

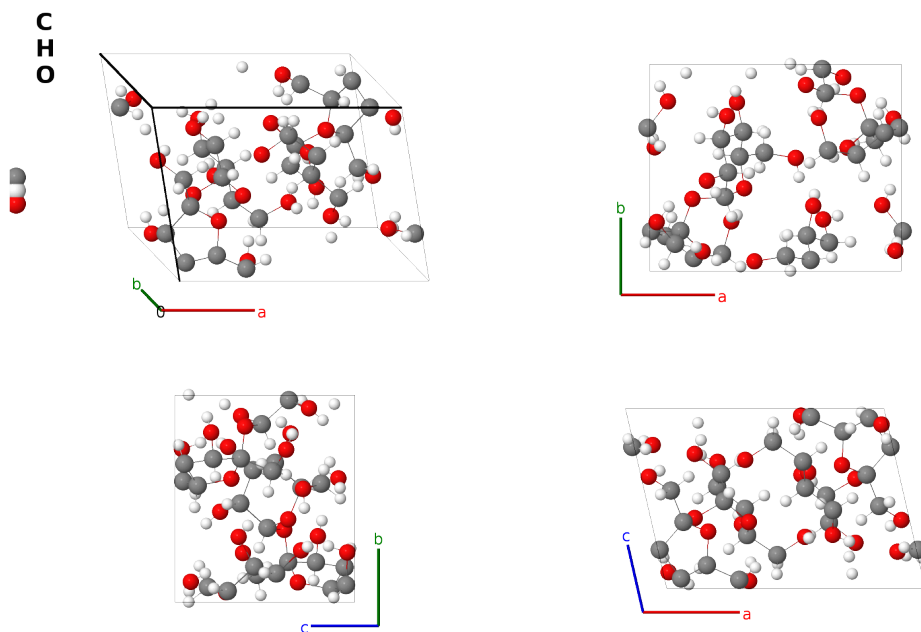
D-Sucrose ($C_{12}H_{22}O_{11}$) Structure: A12B22C11_mP90_4_12a_22a_11a-001

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<https://aflow.org/prototype-encyclopedia/PFH2>

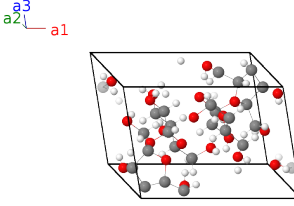
https://aflow.org/prototype-encyclopedia/A12B22C11_mP90_4_12a_22a_11a-001



Prototype	$C_{12}H_{22}O_{11}$
AFLOW prototype label	A12B22C11_mP90_4_12a_22a_11a-001
Mineral name	D-sucrose
CCDC	1263571
Pearson symbol	mP90
Space group number	4
Space group symbol	$P2_1$
AFLOW prototype command	<pre> aflow --proto=A12B22C11_mP90_4_12a_22a_11a-001 --params=a,b/a,c/a,β,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,x_{10},y_{10},z_{10},x_{11},y_{11},z_{11},x_{12},y_{12},z_{12},x_{13},y_{13},z_{13},x_{14},y_{14},z_{14},x_{15}, y_{15},z_{15},x_{16},y_{16},z_{16},x_{17},y_{17},z_{17},x_{18},y_{18},z_{18},x_{19},y_{19},z_{19},x_{20},y_{20},z_{20},x_{21},y_{21},z_{21},x_{22},y_{22}, z_{22},x_{23},y_{23},z_{23},x_{24},y_{24},z_{24},x_{25},y_{25},z_{25},x_{26},y_{26},z_{26},x_{27},y_{27},z_{27},x_{28},y_{28},z_{28},x_{29},y_{29},z_{29}, x_{30},y_{30},z_{30},x_{31},y_{31},z_{31},x_{32},y_{32},z_{32},x_{33},y_{33},z_{33},x_{34},y_{34},z_{34},x_{35},y_{35},z_{35},x_{36},y_{36},z_{36},x_{37}, y_{37},z_{37},x_{38},y_{38},z_{38},x_{39},y_{39},z_{39},x_{40},y_{40},z_{40},x_{41},y_{41},z_{41},x_{42},y_{42},z_{42},x_{43},y_{43},z_{43},x_{44},y_{44}, z_{44},x_{45},y_{45},z_{45} </pre>

- The full name of this compound is β -D-Fructofuranosyl α -D-glucopyranoside. It is a dextrorotatory compound composed of a fructose molecule and a glucose molecule, both $C_6H_{12}O_6$, which share one oxygen atom and shed two hydrogen atoms, making the stoichiometry $C_{12}H_{22}O_{11}$.
- Since this is a chiral compound, we could invert the structure, taking $(x, y, z) \rightarrow (-x, -y, -z)$ and transforming D-sucrose into its enantiomer, L-sucrose (β -L-Fructofuranosyl α -L-glucopyranoside) which would be levorotatory. Only D-sucrose is found in biological systems.
- We use the data in Table 4 of (Hanson, 1973).

