

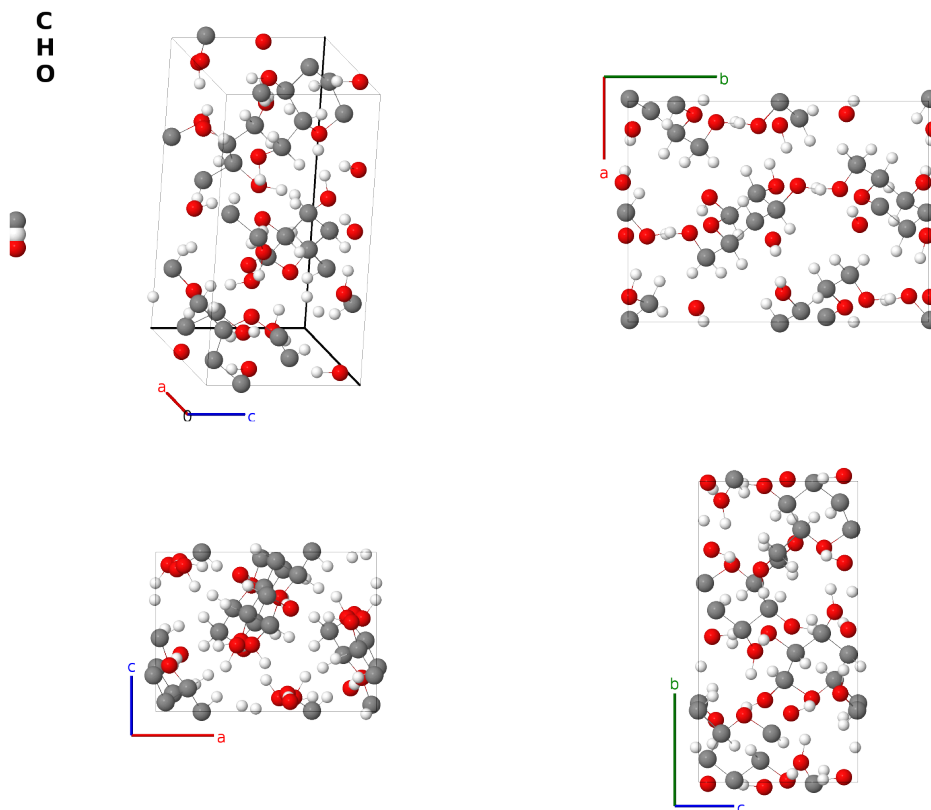
Anhydrous β -D-Glucose ($\text{C}_6\text{H}_{12}\text{O}_6$) Structure: AB2C_oP96_19_6a_12a_6a-002

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<https://aflow.org/prototype-encyclopedia/S0D9>

https://aflow.org/prototype-encyclopedia/AB2C_oP96_19_6a_12a_6a-002

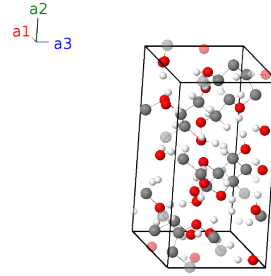


Prototype	CH_2O
AFLOW prototype label	AB2C_oP96_19_6a_12a_6a-002
Mineral name	β -D-glucose
CCDC	1169300
Pearson symbol	oP96
Space group number	19
Space group symbol	$P2_12_12_1$
AFLOW prototype command	<pre>aflow --proto=AB2C_oP96_19_6a_12a_6a-002 --params=a, b/a, c/a, x1, y1, z1, x2, y2, z2, x3, y3, 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 and
 - β -D-glucose (this structure), 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 β -L-glucose is the enantiomer of β -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.
- The hydrogen positions were approximated assuming an O-H bond length of 1Å and knowledge of hydrogen bonding.

