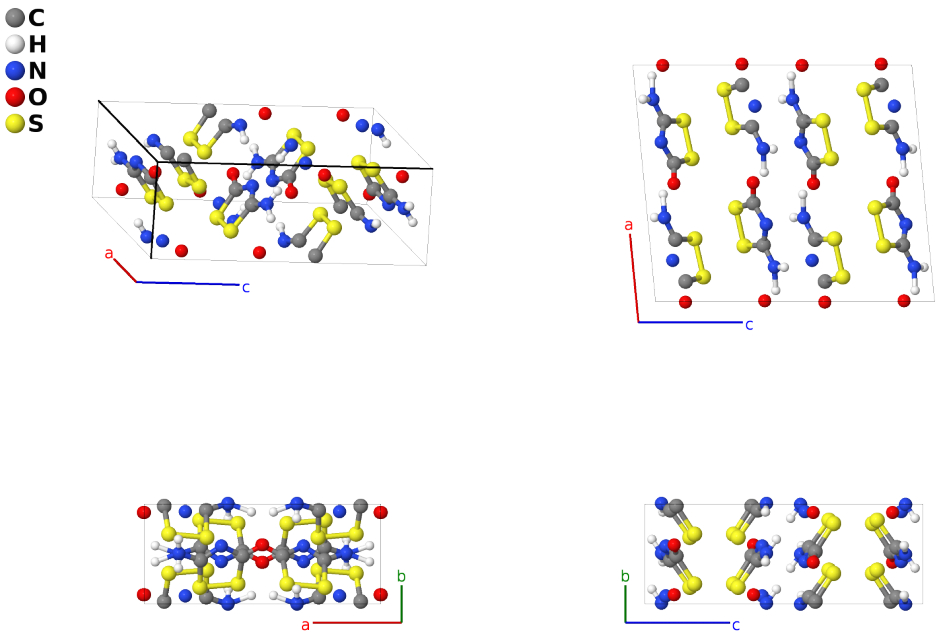
https://aflow.org/p/UX1J

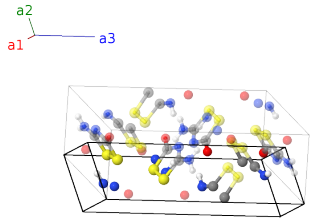
https://aflow.org/p/A2B2C2DE2_mC72_15_2f_2f_2f_f_2f-001



Prototype	$C_2H_2N_2OS_2$
AFLOW prototype label	A2B2C2DE2_mC72_15_2f_2f_2f_f_2f-001
CCDC	1249311
Pearson symbol	mC72
Space group number	15
Space group symbol	$C2/c$
AFLOW prototype command	`aflow --proto=A2B2C2DE2_mC72_15_2f_2f_2f_f_2f-001 --params=`$a, b/a, c/a, \beta, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9$

