

α -Toluene (C₇H₈) Structure: A7B8_mP120_14_14e_16e-001

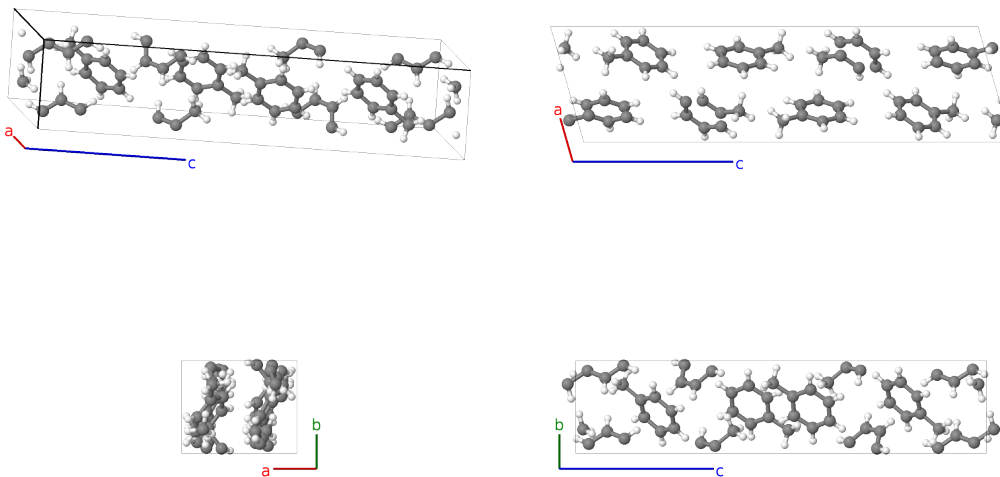
This structure originally had the label A7B8_mP120_14_14e_16e. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

<https://aflow.org/p/NQ3P>

https://aflow.org/p/A7B8_mP120_14_14e_16e-001

● C
● H

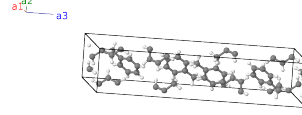


Prototype	C ₇ H ₈
AFLOW prototype label	A7B8_mP120_14_14e_16e-001
Mineral name	toluene
ICSD	none
CCDC	725245
Pearson symbol	mP120
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	<pre>aflow --proto=A7B8_mP120_14_14e_16e-001 --params=a,b/a,c/a,β,x₁,y₁,z₁,x₂,y₂,z₂,x₃,y₃,z₃,x₄,y₄,z₄,x₅,y₅,z₅,x₆,y₆,z₆,x₇, 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,x₂₇,y₂₇,z₂₇,x₂₈,y₂₈,z₂₈,x₂₉,y₂₉,z₂₉, x₃₀,y₃₀,z₃₀</pre>

- α -Toluene is the stable low-temperature crystalline structure of the toluene molecule, C_7H_8 , which crystallizes below 178K. This data was constructed from experiments at 150K. The hydrogen atomic positions were approximated to agree with the chemistry of the toluene molecule.
- There is also a metastable form, β -toluene.

