

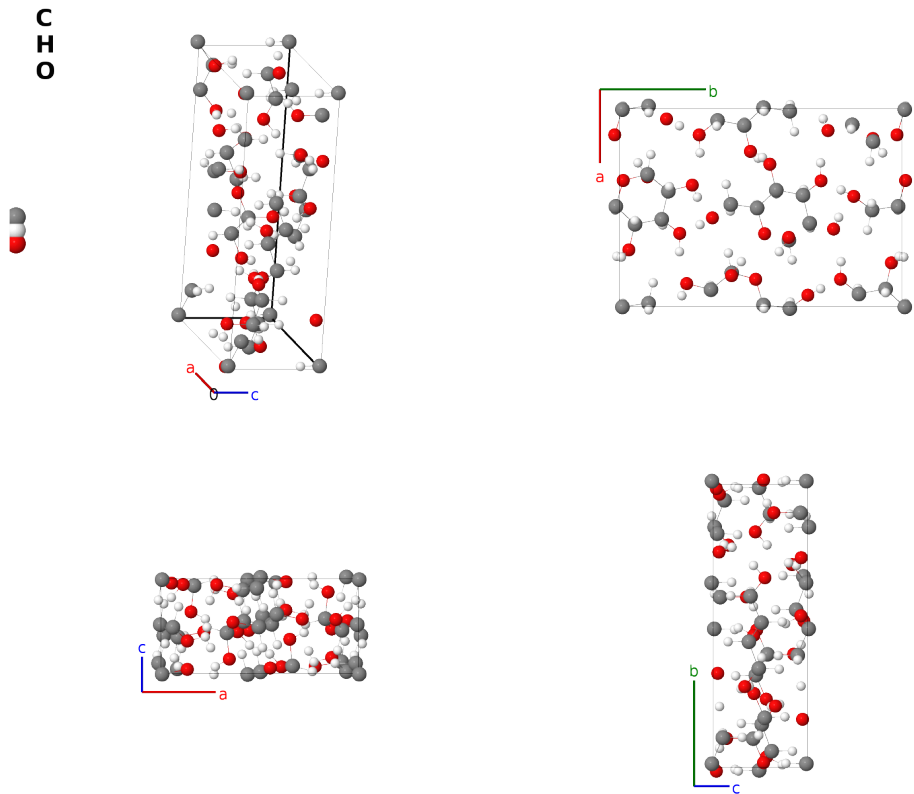
Anhydrous α -D-Glucose ($\text{C}_6\text{H}_{12}\text{O}_6$) Structure: AB2C_oP96_19_6a_12a_6a-001

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<https://aflow.org/prototype-encyclopedia/9N8P>

https://aflow.org/prototype-encyclopedia/AB2C_oP96_19_6a_12a_6a-001

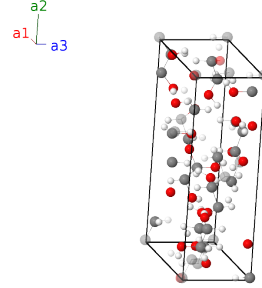


Prototype	CH_2O
AFLOW prototype label	AB2C_oP96_19_6a_12a_6a-001
Mineral name	α -D-glucose
CCDC	1169299
Pearson symbol	oP96
Space group number	19
Space group symbol	$P2_12_12_1$
AFLOW prototype command	<pre>aflow --proto=AB2C_oP96_19_6a_12a_6a-001 --params=a, b/a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, z3, x4, y4, z4, x5, y5, z5, x6, y6, z6, x7, y7, z7, x8, y8, z8, x9, y9, z9, 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</pre>

- Anhydrous glucose can be found in nature in two forms:
 - α -D-glucose (this structure),
 - β -D-glucose and
 - α -D-glucose monohydrate.
- This is a chiral compound.
- The “D” indicates that a solution of this form of glucose will rotate polarized light to the right, while the “L” type rotates light to the left.
- Only D-glucose is found in nature, but the L-type can be synthesized.
- As α -L-glucose is the enantiomer of α -D-glucose its structure should be a mirror image of this one, but we have not been able to find a report of its structure.
- α - and β -D-glucose have the same AFLOW prototype label, AB2C_oP96_19_6a_12a_6a. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