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

$\mathbf{B}_{65} =$	$x_{17} \mathbf{a}_1 + y_{17} \mathbf{a}_2 + z_{17} \mathbf{a}_3$	$=$	$ax_{17} \hat{\mathbf{x}} + by_{17} \hat{\mathbf{y}} + cz_{17} \hat{\mathbf{z}}$	(4a)	H XI
$\mathbf{B}_{66} =$	$-(x_{17} - \frac{1}{2}) \mathbf{a}_1 - y_{17} \mathbf{a}_2 +$ $(z_{17} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{17} - \frac{1}{2}) \hat{\mathbf{x}} - by_{17} \hat{\mathbf{y}} + c(z_{17} + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	H XI
$\mathbf{B}_{67} =$	$-x_{17} \mathbf{a}_1 + (y_{17} + \frac{1}{2}) \mathbf{a}_2 -$ $(z_{17} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{17} \hat{\mathbf{x}} + b(y_{17} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{17} - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	H XI
$\mathbf{B}_{68} =$	$(x_{17} + \frac{1}{2}) \mathbf{a}_1 - (y_{17} - \frac{1}{2}) \mathbf{a}_2 -$ $z_{17} \mathbf{a}_3$	$=$	$a(x_{17} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{17} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{17} \hat{\mathbf{z}}$	(4a)	H XI
$\mathbf{B}_{69} =$	$x_{18} \mathbf{a}_1 + y_{18} \mathbf{a}_2 + z_{18} \mathbf{a}_3$	$=$	$ax_{18} \hat{\mathbf{x}} + by_{18} \hat{\mathbf{y}} + cz_{18} \hat{\mathbf{z}}$	(4a)	H XII
$\mathbf{B}_{70} =$	$-(x_{18} - \frac{1}{2}) \mathbf{a}_1 - y_{18} \mathbf{a}_2 +$ $(z_{18} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{18} - \frac{1}{2}) \hat{\mathbf{x}} - by_{18} \hat{\mathbf{y}} + c(z_{18} + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	H XII
$\mathbf{B}_{71} =$	$-x_{18} \mathbf{a}_1 + (y_{18} + \frac{1}{2}) \mathbf{a}_2 -$ $(z_{18} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{18} \hat{\mathbf{x}} + b(y_{18} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{18} - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	H XII
$\mathbf{B}_{72} =$	$(x_{18} + \frac{1}{2}) \mathbf{a}_1 - (y_{18} - \frac{1}{2}) \mathbf{a}_2 -$ $z_{18} \mathbf{a}_3$	$=$	$a(x_{18} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{18} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{18} \hat{\mathbf{z}}$	(4a)	H XII
$\mathbf{B}_{73} =$	$x_{19} \mathbf{a}_1 + y_{19} \mathbf{a}_2 + z_{19} \mathbf{a}_3$	$=$	$ax_{19} \hat{\mathbf{x}} + by_{19} \hat{\mathbf{y}} + cz_{19} \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_{74} =$	$-(x_{19} - \frac{1}{2}) \mathbf{a}_1 - y_{19} \mathbf{a}_2 +$ $(z_{19} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{19} - \frac{1}{2}) \hat{\mathbf{x}} - by_{19} \hat{\mathbf{y}} + c(z_{19} + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_{75} =$	$-x_{19} \mathbf{a}_1 + (y_{19} + \frac{1}{2}) \mathbf{a}_2 -$ $(z_{19} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{19} \hat{\mathbf{x}} + b(y_{19} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{19} - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_{76} =$	$(x_{19} + \frac{1}{2}) \mathbf{a}_1 - (y_{19} - \frac{1}{2}) \mathbf{a}_2 -$ $z_{19} \mathbf{a}_3$	$=$	$a(x_{19} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{19} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{19} \hat{\mathbf{z}}$	(4a)	O I
$\mathbf{B}_{77} =$	$x_{20} \mathbf{a}_1 + y_{20} \mathbf{a}_2 + z_{20} \mathbf{a}_3$	$=$	$ax_{20} \hat{\mathbf{x}} + by_{20} \hat{\mathbf{y}} + cz_{20} \hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B}_{78} =$	$-(x_{20} - \frac{1}{2}) \mathbf{a}_1 - y_{20} \mathbf{a}_2 +$ $(z_{20} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{20} - \frac{1}{2}) \hat{\mathbf{x}} - by_{20} \hat{\mathbf{y}} + c(z_{20} + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B}_{79} =$	$-x_{20} \mathbf{a}_1 + (y_{20} + \frac{1}{2}) \mathbf{a}_2 -$ $(z_{20} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{20} \hat{\mathbf{x}} + b(y_{20} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{20} - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B}_{80} =$	$(x_{20} + \frac{1}{2}) \mathbf{a}_1 - (y_{20} - \frac{1}{2}) \mathbf{a}_2 -$ $z_{20} \mathbf{a}_3$	$=$	$a(x_{20} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{20} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{20} \hat{\mathbf{z}}$	(4a)	O II
$\mathbf{B}_{81} =$	$x_{21} \mathbf{a}_1 + y_{21} \mathbf{a}_2 + z_{21} \mathbf{a}_3$	$=$	$ax_{21} \hat{\mathbf{x}} + by_{21} \hat{\mathbf{y}} + cz_{21} \hat{\mathbf{z}}$	(4a)	O III
$\mathbf{B}_{82} =$	$-(x_{21} - \frac{1}{2}) \mathbf{a}_1 - y_{21} \mathbf{a}_2 +$ $(z_{21} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{21} - \frac{1}{2}) \hat{\mathbf{x}} - by_{21} \hat{\mathbf{y}} + c(z_{21} + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O III
$\mathbf{B}_{83} =$	$-x_{21} \mathbf{a}_1 + (y_{21} + \frac{1}{2}) \mathbf{a}_2 -$ $(z_{21} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{21} \hat{\mathbf{x}} + b(y_{21} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{21} - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O III
$\mathbf{B}_{84} =$	$(x_{21} + \frac{1}{2}) \mathbf{a}_1 - (y_{21} - \frac{1}{2}) \mathbf{a}_2 -$ $z_{21} \mathbf{a}_3$	$=$	$a(x_{21} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{21} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{21} \hat{\mathbf{z}}$	(4a)	O III
$\mathbf{B}_{85} =$	$x_{22} \mathbf{a}_1 + y_{22} \mathbf{a}_2 + z_{22} \mathbf{a}_3$	$=$	$ax_{22} \hat{\mathbf{x}} + by_{22} \hat{\mathbf{y}} + cz_{22} \hat{\mathbf{z}}$	(4a)	O IV
$\mathbf{B}_{86} =$	$-(x_{22} - \frac{1}{2}) \mathbf{a}_1 - y_{22} \mathbf{a}_2 +$ $(z_{22} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{22} - \frac{1}{2}) \hat{\mathbf{x}} - by_{22} \hat{\mathbf{y}} + c(z_{22} + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O IV
$\mathbf{B}_{87} =$	$-x_{22} \mathbf{a}_1 + (y_{22} + \frac{1}{2}) \mathbf{a}_2 -$ $(z_{22} - \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_{22} \hat{\mathbf{x}} + b(y_{22} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{22} - \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O IV
$\mathbf{B}_{88} =$	$(x_{22} + \frac{1}{2}) \mathbf{a}_1 - (y_{22} - \frac{1}{2}) \mathbf{a}_2 -$ $z_{22} \mathbf{a}_3$	$=$	$a(x_{22} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{22} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{22} \hat{\mathbf{z}}$	(4a)	O IV
$\mathbf{B}_{89} =$	$x_{23} \mathbf{a}_1 + y_{23} \mathbf{a}_2 + z_{23} \mathbf{a}_3$	$=$	$ax_{23} \hat{\mathbf{x}} + by_{23} \hat{\mathbf{y}} + cz_{23} \hat{\mathbf{z}}$	(4a)	O V
$\mathbf{B}_{90} =$	$-(x_{23} - \frac{1}{2}) \mathbf{a}_1 - y_{23} \mathbf{a}_2 +$ $(z_{23} + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_{23} - \frac{1}{2}) \hat{\mathbf{x}} - by_{23} \hat{\mathbf{y}} + c(z_{23} + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	O V