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	$x_1 \mathbf{a}_1 + y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	=	$(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + cz_1 \sin \beta \hat{\mathbf{z}}$	(4e)	C I
\mathbf{B}_2	$-x_1 \mathbf{a}_1 + (y_1 + \frac{1}{2}) \mathbf{a}_2 - (z_1 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_1 + c(z_1 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_1 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_1 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C I
\mathbf{B}_3	$-x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 - z_1 \mathbf{a}_3$	=	$-(ax_1 + cz_1 \cos \beta) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} - cz_1 \sin \beta \hat{\mathbf{z}}$	(4e)	C I
\mathbf{B}_4	$x_1 \mathbf{a}_1 - (y_1 - \frac{1}{2}) \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_1 + c(z_1 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_1 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C I
\mathbf{B}_5	$x_2 \mathbf{a}_1 + y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	=	$(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + cz_2 \sin \beta \hat{\mathbf{z}}$	(4e)	C II
\mathbf{B}_6	$-x_2 \mathbf{a}_1 + (y_2 + \frac{1}{2}) \mathbf{a}_2 - (z_2 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_2 + c(z_2 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_2 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_2 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C II
\mathbf{B}_7	$-x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 - z_2 \mathbf{a}_3$	=	$-(ax_2 + cz_2 \cos \beta) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} - cz_2 \sin \beta \hat{\mathbf{z}}$	(4e)	C II
\mathbf{B}_8	$x_2 \mathbf{a}_1 - (y_2 - \frac{1}{2}) \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_2 + c(z_2 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_2 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C II
\mathbf{B}_9	$x_3 \mathbf{a}_1 + y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	=	$(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + cz_3 \sin \beta \hat{\mathbf{z}}$	(4e)	C III
\mathbf{B}_{10}	$-x_3 \mathbf{a}_1 + (y_3 + \frac{1}{2}) \mathbf{a}_2 - (z_3 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_3 + c(z_3 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_3 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_3 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C III
\mathbf{B}_{11}	$-x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 - z_3 \mathbf{a}_3$	=	$-(ax_3 + cz_3 \cos \beta) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} - cz_3 \sin \beta \hat{\mathbf{z}}$	(4e)	C III
\mathbf{B}_{12}	$x_3 \mathbf{a}_1 - (y_3 - \frac{1}{2}) \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_3 + c(z_3 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_3 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C III
\mathbf{B}_{13}	$x_4 \mathbf{a}_1 + y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	=	$(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + cz_4 \sin \beta \hat{\mathbf{z}}$	(4e)	C IV
\mathbf{B}_{14}	$-x_4 \mathbf{a}_1 + (y_4 + \frac{1}{2}) \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_4 + c(z_4 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_4 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C IV
\mathbf{B}_{15}	$-x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 - z_4 \mathbf{a}_3$	=	$-(ax_4 + cz_4 \cos \beta) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} - cz_4 \sin \beta \hat{\mathbf{z}}$	(4e)	C IV
\mathbf{B}_{16}	$x_4 \mathbf{a}_1 - (y_4 - \frac{1}{2}) \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_4 + c(z_4 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_4 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C IV
\mathbf{B}_{17}	$x_5 \mathbf{a}_1 + y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	=	$(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + cz_5 \sin \beta \hat{\mathbf{z}}$	(4e)	C V
\mathbf{B}_{18}	$-x_5 \mathbf{a}_1 + (y_5 + \frac{1}{2}) \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	=	$-(ax_5 + c(z_5 - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_5 + \frac{1}{2}) \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C V
\mathbf{B}_{19}	$-x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 - z_5 \mathbf{a}_3$	=	$-(ax_5 + cz_5 \cos \beta) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} - cz_5 \sin \beta \hat{\mathbf{z}}$	(4e)	C V
\mathbf{B}_{20}	$x_5 \mathbf{a}_1 - (y_5 - \frac{1}{2}) \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	=	$(ax_5 + c(z_5 + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_5 - \frac{1}{2}) \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \sin \beta \hat{\mathbf{z}}$	(4e)	C V
\mathbf{B}_{21}	$x_6 \mathbf{a}_1 + y_6 \mathbf{a}_2 + z_6 \mathbf{a}_3$	=	$(ax_6 + cz_6 \cos \beta) \hat{\mathbf{x}} + by_6 \hat{\mathbf{y}} + cz_6 \sin \beta \hat{\mathbf{z}}$	(4e)	C VI