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
$\mathbf{B}_1$	$= x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$ax_1 \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	$(4a)$		C I
$\mathbf{B}_2$	$= -\left(x_1 - \frac{1}{2}\right) \mathbf{a}_1 - y_1 \mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_1 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right) \hat{\mathbf{z}}$	$(4a)$		C I
$\mathbf{B}_3$	$= -x_1 \mathbf{a}_1 + \left(y_1 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} + b\left(y_1 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right) \hat{\mathbf{z}}$	$(4a)$		C I
$\mathbf{B}_4$	$= \left(x_1 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_1 - \frac{1}{2}\right) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$a\left(x_1 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_1 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_1 \hat{\mathbf{z}}$	$(4a)$		C I
$\mathbf{B}_5$	$= x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$ax_2 \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	$(4a)$		C II
$\mathbf{B}_6$	$= -\left(x_2 - \frac{1}{2}\right) \mathbf{a}_1 - y_2 \mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_2 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right) \hat{\mathbf{z}}$	$(4a)$		C II
$\mathbf{B}_7$	$= -x_2 \mathbf{a}_1 + \left(y_2 + \frac{1}{2}\right) \mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} + b\left(y_2 + \frac{1}{2}\right) \hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right) \hat{\mathbf{z}}$	$(4a)$		C II
$\mathbf{B}_8$	$= \left(x_2 + \frac{1}{2}\right) \mathbf{a}_1 - \left(y_2 - \frac{1}{2}\right) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$a\left(x_2 + \frac{1}{2}\right) \hat{\mathbf{x}} - b\left(y_2 - \frac{1}{2}\right) \hat{\mathbf{y}} - cz_2 \hat{\mathbf{z}}$	$(4a)$		C II
$\mathbf{B}_9$	$= x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$ax_3 \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	$(4a)$		C III
$\mathbf{B}_{10}$	$= -\left(x_3 - \frac{1}{2}\right) \mathbf{a}_1 - y_3 \mathbf{a}_2 + \left(z_3 + \frac{1}{2}\right) \mathbf{a}_3$	$=$	$-a\left(x_3 - \frac{1}{2}\right) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c\left(z_3 + \frac{1}{2}\right) \hat{\mathbf{z}}$	$(4a)$		C III

$\mathbf{B}_{11} =$	$-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-ax_3 \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	C III
	$(z_3 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{12} =$	$(x_3 + \frac{1}{2}) \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \hat{\mathbf{z}}$	(4a)	C III
$\mathbf{B}_{13} =$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$ax_4 \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4a)	C IV
$\mathbf{B}_{14} =$	$-(x_4 - \frac{1}{2}) \mathbf{a}_1 - y_4 \mathbf{a}_2 +$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	C IV
	$(z_4 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{15} =$	$-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-ax_4 \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	C IV
	$(z_4 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{16} =$	$(x_4 + \frac{1}{2}) \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4a)	C IV
$\mathbf{B}_{17} =$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$ax_5 \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4a)	C V
$\mathbf{B}_{18} =$	$-(x_5 - \frac{1}{2}) \mathbf{a}_1 - y_5 \mathbf{a}_2 +$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	C V
	$(z_5 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{19} =$	$-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-ax_5 \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	C V
	$(z_5 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{20} =$	$(x_5 + \frac{1}{2}) \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4a)	C V
$\mathbf{B}_{21} =$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$ax_6 \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4a)	C VI
$\mathbf{B}_{22} =$	$-(x_6 - \frac{1}{2}) \mathbf{a}_1 - y_6 \mathbf{a}_2 +$	$=$	$-a(x_6 - \frac{1}{2}) \hat{\mathbf{x}} - by_6 \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	C VI
	$(z_6 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{23} =$	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-ax_6 \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	C VI
	$(z_6 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{24} =$	$(x_6 + \frac{1}{2}) \mathbf{a}_1 - (y_6 - \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$a(x_6 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_6 - \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4a)	C VI
$\mathbf{B}_{25} =$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$ax_7 \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4a)	H I
$\mathbf{B}_{26} =$	$-(x_7 - \frac{1}{2}) \mathbf{a}_1 - y_7 \mathbf{a}_2 +$	$=$	$-a(x_7 - \frac{1}{2}) \hat{\mathbf{x}} - by_7 \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	H I
	$(z_7 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{27} =$	$-x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-ax_7 \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	H I
	$(z_7 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{28} =$	$(x_7 + \frac{1}{2}) \mathbf{a}_1 - (y_7 - \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$a(x_7 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_7 - \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(4a)	H I
$\mathbf{B}_{29} =$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$ax_8 \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(4a)	H II
$\mathbf{B}_{30} =$	$-(x_8 - \frac{1}{2}) \mathbf{a}_1 - y_8 \mathbf{a}_2 +$	$=$	$-a(x_8 - \frac{1}{2}) \hat{\mathbf{x}} - by_8 \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	H II
	$(z_8 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{31} =$	$-x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-ax_8 \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	H II
	$(z_8 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{32} =$	$(x_8 + \frac{1}{2}) \mathbf{a}_1 - (y_8 - \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$a(x_8 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_8 - \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(4a)	H II
$\mathbf{B}_{33} =$	$x_9 \mathbf{a}_1 + y_9 \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$ax_9 \hat{\mathbf{x}} + by_9 \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(4a)	H III
$\mathbf{B}_{34} =$	$-(x_9 - \frac{1}{2}) \mathbf{a}_1 - y_9 \mathbf{a}_2 +$	$=$	$-a(x_9 - \frac{1}{2}) \hat{\mathbf{x}} - by_9 \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	H III
	$(z_9 + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{35} =$	$-x_9 \mathbf{a}_1 + (y_9 + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-ax_9 \hat{\mathbf{x}} + b(y_9 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	H III
	$(z_9 - \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{36} =$	$(x_9 + \frac{1}{2}) \mathbf{a}_1 - (y_9 - \frac{1}{2}) \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$a(x_9 + \frac{1}{2}) \hat{\mathbf{x}} - b(y_9 - \frac{1}{2}) \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(4a)	H III
$\mathbf{B}_{37} =$	$x_{10} \mathbf{a}_1 + y_{10} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$ax_{10} \hat{\mathbf{x}} + by_{10} \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(4a)	H IV
$\mathbf{B}_{38} =$	$-(x_{10} - \frac{1}{2}) \mathbf{a}_1 - y_{10} \mathbf{a}_2 +$	$=$	$-a(x_{10} - \frac{1}{2}) \hat{\mathbf{x}} - by_{10} \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	H IV
	$(z_{10} + \frac{1}{2}) \mathbf{a}_3$				
$\mathbf{B}_{39} =$	$-x_{10} \mathbf{a}_1 + (y_{10} + \frac{1}{2}) \mathbf{a}_2 -$	$=$	$-ax_{10} \hat{\mathbf{x}} + b(y_{10} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	H IV
	$(z_{10} - \frac{1}{2}) \mathbf{a}_3$				

