

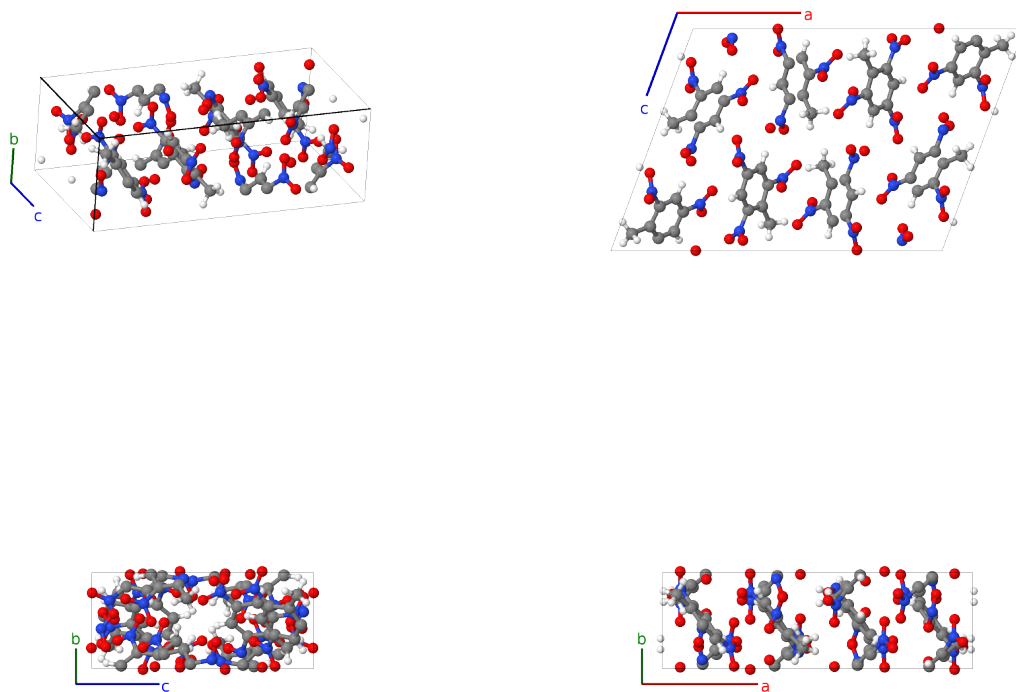
Monoclinic 2-4-6 Trinitrotoluene ($C_7H_5N_3O_6$) Structure: A7B5C3D6_mP168_14_14e_10e_6e_12e-001

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/MUZR>

https://aflow.org/p/A7B5C3D6_mP168_14_14e_10e_6e_12e-001

● C
● H
● N
● O



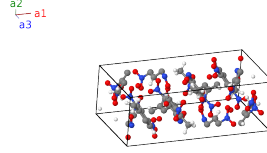
Prototype	$C_7H_5N_3O_6$
AFLOW prototype label	A7B5C3D6_mP168_14_14e_10e_6e_12e-001
Mineral name	2-4-6 trinitrotoluene
CCDC	227799
Pearson symbol	mP168
Space group number	14
Space group symbol	$P2_1/c$
AFLOW prototype command	<code>aflow --proto=A7B5C3D6_mP168_14_14e_10e_6e_12e-001</code> <code>--params=a, b/a, c/a, β, $x_1, y_1, z_1, x_2, y_2, z_2, x_3, y_3, z_3, x_4, y_4, z_4, x_5, y_5, z_5, x_6, y_6, z_6, x_7,$</code> <code>$y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}, x_{11}, y_{11}, z_{11}, x_{12}, y_{12}, z_{12}, x_{13}, y_{13}, z_{13}, x_{14}, y_{14}, z_{14}, x_{15},$</code>