Simple Monoclinic primitive vectors

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


Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(2a)	C I
$\mathbf{B}_2$	$-x_1 \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 - z_1 \mathbf{a}_3$	$=$	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(2a)	C I
$\mathbf{B}_3$	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(2a)	C II
$\mathbf{B}_4$	$-x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - z_2 \mathbf{a}_3$	$=$	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(2a)	C II
$\mathbf{B}_5$	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(2a)	C III
$\mathbf{B}_6$	$-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - z_3 \mathbf{a}_3$	$=$	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(2a)	C III
$\mathbf{B}_7$	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(2a)	C IV
$\mathbf{B}_8$	$-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(2a)	C IV
$\mathbf{B}_9$	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(2a)	C V
$\mathbf{B}_{10}$	$-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(2a)	C V
$\mathbf{B}_{11}$	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(2a)	C VI
$\mathbf{B}_{12}$	$-x_6 \mathbf{a}_1 + (y_6 + \frac{1}{2}) \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$-(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + b(y_6 + \frac{1}{2}) \hat{\mathbf{y}} - cz_6 \sin \beta \hat{\mathbf{z}}$	(2a)	C VI
$\mathbf{B}_{13}$	$x_7 \mathbf{a}_1 + y_7 \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + by_7 \hat{\mathbf{y}} + cz_7 \sin \beta \hat{\mathbf{z}}$	(2a)	C VII
$\mathbf{B}_{14}$	$-x_7 \mathbf{a}_1 + (y_7 + \frac{1}{2}) \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$-(ax_7 + cz_7 \cos \beta) \hat{\mathbf{x}} + b(y_7 + \frac{1}{2}) \hat{\mathbf{y}} - cz_7 \sin \beta \hat{\mathbf{z}}$	(2a)	C VII
$\mathbf{B}_{15}$	$x_8 \mathbf{a}_1 + y_8 \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + by_8 \hat{\mathbf{y}} + cz_8 \sin \beta \hat{\mathbf{z}}$	(2a)	C VIII
$\mathbf{B}_{16}$	$-x_8 \mathbf{a}_1 + (y_8 + \frac{1}{2}) \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$-(ax_8 + cz_8 \cos \beta) \hat{\mathbf{x}} + b(y_8 + \frac{1}{2}) \hat{\mathbf{y}} - cz_8 \sin \beta \hat{\mathbf{z}}$	(2a)	C VIII