Base-centered Monoclinic primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$(x_1 - y_1)\,\mathbf{a}_1 + (x_1 + y_1)\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} + cz_1\sin\beta\,\hat{\mathbf{z}}$	(8f)	C I
$\mathbf{B_2}$	=	$-(x_1 + y_1)\,\mathbf{a}_1 - (x_1 - y_1)\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\mathbf{a}_3$	=	$-\left(ax_1 + c\left(z_1 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + by_1\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	C I
$\mathbf{B_3}$	=	$-(x_1 - y_1)\,\mathbf{a}_1 - (x_1 + y_1)\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-(ax_1 + cz_1\cos\beta)\,\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} - cz_1\sin\beta\,\hat{\mathbf{z}}$	(8f)	C I
$\mathbf{B_4}$	=	$(x_1 + y_1)\,\mathbf{a}_1 + (x_1 - y_1)\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\mathbf{a}_3$	=	$\left(ax_1 + c\left(z_1 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - by_1\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	C I
$\mathbf{B_5}$	=	$(x_2 - y_2)\,\mathbf{a}_1 + (x_2 + y_2)\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} + cz_2\sin\beta\,\hat{\mathbf{z}}$	(8f)	C II
$\mathbf{B_6}$	=	$-(x_2 + y_2)\,\mathbf{a}_1 - (x_2 - y_2)\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\mathbf{a}_3$	=	$-\left(ax_2 + c\left(z_2 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + by_2\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	C II
$\mathbf{B_7}$	=	$-(x_2 - y_2)\,\mathbf{a}_1 - (x_2 + y_2)\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + cz_2\cos\beta)\,\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} - cz_2\sin\beta\,\hat{\mathbf{z}}$	(8f)	C II
$\mathbf{B_8}$	=	$(x_2 + y_2)\,\mathbf{a}_1 + (x_2 - y_2)\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\mathbf{a}_3$	=	$\left(ax_2 + c\left(z_2 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - by_2\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	C II
$\mathbf{B_9}$	=	$(x_3 - y_3)\,\mathbf{a}_1 + (x_3 + y_3)\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} + cz_3\sin\beta\,\hat{\mathbf{z}}$	(8f)	H I
$\mathbf{B_{10}}$	=	$-(x_3 + y_3)\,\mathbf{a}_1 - (x_3 - y_3)\,\mathbf{a}_2 - \left(z_3 - \frac{1}{2}\right)\mathbf{a}_3$	=	$-\left(ax_3 + c\left(z_3 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + by_3\,\hat{\mathbf{y}} - c\left(z_3 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	H I
$\mathbf{B_{11}}$	=	$-(x_3 - y_3)\,\mathbf{a}_1 - (x_3 + y_3)\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + cz_3\cos\beta)\,\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} - cz_3\sin\beta\,\hat{\mathbf{z}}$	(8f)	H I
$\mathbf{B_{12}}$	=	$(x_3 + y_3)\,\mathbf{a}_1 + (x_3 - y_3)\,\mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right)\mathbf{a}_3$	=	$\left(ax_3 + c\left(z_3 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - by_3\,\hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	H I
$\mathbf{B_{13}}$	=	$(x_4 - y_4)\,\mathbf{a}_1 + (x_4 + y_4)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} + cz_4\sin\beta\,\hat{\mathbf{z}}$	(8f)	H II
$\mathbf{B_{14}}$	=	$-(x_4 + y_4)\,\mathbf{a}_1 - (x_4 - y_4)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\mathbf{a}_3$	=	$-\left(ax_4 + c\left(z_4 - \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} + by_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	H II
$\mathbf{B_{15}}$	=	$-(x_4 - y_4)\,\mathbf{a}_1 - (x_4 + y_4)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + cz_4\cos\beta)\,\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} - cz_4\sin\beta\,\hat{\mathbf{z}}$	(8f)	H II
$\mathbf{B_{16}}$	=	$(x_4 + y_4)\,\mathbf{a}_1 + (x_4 - y_4)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\mathbf{a}_3$	=	$\left(ax_4 + c\left(z_4 + \frac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}} - by_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}}$	(8f)	H II
$\mathbf{B_{17}}$	=	$(x_5 - y_5)\,\mathbf{a}_1 + (x_5 + y_5)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + cz_5\cos\beta)\,\hat{\mathbf{x}} + by_5\,\hat{\mathbf{y}} + cz_5\sin\beta\,\hat{\mathbf{z}}$	(8f)	N I

$$\mathbf{B_{18}} = -(x_5+y_5)\,\mathbf{a}_1-(x_5-y_5)\,\mathbf{a}_2-\left(z_5-\tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_5+c\left(z_5-\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}+by_5\,\hat{\mathbf{y}}-c\left(z_5-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{N I}$$

$$\mathbf{B_{19}} = -(x_5-y_5)\,\mathbf{a}_1-(x_5+y_5)\,\mathbf{a}_2-z_5\,\mathbf{a}_3 = -(ax_5+cz_5\cos\beta)\,\hat{\mathbf{x}}-by_5\,\hat{\mathbf{y}}-cz_5\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{N I}$$

$$\mathbf{B_{20}} = (x_5+y_5)\,\mathbf{a}_1+(x_5-y_5)\,\mathbf{a}_2+\left(z_5+\tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_5+c\left(z_5+\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}-by_5\,\hat{\mathbf{y}}+c\left(z_5+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{N I}$$

$$\mathbf{B_{21}} = (x_6-y_6)\,\mathbf{a}_1+(x_6+y_6)\,\mathbf{a}_2+z_6\,\mathbf{a}_3 = (ax_6+cz_6\cos\beta)\,\hat{\mathbf{x}}+by_6\,\hat{\mathbf{y}}+cz_6\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{N II}$$

$$\mathbf{B_{22}} = -(x_6+y_6)\,\mathbf{a}_1-(x_6-y_6)\,\mathbf{a}_2-\left(z_6-\tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_6+c\left(z_6-\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}+by_6\,\hat{\mathbf{y}}-c\left(z_6-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{N II}$$

