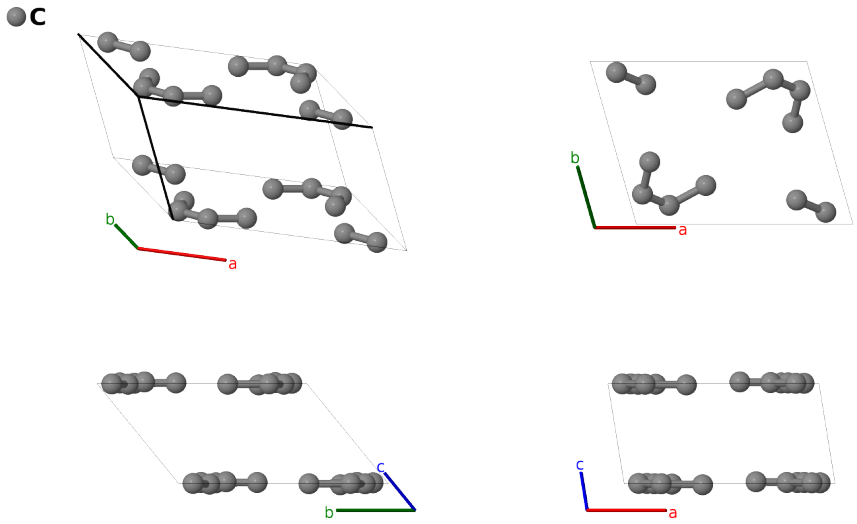
Hexamethylbenzene II ($C_{12}H_{18}$) Structure: A_aP12_2_6i-001

Cite this page as: H. Eckert, S. Divilov, A. Zettel, M. J. Mehl, D. Hicks, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 4*. In preparation.

https://aflow.org/p/7LZP

https://aflow.org/p/A_aP12_2_6i-001



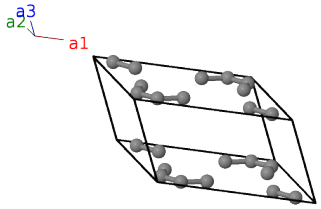
Prototype	C_2H_3
AFLOW prototype label	A_aP12_2_6i-001
Mineral name	hexamethylbenzene
CCDC	1176976
Pearson symbol	aP12
Space group number	2
Space group symbol	$P\bar{1}$
AFLOW prototype command	`aflow --proto=A_aP12_2_6i-001 --params=`$a, b/a, c/a, \alpha, \beta, \gamma, x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6$

- Solid hexamethylbenzene is found in three forms (Woodruff, 1977):
  - Phase I (Watanabe, 1949) a triclinic high-temperature phase.
  - Phase II (Brockway, 1939) is also triclinic, and is the room temperature phase.
  - Phase III (Woodruff, 1977) is trigonal and stable below 115K.
- All three structures can be considered as a benzene ring with the hydrogen atoms replaced by methyl (CH_3) groups.
- Unfortunately we have not been able to obtain a copy of (Watanabe, 1949), and (Woodruff, 1977) only has Raman data and therefore cannot completely describe the structure of Phase III.

- (Lonsdale, 1928-1929) studied hexamethylbenzene as a means of understanding the crystal structure of benzene, which is liquid at room temperature. She determined that the carbon atoms were all co-planar, and by inference extended this finding to benzene. (Brockway, 1939) presented a refinement of the structure, and we use their results here.
- Each of the outer carbon atoms is connected to three hydrogen atoms, but those positions were never determined in either paper. We do not even know if they are organized to maintain the inversion symmetry of the $P\bar{1}$ #2 space group, or if the inversion is lost and the space group becomes $P1$ #1.
- The CCSD CIF file has no atomic positions.