$$\begin{aligned}
\mathbf{B}_{91} &= \begin{matrix} -x_{23} \mathbf{a}_1 + (y_{23} + \frac{1}{2}) \mathbf{a}_2 - \\ (z_{23} - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ax_{23} \hat{\mathbf{x}} + b(y_{23} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{23} - \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O V} \\
\mathbf{B}_{92} &= \begin{matrix} (x_{23} + \frac{1}{2}) \mathbf{a}_1 - (y_{23} - \frac{1}{2}) \mathbf{a}_2 - \\ z_{23} \mathbf{a}_3 \end{matrix} = a(x_{23} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{23} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{23} \hat{\mathbf{z}} & (4a) & \text{O V} \\
\mathbf{B}_{93} &= x_{24} \mathbf{a}_1 + y_{24} \mathbf{a}_2 + z_{24} \mathbf{a}_3 = ax_{24} \hat{\mathbf{x}} + by_{24} \hat{\mathbf{y}} + cz_{24} \hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B}_{94} &= \begin{matrix} -(x_{24} - \frac{1}{2}) \mathbf{a}_1 - y_{24} \mathbf{a}_2 + \\ (z_{24} + \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -a(x_{24} - \frac{1}{2}) \hat{\mathbf{x}} - by_{24} \hat{\mathbf{y}} + c(z_{24} + \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B}_{95} &= \begin{matrix} -x_{24} \mathbf{a}_1 + (y_{24} + \frac{1}{2}) \mathbf{a}_2 - \\ (z_{24} - \frac{1}{2}) \mathbf{a}_3 \end{matrix} = -ax_{24} \hat{\mathbf{x}} + b(y_{24} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{24} - \frac{1}{2}) \hat{\mathbf{z}} & (4a) & \text{O VI} \\
\mathbf{B}_{96} &= \begin{matrix} (x_{24} + \frac{1}{2}) \mathbf{a}_1 - (y_{24} - \frac{1}{2}) \mathbf{a}_2 - \\ z_{24} \mathbf{a}_3 \end{matrix} = a(x_{24} + \frac{1}{2}) \hat{\mathbf{x}} - b(y_{24} - \frac{1}{2}) \hat{\mathbf{y}} - cz_{24} \hat{\mathbf{z}} & (4a) & \text{O VI}
\end{aligned}$$

References

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