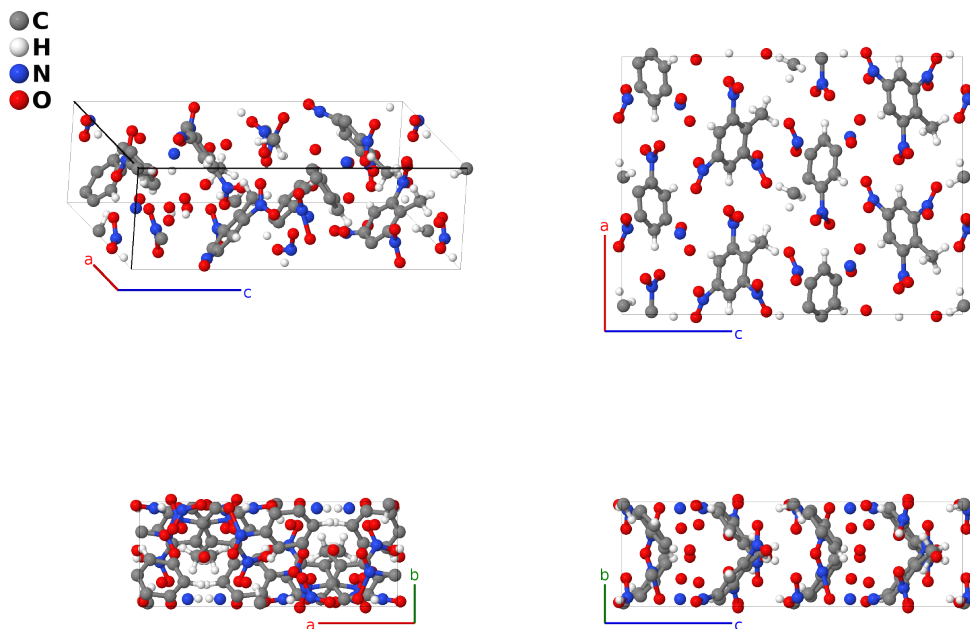


Orthorhombic 2-4-6 Trinitrotoluene ($C_7H_5N_3O_6$) Structure: A7B5C3D6_oP168_29_14a_10a_6a_12a-001

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/EY4Y>

https://aflow.org/p/A7B5C3D6_oP168_29_14a_10a_6a_12a-001



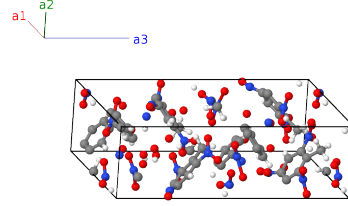
Prototype	$C_7H_5N_3O_6$
AFLOW prototype label	A7B5C3D6_oP168_29_14a_10a_6a_12a-001
Mineral name	2-4-6 trinitrotoluene
CCDC	227800
Pearson symbol	oP168
Space group number	29
Space group symbol	$Pca2_1$
AFLOW prototype command	<pre>aflow --proto=A7B5C3D6_oP168_29_14a_10a_6a_12a-001 --params=a, b/a, c/a, 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, x25, y25, z25, x26, y26, z26, x27, y27, z27, x28, y28, z28, x29, y29, z29, x30, y30, z30, x31, y31, z31, x32, y32, z32, x33, y33, z33, x34, y34, z34, x35, y35, z35, x36, y36, z36, x37, y37, z37, x38, y38, z38, x39, y39, z39, x40, y40, z40, x41, y41, z41, x42, y42, z42</pre>

- The solid form of 2-4-6 Trinitrotoluene (TNT) has two polymorphs (Vrcelj, 2003):

- The low temperature monoclinic structure, and
 - this somewhat higher temperature orthorhombic structure.
- Both can be prepared at room temperature, from ethyl acetate and ethanol solutions, respectively.
 - Data for the orthorhombic phase was taken at 123K.

