

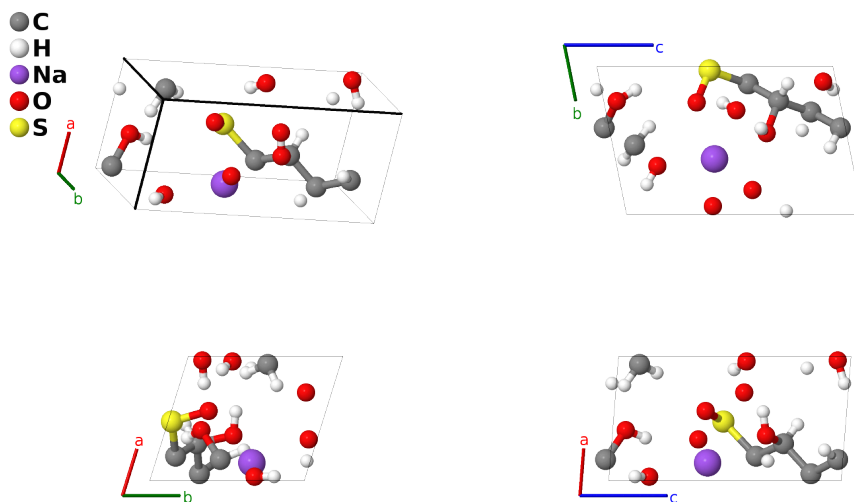
NaC₅H₁₁O₈S Structure: A5B11CD8E_aP26_1_5a_11a_a_8a_a-001

This structure originally had the label A5B11CD8E_aP26_1_5a_11a_a_8a_a. Calls to that address will be redirected here.

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

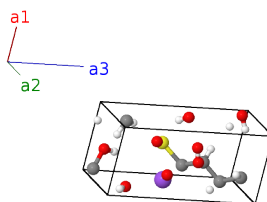
https://aflow.org/p/A5B11CD8E_aP26_1_5a_11a_a_8a_a-001



Prototype	C ₅ H ₁₁ NaO ₈ S
AFLOW prototype label	A5B11CD8E_aP26_1_5a_11a_a_8a_a-001
CCDC	1471425
Pearson symbol	aP26
Space group number	1
Space group symbol	<i>P</i> 1
AFLOW prototype command	<pre>aflow --proto=A5B11CD8E_aP26_1_5a_11a_a_8a_a-001 --params=a,b/a,c/a,α,β,γ,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,x₁₀,y₁₀,z₁₀,x₁₁,y₁₁,z₁₁,x₁₂,y₁₂,z₁₂,x₁₃,y₁₃,z₁₃,x₁₄,y₁₄,z₁₄, x₁₅,y₁₅,z₁₅,x₁₆,y₁₆,z₁₆,x₁₇,y₁₇,z₁₇,x₁₈,y₁₈,z₁₈,x₁₉,y₁₉,z₁₉,x₂₀,y₂₀,z₂₀,x₂₁,y₂₁,z₂₁,x₂₂, y₂₂,z₂₂,x₂₃,y₂₃,z₂₃,x₂₄,y₂₄,z₂₄,x₂₅,y₂₅,z₂₅,x₂₆,y₂₆,z₂₆</pre>