$$\begin{aligned}
\mathbf{B}_{102} &= -x_{26} \mathbf{a}_1 + \left(y_{26} + \frac{1}{2}\right) \mathbf{a}_2 - &= & - \left(ax_{26} + c \left(z_{26} - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + & (4e) & \text{H XII} \\
&\quad \left(z_{26} - \frac{1}{2}\right) \mathbf{a}_3 & & b \left(y_{26} + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_{26} - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{103} &= -x_{26} \mathbf{a}_1 - y_{26} \mathbf{a}_2 - z_{26} \mathbf{a}_3 &= & - \left(ax_{26} + cz_{26} \cos \beta\right) \hat{\mathbf{x}} - by_{26} \hat{\mathbf{y}} - & (4e) & \text{H XII} \\
& & & cz_{26} \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{104} &= x_{26} \mathbf{a}_1 - \left(y_{26} - \frac{1}{2}\right) \mathbf{a}_2 + &= & \left(ax_{26} + c \left(z_{26} + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - & (4e) & \text{H XII} \\
&\quad \left(z_{26} + \frac{1}{2}\right) \mathbf{a}_3 & & b \left(y_{26} - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{26} + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{105} &= x_{27} \mathbf{a}_1 + y_{27} \mathbf{a}_2 + z_{27} \mathbf{a}_3 &= & \left(ax_{27} + cz_{27} \cos \beta\right) \hat{\mathbf{x}} + by_{27} \hat{\mathbf{y}} + cz_{27} \sin \beta \hat{\mathbf{z}} & (4e) & \text{H XIII} \\
\mathbf{B}_{106} &= -x_{27} \mathbf{a}_1 + \left(y_{27} + \frac{1}{2}\right) \mathbf{a}_2 - &= & - \left(ax_{27} + c \left(z_{27} - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + & (4e) & \text{H XIII} \\
&\quad \left(z_{27} - \frac{1}{2}\right) \mathbf{a}_3 & & b \left(y_{27} + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_{27} - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{107} &= -x_{27} \mathbf{a}_1 - y_{27} \mathbf{a}_2 - z_{27} \mathbf{a}_3 &= & - \left(ax_{27} + cz_{27} \cos \beta\right) \hat{\mathbf{x}} - by_{27} \hat{\mathbf{y}} - & (4e) & \text{H XIII} \\
& & & cz_{27} \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{108} &= x_{27} \mathbf{a}_1 - \left(y_{27} - \frac{1}{2}\right) \mathbf{a}_2 + &= & \left(ax_{27} + c \left(z_{27} + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - & (4e) & \text{H XIII} \\
&\quad \left(z_{27} + \frac{1}{2}\right) \mathbf{a}_3 & & b \left(y_{27} - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{27} + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{109} &= x_{28} \mathbf{a}_1 + y_{28} \mathbf{a}_2 + z_{28} \mathbf{a}_3 &= & \left(ax_{28} + cz_{28} \cos \beta\right) \hat{\mathbf{x}} + by_{28} \hat{\mathbf{y}} + cz_{28} \sin \beta \hat{\mathbf{z}} & (4e) & \text{H XIV} \\
\mathbf{B}_{110} &= -x_{28} \mathbf{a}_1 + \left(y_{28} + \frac{1}{2}\right) \mathbf{a}_2 - &= & - \left(ax_{28} + c \left(z_{28} - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + & (4e) & \text{H XIV} \\
&\quad \left(z_{28} - \frac{1}{2}\right) \mathbf{a}_3 & & b \left(y_{28} + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_{28} - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{111} &= -x_{28} \mathbf{a}_1 - y_{28} \mathbf{a}_2 - z_{28} \mathbf{a}_3 &= & - \left(ax_{28} + cz_{28} \cos \beta\right) \hat{\mathbf{x}} - by_{28} \hat{\mathbf{y}} - & (4e) & \text{H XIV} \\