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	$= -x_1 \mathbf{a}_1 - y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_1 \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	C I
\mathbf{B}_3	$= (x_1 + \frac{1}{2}) \mathbf{a}_1 - y_1 \mathbf{a}_2 + z_1 \mathbf{a}_3$	$=$	$a(x_1 + \frac{1}{2}) \hat{\mathbf{x}} - by_1 \hat{\mathbf{y}} + cz_1 \hat{\mathbf{z}}$	(4a)	C I
\mathbf{B}_4	$= -(x_1 - \frac{1}{2}) \mathbf{a}_1 + y_1 \mathbf{a}_2 + (z_1 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_1 - \frac{1}{2}) \hat{\mathbf{x}} + by_1 \hat{\mathbf{y}} + c(z_1 + \frac{1}{2}) \hat{\mathbf{z}}$	(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	$= -x_2 \mathbf{a}_1 - y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_2 \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	C II
\mathbf{B}_7	$= (x_2 + \frac{1}{2}) \mathbf{a}_1 - y_2 \mathbf{a}_2 + z_2 \mathbf{a}_3$	$=$	$a(x_2 + \frac{1}{2}) \hat{\mathbf{x}} - by_2 \hat{\mathbf{y}} + cz_2 \hat{\mathbf{z}}$	(4a)	C II
\mathbf{B}_8	$= -(x_2 - \frac{1}{2}) \mathbf{a}_1 + y_2 \mathbf{a}_2 + (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_2 - \frac{1}{2}) \hat{\mathbf{x}} + by_2 \hat{\mathbf{y}} + c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(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}	$= -x_3 \mathbf{a}_1 - y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_3 \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	C III
\mathbf{B}_{11}	$= (x_3 + \frac{1}{2}) \mathbf{a}_1 - y_3 \mathbf{a}_2 + z_3 \mathbf{a}_3$	$=$	$a(x_3 + \frac{1}{2}) \hat{\mathbf{x}} - by_3 \hat{\mathbf{y}} + cz_3 \hat{\mathbf{z}}$	(4a)	C III
\mathbf{B}_{12}	$= -(x_3 - \frac{1}{2}) \mathbf{a}_1 + y_3 \mathbf{a}_2 + (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_3 - \frac{1}{2}) \hat{\mathbf{x}} + by_3 \hat{\mathbf{y}} + c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(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}	$= -x_4 \mathbf{a}_1 - y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_4 \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	C IV
\mathbf{B}_{15}	$= (x_4 + \frac{1}{2}) \mathbf{a}_1 - y_4 \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$a(x_4 + \frac{1}{2}) \hat{\mathbf{x}} - by_4 \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4a)	C IV
\mathbf{B}_{16}	$= -(x_4 - \frac{1}{2}) \mathbf{a}_1 + y_4 \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_4 - \frac{1}{2}) \hat{\mathbf{x}} + by_4 \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	C IV
\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}	$= -x_5 \mathbf{a}_1 - y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-ax_5 \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	C V
\mathbf{B}_{19}	$= (x_5 + \frac{1}{2}) \mathbf{a}_1 - y_5 \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$a(x_5 + \frac{1}{2}) \hat{\mathbf{x}} - by_5 \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4a)	C V
\mathbf{B}_{20}	$= -(x_5 - \frac{1}{2}) \mathbf{a}_1 + y_5 \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$-a(x_5 - \frac{1}{2}) \hat{\mathbf{x}} + by_5 \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4a)	C V
\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