Triclinic primitive vectors

$$\begin{aligned}
 \mathbf{a}_1 &= a \hat{\mathbf{x}} \\
 \mathbf{a}_2 &= b \cos \gamma \hat{\mathbf{x}} + b \sin \gamma \hat{\mathbf{y}} \\
 \mathbf{a}_3 &= c_x \hat{\mathbf{x}} + c_y \hat{\mathbf{y}} + c_z \hat{\mathbf{z}} \\
 c_x &= c \cos \beta \\
 c_y &= c(\cos \alpha - \cos \beta \cos \gamma) / \sin \gamma \\
 c_z &= \sqrt{c^2 - c_x^2 - c_y^2}
 \end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$(ax_1 + by_1 \cos \gamma + c_x z_1) \hat{\mathbf{x}} + (by_1 \sin \gamma + c_y z_1) \hat{\mathbf{y}} + c_z z_1 \hat{\mathbf{z}}$	(1a)	C I
\mathbf{B}_2	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + by_2 \cos \gamma + c_x z_2) \hat{\mathbf{x}} + (by_2 \sin \gamma + c_y z_2) \hat{\mathbf{y}} + c_z z_2 \hat{\mathbf{z}}$	(1a)	C II
\mathbf{B}_3	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + by_3 \cos \gamma + c_x z_3) \hat{\mathbf{x}} + (by_3 \sin \gamma + c_y z_3) \hat{\mathbf{y}} + c_z z_3 \hat{\mathbf{z}}$	(1a)	C III
\mathbf{B}_4	$= x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + by_4 \cos \gamma + c_x z_4) \hat{\mathbf{x}} + (by_4 \sin \gamma + c_y z_4) \hat{\mathbf{y}} + c_z z_4 \hat{\mathbf{z}}$	(1a)	C IV
\mathbf{B}_5	$= x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + by_5 \cos \gamma + c_x z_5) \hat{\mathbf{x}} + (by_5 \sin \gamma + c_y z_5) \hat{\mathbf{y}} + c_z z_5 \hat{\mathbf{z}}$	(1a)	C V
\mathbf{B}_6	$= x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + by_6 \cos \gamma + c_x z_6) \hat{\mathbf{x}} + (by_6 \sin \gamma + c_y z_6) \hat{\mathbf{y}} + c_z z_6 \hat{\mathbf{z}}$	(1a)	H I
\mathbf{B}_7	$= x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + by_7 \cos \gamma + c_x z_7) \hat{\mathbf{x}} + (by_7 \sin \gamma + c_y z_7) \hat{\mathbf{y}} + c_z z_7 \hat{\mathbf{z}}$	(1a)	H II
\mathbf{B}_8	$= x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + by_8 \cos \gamma + c_x z_8) \hat{\mathbf{x}} + (by_8 \sin \gamma + c_y z_8) \hat{\mathbf{y}} + c_z z_8 \hat{\mathbf{z}}$	(1a)	H III
\mathbf{B}_9	$= x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$(ax_9 + by_9 \cos \gamma + c_x z_9) \hat{\mathbf{x}} + (by_9 \sin \gamma + c_y z_9) \hat{\mathbf{y}} + c_z z_9 \hat{\mathbf{z}}$	(1a)	H IV
\mathbf{B}_{10}	$= x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$(ax_{10} + by_{10} \cos \gamma + c_x z_{10}) \hat{\mathbf{x}} + (by_{10} \sin \gamma + c_y z_{10}) \hat{\mathbf{y}} + c_z z_{10} \hat{\mathbf{z}}$	(1a)	H V
\mathbf{B}_{11}	$= x_{11} \mathbf{a}_1 + y_{11} \mathbf{a}_2 + z_{11} \mathbf{a}_3$	$=$	$(ax_{11} + by_{11} \cos \gamma + c_x z_{11}) \hat{\mathbf{x}} + (by_{11} \sin \gamma + c_y z_{11}) \hat{\mathbf{y}} + c_z z_{11} \hat{\mathbf{z}}$	(1a)	H VI
\mathbf{B}_{12}	$= x_{12} \mathbf{a}_1 + y_{12} \mathbf{a}_2 + z_{12} \mathbf{a}_3$	$=$	$(ax_{12} + by_{12} \cos \gamma + c_x z_{12}) \hat{\mathbf{x}} + (by_{12} \sin \gamma + c_y z_{12}) \hat{\mathbf{y}} + c_z z_{12} \hat{\mathbf{z}}$	(1a)	H VII
\mathbf{B}_{13}	$= x_{13} \mathbf{a}_1 + y_{13} \mathbf{a}_2 + z_{13} \mathbf{a}_3$	$=$	$(ax_{13} + by_{13} \cos \gamma + c_x z_{13}) \hat{\mathbf{x}} + (by_{13} \sin \gamma + c_y z_{13}) \hat{\mathbf{y}} + c_z z_{13} \hat{\mathbf{z}}$	(1a)	H VIII
\mathbf{B}_{14}	$= x_{14} \mathbf{a}_1 + y_{14} \mathbf{a}_2 + z_{14} \mathbf{a}_3$	$=$	$(ax_{14} + by_{14} \cos \gamma + c_x z_{14}) \hat{\mathbf{x}} + (by_{14} \sin \gamma + c_y z_{14}) \hat{\mathbf{y}} + c_z z_{14} \hat{\mathbf{z}}$	(1a)	H IX
\mathbf{B}_{15}	$= x_{15} \mathbf{a}_1 + y_{15} \mathbf{a}_2 + z_{15} \mathbf{a}_3$	$=$	$(ax_{15} + by_{15} \cos \gamma + c_x z_{15}) \hat{\mathbf{x}} + (by_{15} \sin \gamma + c_y z_{15}) \hat{\mathbf{y}} + c_z z_{15} \hat{\mathbf{z}}$	(1a)	H X
\mathbf{B}_{16}	$= x_{16} \mathbf{a}_1 + y_{16} \mathbf{a}_2 + z_{16} \mathbf{a}_3$	$=$	$(ax_{16} + by_{16} \cos \gamma + c_x z_{16}) \hat{\mathbf{x}} + (by_{16} \sin \gamma + c_y z_{16}) \hat{\mathbf{y}} + c_z z_{16} \hat{\mathbf{z}}$	(1a)	H XI
\mathbf{B}_{17}	$= x_{17} \mathbf{a}_1 + y_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3$	$=$	$(ax_{17} + by_{17} \cos \gamma + c_x z_{17}) \hat{\mathbf{x}} + (by_{17} \sin \gamma + c_y z_{17}) \hat{\mathbf{y}} + c_z z_{17} \hat{\mathbf{z}}$	(1a)	Na I
\mathbf{B}_{18}	$= x_{18} \mathbf{a}_1 + y_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3$	$=$	$(ax_{18} + by_{18} \cos \gamma + c_x z_{18}) \hat{\mathbf{x}} + (by_{18} \sin \gamma + c_y z_{18}) \hat{\mathbf{y}} + c_z z_{18} \hat{\mathbf{z}}$	(1a)	O I
\mathbf{B}_{19}	$= x_{19} \mathbf{a}_1 + y_{19} \mathbf{a}_2 + z_{19} \mathbf{a}_3$	$=$	$(ax_{19} + by_{19} \cos \gamma + c_x z_{19}) \hat{\mathbf{x}} + (by_{19} \sin \gamma + c_y z_{19}) \hat{\mathbf{y}} + c_z z_{19} \hat{\mathbf{z}}$	(1a)	O II
\mathbf{B}_{20}	$= x_{20} \mathbf{a}_1 + y_{20} \mathbf{a}_2 + z_{20} \mathbf{a}_3$	$=$	$(ax_{20} + by_{20} \cos \gamma + c_x z_{20}) \hat{\mathbf{x}} + (by_{20} \sin \gamma + c_y z_{20}) \hat{\mathbf{y}} + c_z z_{20} \hat{\mathbf{z}}$	(1a)	O III
\mathbf{B}_{21}	$= x_{21} \mathbf{a}_1 + y_{21} \mathbf{a}_2 + z_{21} \mathbf{a}_3$	$=$	$(ax_{21} + by_{21} \cos \gamma + c_x z_{21}) \hat{\mathbf{x}} + (by_{21} \sin \gamma + c_y z_{21}) \hat{\mathbf{y}} + c_z z_{21} \hat{\mathbf{z}}$	(1a)	O IV
\mathbf{B}_{22}	$= x_{22} \mathbf{a}_1 + y_{22} \mathbf{a}_2 + z_{22} \mathbf{a}_3$	$=$	$(ax_{22} + by_{22} \cos \gamma + c_x z_{22}) \hat{\mathbf{x}} + (by_{22} \sin \gamma + c_y z_{22}) \hat{\mathbf{y}} + c_z z_{22} \hat{\mathbf{z}}$	(1a)	O V