$$\mathbf{B_{23}} = -(x_6-y_6)\,\mathbf{a}_1-(x_6+y_6)\,\mathbf{a}_2-z_6\,\mathbf{a}_3 = -(ax_6+cz_6\cos\beta)\,\hat{\mathbf{x}}-by_6\,\hat{\mathbf{y}}-cz_6\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{N II}$$

$$\mathbf{B_{24}} = (x_6+y_6)\,\mathbf{a}_1+(x_6-y_6)\,\mathbf{a}_2+\left(z_6+\tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_6+c\left(z_6+\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}-by_6\,\hat{\mathbf{y}}+c\left(z_6+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{N II}$$

$$\mathbf{B_{25}} = (x_7-y_7)\,\mathbf{a}_1+(x_7+y_7)\,\mathbf{a}_2+z_7\,\mathbf{a}_3 = (ax_7+cz_7\cos\beta)\,\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}+cz_7\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O I}$$

$$\mathbf{B_{26}} = -(x_7+y_7)\,\mathbf{a}_1-(x_7-y_7)\,\mathbf{a}_2-\left(z_7-\tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_7+c\left(z_7-\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}+by_7\,\hat{\mathbf{y}}-c\left(z_7-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O I}$$

$$\mathbf{B_{27}} = -(x_7-y_7)\,\mathbf{a}_1-(x_7+y_7)\,\mathbf{a}_2-z_7\,\mathbf{a}_3 = -(ax_7+cz_7\cos\beta)\,\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}-cz_7\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O I}$$

$$\mathbf{B_{28}} = (x_7+y_7)\,\mathbf{a}_1+(x_7-y_7)\,\mathbf{a}_2+\left(z_7+\tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_7+c\left(z_7+\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}-by_7\,\hat{\mathbf{y}}+c\left(z_7+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{O I}$$

$$\mathbf{B_{29}} = (x_8-y_8)\,\mathbf{a}_1+(x_8+y_8)\,\mathbf{a}_2+z_8\,\mathbf{a}_3 = (ax_8+cz_8\cos\beta)\,\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}+cz_8\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{S I}$$

$$\mathbf{B_{30}} = -(x_8+y_8)\,\mathbf{a}_1-(x_8-y_8)\,\mathbf{a}_2-\left(z_8-\tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_8+c\left(z_8-\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}+by_8\,\hat{\mathbf{y}}-c\left(z_8-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{S I}$$

$$\mathbf{B_{31}} = -(x_8-y_8)\,\mathbf{a}_1-(x_8+y_8)\,\mathbf{a}_2-z_8\,\mathbf{a}_3 = -(ax_8+cz_8\cos\beta)\,\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}-cz_8\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{S I}$$

$$\mathbf{B_{32}} = (x_8+y_8)\,\mathbf{a}_1+(x_8-y_8)\,\mathbf{a}_2+\left(z_8+\tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_8+c\left(z_8+\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}-by_8\,\hat{\mathbf{y}}+c\left(z_8+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{S I}$$

$$\mathbf{B_{33}} = (x_9-y_9)\,\mathbf{a}_1+(x_9+y_9)\,\mathbf{a}_2+z_9\,\mathbf{a}_3 = (ax_9+cz_9\cos\beta)\,\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}+cz_9\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{S II}$$

$$\mathbf{B_{34}} = -(x_9+y_9)\,\mathbf{a}_1-(x_9-y_9)\,\mathbf{a}_2-\left(z_9-\tfrac{1}{2}\right)\mathbf{a}_3 = -\left(ax_9+c\left(z_9-\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}+by_9\,\hat{\mathbf{y}}-c\left(z_9-\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{S II}$$

$$\mathbf{B_{35}} = -(x_9-y_9)\,\mathbf{a}_1-(x_9+y_9)\,\mathbf{a}_2-z_9\,\mathbf{a}_3 = -(ax_9+cz_9\cos\beta)\,\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}-cz_9\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{S II}$$

$$\mathbf{B_{36}} = (x_9+y_9)\,\mathbf{a}_1+(x_9-y_9)\,\mathbf{a}_2+\left(z_9+\tfrac{1}{2}\right)\mathbf{a}_3 = \left(ax_9+c\left(z_9+\tfrac{1}{2}\right)\cos\beta\right)\hat{\mathbf{x}}-by_9\,\hat{\mathbf{y}}+c\left(z_9+\tfrac{1}{2}\right)\sin\beta\,\hat{\mathbf{z}} \quad (8f) \quad \text{S II}$$

References

[1] A. Hordvik, *The Crystal and Molecular Structure of Rhodan Hydrate*, Acta Chem. Scand. **20**, 754–770 (1966), doi:10.3891/acta.chem.scand.20-0754.