$$\begin{aligned}
\mathbf{B}_{158} &= -x_{40} \mathbf{a}_1 - y_{40} \mathbf{a}_2 + \left(z_{40} + \frac{1}{2}\right) \mathbf{a}_3 &= & -ax_{40} \hat{\mathbf{x}} - by_{40} \hat{\mathbf{y}} + c \left(z_{40} + \frac{1}{2}\right) \hat{\mathbf{z}} & (4a) & \text{O X} \\
\mathbf{B}_{159} &= \left(x_{40} + \frac{1}{2}\right) \mathbf{a}_1 - y_{40} \mathbf{a}_2 + z_{40} \mathbf{a}_3 &= & a \left(x_{40} + \frac{1}{2}\right) \hat{\mathbf{x}} - by_{40} \hat{\mathbf{y}} + cz_{40} \hat{\mathbf{z}} & (4a) & \text{O X} \\
\mathbf{B}_{160} &= -\left(x_{40} - \frac{1}{2}\right) \mathbf{a}_1 + y_{40} \mathbf{a}_2 + &= & -a \left(x_{40} - \frac{1}{2}\right) \hat{\mathbf{x}} + by_{40} \hat{\mathbf{y}} + c \left(z_{40} + \frac{1}{2}\right) \hat{\mathbf{z}} & (4a) & \text{O X} \\
&\quad \left(z_{40} + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{161} &= x_{41} \mathbf{a}_1 + y_{41} \mathbf{a}_2 + z_{41} \mathbf{a}_3 &= & ax_{41} \hat{\mathbf{x}} + by_{41} \hat{\mathbf{y}} + cz_{41} \hat{\mathbf{z}} & (4a) & \text{O XI} \\
\mathbf{B}_{162} &= -x_{41} \mathbf{a}_1 - y_{41} \mathbf{a}_2 + \left(z_{41} + \frac{1}{2}\right) \mathbf{a}_3 &= & -ax_{41} \hat{\mathbf{x}} - by_{41} \hat{\mathbf{y}} + c \left(z_{41} + \frac{1}{2}\right) \hat{\mathbf{z}} & (4a) & \text{O XI} \\
\mathbf{B}_{163} &= \left(x_{41} + \frac{1}{2}\right) \mathbf{a}_1 - y_{41} \mathbf{a}_2 + z_{41} \mathbf{a}_3 &= & a \left(x_{41} + \frac{1}{2}\right) \hat{\mathbf{x}} - by_{41} \hat{\mathbf{y}} + cz_{41} \hat{\mathbf{z}} & (4a) & \text{O XI} \\
\mathbf{B}_{164} &= -\left(x_{41} - \frac{1}{2}\right) \mathbf{a}_1 + y_{41} \mathbf{a}_2 + &= & -a \left(x_{41} - \frac{1}{2}\right) \hat{\mathbf{x}} + by_{41} \hat{\mathbf{y}} + c \left(z_{41} + \frac{1}{2}\right) \hat{\mathbf{z}} & (4a) & \text{O XI} \\
&\quad \left(z_{41} + \frac{1}{2}\right) \mathbf{a}_3 \\
\mathbf{B}_{165} &= x_{42} \mathbf{a}_1 + y_{42} \mathbf{a}_2 + z_{42} \mathbf{a}_3 &= & ax_{42} \hat{\mathbf{x}} + by_{42} \hat{\mathbf{y}} + cz_{42} \hat{\mathbf{z}} & (4a) & \text{O XII} \\
\mathbf{B}_{166} &= -x_{42} \mathbf{a}_1 - y_{42} \mathbf{a}_2 + \left(z_{42} + \frac{1}{2}\right) \mathbf{a}_3 &= & -ax_{42} \hat{\mathbf{x}} - by_{42} \hat{\mathbf{y}} + c \left(z_{42} + \frac{1}{2}\right) \hat{\mathbf{z}} & (4a) & \text{O XII} \\
\mathbf{B}_{167} &= \left(x_{42} + \frac{1}{2}\right) \mathbf{a}_1 - y_{42} \mathbf{a}_2 + z_{42} \mathbf{a}_3 &= & a \left(x_{42} + \frac{1}{2}\right) \hat{\mathbf{x}} - by_{42} \hat{\mathbf{y}} + cz_{42} \hat{\mathbf{z}} & (4a) & \text{O XII} \\
\mathbf{B}_{168} &= -\left(x_{42} - \frac{1}{2}\right) \mathbf{a}_1 + y_{42} \mathbf{a}_2 + &= & -a \left(x_{42} - \frac{1}{2}\right) \hat{\mathbf{x}} + by_{42} \hat{\mathbf{y}} + c \left(z_{42} + \frac{1}{2}\right) \hat{\mathbf{z}} & (4a) & \text{O XII} \\
&\quad \left(z_{42} + \frac{1}{2}\right) \mathbf{a}_3
\end{aligned}$$

References

- [1] R. M. Vrcelj, J. N. Sherwood, A. R. Kennedy, H. G. Gallagher, and T. Gelbrich, *Polymorphism in 2-4-6 Trinitrotoluene*, *Crystal Growth & Design* **3**, 1027–1032 (2003), doi:10.1021/cg0340704.