$$\begin{aligned}
\mathbf{B}_{77} &= x_{39} \mathbf{a}_1 + y_{39} \mathbf{a}_2 + z_{39} \mathbf{a}_3 &= (ax_{39} + cz_{39} \cos \beta) \hat{\mathbf{x}} + by_{39} \hat{\mathbf{y}} + cz_{39} \sin \beta \hat{\mathbf{z}} &(2a) &\text{O V} \\
\mathbf{B}_{78} &= -x_{39} \mathbf{a}_1 + \left(y_{39} + \frac{1}{2}\right) \mathbf{a}_2 - z_{39} \mathbf{a}_3 &= -(ax_{39} + cz_{39} \cos \beta) \hat{\mathbf{x}} + b \left(y_{39} + \frac{1}{2}\right) \hat{\mathbf{y}} - &(2a) &\text{O V} \\
&&& cz_{39} \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{79} &= x_{40} \mathbf{a}_1 + y_{40} \mathbf{a}_2 + z_{40} \mathbf{a}_3 &= (ax_{40} + cz_{40} \cos \beta) \hat{\mathbf{x}} + by_{40} \hat{\mathbf{y}} + cz_{40} \sin \beta \hat{\mathbf{z}} &(2a) &\text{O VI} \\
\mathbf{B}_{80} &= -x_{40} \mathbf{a}_1 + \left(y_{40} + \frac{1}{2}\right) \mathbf{a}_2 - z_{40} \mathbf{a}_3 &= -(ax_{40} + cz_{40} \cos \beta) \hat{\mathbf{x}} + b \left(y_{40} + \frac{1}{2}\right) \hat{\mathbf{y}} - &(2a) &\text{O VI} \\
&&& cz_{40} \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{81} &= x_{41} \mathbf{a}_1 + y_{41} \mathbf{a}_2 + z_{41} \mathbf{a}_3 &= (ax_{41} + cz_{41} \cos \beta) \hat{\mathbf{x}} + by_{41} \hat{\mathbf{y}} + cz_{41} \sin \beta \hat{\mathbf{z}} &(2a) &\text{O VII} \\
\mathbf{B}_{82} &= -x_{41} \mathbf{a}_1 + \left(y_{41} + \frac{1}{2}\right) \mathbf{a}_2 - z_{41} \mathbf{a}_3 &= -(ax_{41} + cz_{41} \cos \beta) \hat{\mathbf{x}} + b \left(y_{41} + \frac{1}{2}\right) \hat{\mathbf{y}} - &(2a) &\text{O VII} \\
&&& cz_{41} \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{83} &= x_{42} \mathbf{a}_1 + y_{42} \mathbf{a}_2 + z_{42} \mathbf{a}_3 &= (ax_{42} + cz_{42} \cos \beta) \hat{\mathbf{x}} + by_{42} \hat{\mathbf{y}} + cz_{42} \sin \beta \hat{\mathbf{z}} &(2a) &\text{O VIII} \\
\mathbf{B}_{84} &= -x_{42} \mathbf{a}_1 + \left(y_{42} + \frac{1}{2}\right) \mathbf{a}_2 - z_{42} \mathbf{a}_3 &= -(ax_{42} + cz_{42} \cos \beta) \hat{\mathbf{x}} + b \left(y_{42} + \frac{1}{2}\right) \hat{\mathbf{y}} - &(2a) &\text{O VIII} \\
&&& cz_{42} \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{85} &= x_{43} \mathbf{a}_1 + y_{43} \mathbf{a}_2 + z_{43} \mathbf{a}_3 &= (ax_{43} + cz_{43} \cos \beta) \hat{\mathbf{x}} + by_{43} \hat{\mathbf{y}} + cz_{43} \sin \beta \hat{\mathbf{z}} &(2a) &\text{O IX} \\
\mathbf{B}_{86} &= -x_{43} \mathbf{a}_1 + \left(y_{43} + \frac{1}{2}\right) \mathbf{a}_2 - z_{43} \mathbf{a}_3 &= -(ax_{43} + cz_{43} \cos \beta) \hat{\mathbf{x}} + b \left(y_{43} + \frac{1}{2}\right) \hat{\mathbf{y}} - &(2a) &\text{O IX} \\
&&& cz_{43} \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{87} &= x_{44} \mathbf{a}_1 + y_{44} \mathbf{a}_2 + z_{44} \mathbf{a}_3 &= (ax_{44} + cz_{44} \cos \beta) \hat{\mathbf{x}} + by_{44} \hat{\mathbf{y}} + cz_{44} \sin \beta \hat{\mathbf{z}} &(2a) &\text{O X} \\
\mathbf{B}_{88} &= -x_{44} \mathbf{a}_1 + \left(y_{44} + \frac{1}{2}\right) \mathbf{a}_2 - z_{44} \mathbf{a}_3 &= -(ax_{44} + cz_{44} \cos \beta) \hat{\mathbf{x}} + b \left(y_{44} + \frac{1}{2}\right) \hat{\mathbf{y}} - &(2a) &\text{O X} \\
&&& cz_{44} \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{89} &= x_{45} \mathbf{a}_1 + y_{45} \mathbf{a}_2 + z_{45} \mathbf{a}_3 &= (ax_{45} + cz_{45} \cos \beta) \hat{\mathbf{x}} + by_{45} \hat{\mathbf{y}} + cz_{45} \sin \beta \hat{\mathbf{z}} &(2a) &\text{O XI} \\
\mathbf{B}_{90} &= -x_{45} \mathbf{a}_1 + \left(y_{45} + \frac{1}{2}\right) \mathbf{a}_2 - z_{45} \mathbf{a}_3 &= -(ax_{45} + cz_{45} \cos \beta) \hat{\mathbf{x}} + b \left(y_{45} + \frac{1}{2}\right) \hat{\mathbf{y}} - &(2a) &\text{O XI} \\
&&& cz_{45} \sin \beta \hat{\mathbf{z}}
\end{aligned}$$

References

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