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
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + y_1\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$(ax_1 + by_1\cos\gamma + c_x z_1)\,\hat{\mathbf{x}} + (by_1\sin\gamma + c_y z_1)\,\hat{\mathbf{y}} + c_z z_1\,\hat{\mathbf{z}}$	(2i)	C I
$\mathbf{B_2}$	=	$-x_1\,\mathbf{a}_1 - y_1\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-(ax_1 + by_1\cos\gamma + c_x z_1)\,\hat{\mathbf{x}} - (by_1\sin\gamma + c_y z_1)\,\hat{\mathbf{y}} - c_z z_1\,\hat{\mathbf{z}}$	(2i)	C I
$\mathbf{B_3}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$(ax_2 + by_2\cos\gamma + c_x z_2)\,\hat{\mathbf{x}} + (by_2\sin\gamma + c_y z_2)\,\hat{\mathbf{y}} + c_z z_2\,\hat{\mathbf{z}}$	(2i)	C II
$\mathbf{B_4}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-(ax_2 + by_2\cos\gamma + c_x z_2)\,\hat{\mathbf{x}} - (by_2\sin\gamma + c_y z_2)\,\hat{\mathbf{y}} - c_z z_2\,\hat{\mathbf{z}}$	(2i)	C II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$(ax_3 + by_3\cos\gamma + c_x z_3)\,\hat{\mathbf{x}} + (by_3\sin\gamma + c_y z_3)\,\hat{\mathbf{y}} + c_z z_3\,\hat{\mathbf{z}}$	(2i)	C III
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$-(ax_3 + by_3\cos\gamma + c_x z_3)\,\hat{\mathbf{x}} - (by_3\sin\gamma + c_y z_3)\,\hat{\mathbf{y}} - c_z z_3\,\hat{\mathbf{z}}$	(2i)	C III
$\mathbf{B_7}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$(ax_4 + by_4\cos\gamma + c_x z_4)\,\hat{\mathbf{x}} + (by_4\sin\gamma + c_y z_4)\,\hat{\mathbf{y}} + c_z z_4\,\hat{\mathbf{z}}$	(2i)	C IV
$\mathbf{B_8}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-(ax_4 + by_4\cos\gamma + c_x z_4)\,\hat{\mathbf{x}} - (by_4\sin\gamma + c_y z_4)\,\hat{\mathbf{y}} - c_z z_4\,\hat{\mathbf{z}}$	(2i)	C IV
$\mathbf{B_9}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$(ax_5 + by_5\cos\gamma + c_x z_5)\,\hat{\mathbf{x}} + (by_5\sin\gamma + c_y z_5)\,\hat{\mathbf{y}} + c_z z_5\,\hat{\mathbf{z}}$	(2i)	C V
$\mathbf{B_{10}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-(ax_5 + by_5\cos\gamma + c_x z_5)\,\hat{\mathbf{x}} - (by_5\sin\gamma + c_y z_5)\,\hat{\mathbf{y}} - c_z z_5\,\hat{\mathbf{z}}$	(2i)	C V
$\mathbf{B_{11}}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$(ax_6 + by_6\cos\gamma + c_x z_6)\,\hat{\mathbf{x}} + (by_6\sin\gamma + c_y z_6)\,\hat{\mathbf{y}} + c_z z_6\,\hat{\mathbf{z}}$	(2i)	C VI
$\mathbf{B_{12}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-(ax_6 + by_6\cos\gamma + c_x z_6)\,\hat{\mathbf{x}} - (by_6\sin\gamma + c_y z_6)\,\hat{\mathbf{y}} - c_z z_6\,\hat{\mathbf{z}}$	(2i)	C VI

References

[1] L. O. Brockway and J. M. Robertson, *The crystal structure of hexamethylbenzene and the length of the methyl group bond to aromatic carbon atoms*, J. Chem. Soc. pp. 1324–1332 (1939), doi:10.1039/JR9390001324.

[2] K. Londsdale, *The Structure of the Benzene Ring*, Nature **122**, 810 (1928), doi:10.1038/122810c0.

[3] K. Lonsdale, *The Structure of the Benzene Ring in* $C_6(CH_3)_6$, Proc. R. Soc. A **123**, 494–515 (1929), doi:10.1098/rspa.1929.0081.

[4] S. D. Woodtruff and R. Kopelman, *Phase III crystal structure and 115 K phase transition of hexamethylbenzene*, J. Cryst. Mol. Struc. **7**, 29–40 (1977), doi:10.1007/BF01239675.

[5] T. Watanabe, Y. Saito, and H. Chihra, , Sci. Papers Osaka Univ. **1**, 9 (1949).