$$\begin{aligned}
\mathbf{B}_{92} &= \begin{pmatrix} x_{23} + \frac{1}{2} \\ z_{23} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_{23} - \frac{1}{2} \\ \mathbf{a}_3 \end{pmatrix} \mathbf{a}_2 - &= & a \left(x_{23} + \frac{1}{2} \right) \hat{\mathbf{x}} - b \left(y_{23} - \frac{1}{2} \right) \hat{\mathbf{y}} - cz_{23} \hat{\mathbf{z}} & (4a) & \text{O V} \\
\mathbf{B}_{93} &= x_{24} \mathbf{a}_1 + y_{24} \mathbf{a}_2 + z_{24} \mathbf{a}_3 &= & ax_{24} \hat{\mathbf{x}} + by_{24} \hat{\mathbf{y}} + cz_{24} \hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B}_{94} &= \begin{pmatrix} -\left(x_{24} - \frac{1}{2}\right) \\ z_{24} + \frac{1}{2} \end{pmatrix} \mathbf{a}_1 - y_{24} \mathbf{a}_2 + &= & -a \left(x_{24} - \frac{1}{2} \right) \hat{\mathbf{x}} - by_{24} \hat{\mathbf{y}} + c \left(z_{24} + \frac{1}{2} \right) \hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B}_{95} &= \begin{pmatrix} -x_{24} \\ z_{24} - \frac{1}{2} \end{pmatrix} \mathbf{a}_1 + \begin{pmatrix} y_{24} + \frac{1}{2} \\ \mathbf{a}_3 \end{pmatrix} \mathbf{a}_2 - &= & -ax_{24} \hat{\mathbf{x}} + b \left(y_{24} + \frac{1}{2} \right) \hat{\mathbf{y}} - c \left(z_{24} - \frac{1}{2} \right) \hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B}_{96} &= \begin{pmatrix} x_{24} + \frac{1}{2} \\ z_{24} \end{pmatrix} \mathbf{a}_1 - \begin{pmatrix} y_{24} - \frac{1}{2} \\ \mathbf{a}_3 \end{pmatrix} \mathbf{a}_2 - &= & a \left(x_{24} + \frac{1}{2} \right) \hat{\mathbf{x}} - b \left(y_{24} - \frac{1}{2} \right) \hat{\mathbf{y}} - cz_{24} \hat{\mathbf{z}} & (4a) & \text{O VI}
\end{aligned}$$

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