& & & cz_{28} \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{112} &= x_{28} \mathbf{a}_1 - \left(y_{28} - \frac{1}{2}\right) \mathbf{a}_2 + &= & \left(ax_{28} + c \left(z_{28} + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - & (4e) & \text{H XIV} \\
&\quad \left(z_{28} + \frac{1}{2}\right) \mathbf{a}_3 & & b \left(y_{28} - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{28} + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{113} &= x_{29} \mathbf{a}_1 + y_{29} \mathbf{a}_2 + z_{29} \mathbf{a}_3 &= & \left(ax_{29} + cz_{29} \cos \beta\right) \hat{\mathbf{x}} + by_{29} \hat{\mathbf{y}} + cz_{29} \sin \beta \hat{\mathbf{z}} & (4e) & \text{H XV} \\
\mathbf{B}_{114} &= -x_{29} \mathbf{a}_1 + \left(y_{29} + \frac{1}{2}\right) \mathbf{a}_2 - &= & - \left(ax_{29} + c \left(z_{29} - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + & (4e) & \text{H XV} \\
&\quad \left(z_{29} - \frac{1}{2}\right) \mathbf{a}_3 & & b \left(y_{29} + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_{29} - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{115} &= -x_{29} \mathbf{a}_1 - y_{29} \mathbf{a}_2 - z_{29} \mathbf{a}_3 &= & - \left(ax_{29} + cz_{29} \cos \beta\right) \hat{\mathbf{x}} - by_{29} \hat{\mathbf{y}} - & (4e) & \text{H XV} \\
& & & cz_{29} \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{116} &= x_{29} \mathbf{a}_1 - \left(y_{29} - \frac{1}{2}\right) \mathbf{a}_2 + &= & \left(ax_{29} + c \left(z_{29} + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - & (4e) & \text{H XV} \\
&\quad \left(z_{29} + \frac{1}{2}\right) \mathbf{a}_3 & & b \left(y_{29} - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{29} + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{117} &= x_{30} \mathbf{a}_1 + y_{30} \mathbf{a}_2 + z_{30} \mathbf{a}_3 &= & \left(ax_{30} + cz_{30} \cos \beta\right) \hat{\mathbf{x}} + by_{30} \hat{\mathbf{y}} + cz_{30} \sin \beta \hat{\mathbf{z}} & (4e) & \text{H XVI} \\
\mathbf{B}_{118} &= -x_{30} \mathbf{a}_1 + \left(y_{30} + \frac{1}{2}\right) \mathbf{a}_2 - &= & - \left(ax_{30} + c \left(z_{30} - \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} + & (4e) & \text{H XVI} \\
&\quad \left(z_{30} - \frac{1}{2}\right) \mathbf{a}_3 & & b \left(y_{30} + \frac{1}{2}\right) \hat{\mathbf{y}} - c \left(z_{30} - \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{119} &= -x_{30} \mathbf{a}_1 - y_{30} \mathbf{a}_2 - z_{30} \mathbf{a}_3 &= & - \left(ax_{30} + cz_{30} \cos \beta\right) \hat{\mathbf{x}} - by_{30} \hat{\mathbf{y}} - & (4e) & \text{H XVI} \\
& & & cz_{30} \sin \beta \hat{\mathbf{z}} \\
\mathbf{B}_{120} &= x_{30} \mathbf{a}_1 - \left(y_{30} - \frac{1}{2}\right) \mathbf{a}_2 + &= & \left(ax_{30} + c \left(z_{30} + \frac{1}{2}\right) \cos \beta\right) \hat{\mathbf{x}} - & (4e) & \text{H XVI} \\
&\quad \left(z_{30} + \frac{1}{2}\right) \mathbf{a}_3 & & b \left(y_{30} - \frac{1}{2}\right) \hat{\mathbf{y}} + c \left(z_{30} + \frac{1}{2}\right) \sin \beta \hat{\mathbf{z}}
\end{aligned}$$

References

- [1] S. K. Nayak, R. Sathishkumar, and T. N. G. Row, *Directing role of functional groups in selective generation of C-H- π interactions: In situ cryo-crystallographic studies on benzyl derivatives*, CrystEngComm **12**, 3112–3118 (2010), doi:10.1039/c001190h.

Found in

- [1] *Cambridge Structural Database*. CCDC 725244.