$$\begin{aligned}
\mathbf{B}_{23} &= x_{23} \mathbf{a}_1 + y_{23} \mathbf{a}_2 + z_{23} \mathbf{a}_3 &= (ax_{23} + by_{23} \cos \gamma + c_x z_{23}) \hat{\mathbf{x}} + & (1a) & \text{O VI} \\
&&& (by_{23} \sin \gamma + c_y z_{23}) \hat{\mathbf{y}} + c_z z_{23} \hat{\mathbf{z}} \\
\mathbf{B}_{24} &= x_{24} \mathbf{a}_1 + y_{24} \mathbf{a}_2 + z_{24} \mathbf{a}_3 &= (ax_{24} + by_{24} \cos \gamma + c_x z_{24}) \hat{\mathbf{x}} + & (1a) & \text{O VII} \\
&&& (by_{24} \sin \gamma + c_y z_{24}) \hat{\mathbf{y}} + c_z z_{24} \hat{\mathbf{z}} \\
\mathbf{B}_{25} &= x_{25} \mathbf{a}_1 + y_{25} \mathbf{a}_2 + z_{25} \mathbf{a}_3 &= (ax_{25} + by_{25} \cos \gamma + c_x z_{25}) \hat{\mathbf{x}} + & (1a) & \text{O VIII} \\
&&& (by_{25} \sin \gamma + c_y z_{25}) \hat{\mathbf{y}} + c_z z_{25} \hat{\mathbf{z}} \\
\mathbf{B}_{26} &= x_{26} \mathbf{a}_1 + y_{26} \mathbf{a}_2 + z_{26} \mathbf{a}_3 &= (ax_{26} + by_{26} \cos \gamma + c_x z_{26}) \hat{\mathbf{x}} + & (1a) & \text{S I} \\
&&& (by_{26} \sin \gamma + c_y z_{26}) \hat{\mathbf{y}} + c_z z_{26} \hat{\mathbf{z}}
\end{aligned}$$

References

- [1] A. H. Haines and D. L. Hughes, *Crystal structure of sodium (1S)-D-lyxit-1-ylsulfonate* **72**, 628–631 (2016), doi:10.1107/S2056989016005375.