$y_{15}, z_{15}, x_{16}, y_{16}, z_{16}, x_{17}, y_{17}, z_{17}, x_{18}, y_{18}, z_{18}, x_{19}, y_{19}, z_{19}, x_{20}, y_{20}, z_{20}, x_{21}, y_{21}, z_{21}, x_{22}, y_{22}, z_{22}, x_{23}, y_{23}, z_{23}, x_{24}, y_{24}, z_{24}, x_{25}, y_{25}, z_{25}, x_{26}, y_{26}, z_{26}, x_{27}, y_{27}, z_{27}, x_{28}, y_{28}, z_{28}, x_{29}, y_{29}, z_{29}, x_{30}, y_{30}, z_{30}, x_{31}, y_{31}, z_{31}, x_{32}, y_{32}, z_{32}, x_{33}, y_{33}, z_{33}, x_{34}, y_{34}, z_{34}, x_{35}, y_{35}, z_{35}, x_{36}, y_{36}, z_{36}, x_{37}, y_{37}, z_{37}, x_{38}, y_{38}, z_{38}, x_{39}, y_{39}, z_{39}, x_{40}, y_{40}, z_{40}, x_{41}, y_{41}, z_{41}, x_{42}, y_{42}, z_{42}$

- The solid form of 2-4-6 Trinitrotoluene (TNT) has two polymorphs (Vrcelj, 2003):
 - This low temperature monoclinic structure, and
 - the somewhat higher temperature orthorhombic structure.
- Both can be prepared at room temperature, from ethyl acetate and ethanol solutions, respectively.
- Data for the monoclinic phase was taken at 100K.
- (Vrcelj, 2003) gave the structure for the monoclinic phase in the $P2_1/a$ setting of space group #14. We used FINDSYM to translate this to the standard $P2_1/c$ setting.

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

$$\begin{aligned}
\mathbf{B}_{95} &= -x_{24} \mathbf{a}_1 - y_{24} \mathbf{a}_2 - z_{24} \mathbf{a}_3 &= - (ax_{24} + cz_{24} \cos \beta) \hat{\mathbf{x}} - by_{24} \hat{\mathbf{y}} - cz_{24} \sin \beta \hat{\mathbf{z}} &(4e) & \text{H X} \\
\mathbf{B}_{96} &= x_{24} \mathbf{a}_1 - (y_{24} - \frac{1}{2}) \mathbf{a}_2 + (z_{24} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{24} + c(z_{24} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{24} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{24} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4e) & \text{H X} \\
\mathbf{B}_{97} &= x_{25} \mathbf{a}_1 + y_{25} \mathbf{a}_2 + z_{25} \mathbf{a}_3 &= (ax_{25} + cz_{25} \cos \beta) \hat{\mathbf{x}} + by_{25} \hat{\mathbf{y}} + cz_{25} \sin \beta \hat{\mathbf{z}} &(4e) & \text{N I} \\
\mathbf{B}_{98} &= -x_{25} \mathbf{a}_1 + (y_{25} + \frac{1}{2}) \mathbf{a}_2 - (z_{25} - \frac{1}{2}) \mathbf{a}_3 &= - (ax_{25} + c(z_{25} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{25} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{25} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4e) & \text{N I} \\
\mathbf{B}_{99} &= -x_{25} \mathbf{a}_1 - y_{25} \mathbf{a}_2 - z_{25} \mathbf{a}_3 &= - (ax_{25} + cz_{25} \cos \beta) \hat{\mathbf{x}} - by_{25} \hat{\mathbf{y}} - cz_{25} \sin \beta \hat{\mathbf{z}} &(4e) & \text{N I} \\
\mathbf{B}_{100} &= x_{25} \mathbf{a}_1 - (y_{25} - \frac{1}{2}) \mathbf{a}_2 + (z_{25} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{25} + c(z_{25} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{25} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{25} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4e) & \text{N I} \\
\mathbf{B}_{101} &= x_{26} \mathbf{a}_1 + y_{26} \mathbf{a}_2 + z_{26} \mathbf{a}_3 &= (ax_{26} + cz_{26} \cos \beta) \hat{\mathbf{x}} + by_{26} \hat{\mathbf{y}} + cz_{26} \sin \beta \hat{\mathbf{z}} &(4e) & \text{N II} \\
\mathbf{B}_{102} &= -x_{26} \mathbf{a}_1 + (y_{26} + \frac{1}{2}) \mathbf{a}_2 - (z_{26} - \frac{1}{2}) \mathbf{a}_3 &= - (ax_{26} + c(z_{26} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{26} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{26} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4e) & \text{N II} \\
\mathbf{B}_{103} &= -x_{26} \mathbf{a}_1 - y_{26} \mathbf{a}_2 - z_{26} \mathbf{a}_3 &= - (ax_{26} + cz_{26} \cos \beta) \hat{\mathbf{x}} - by_{26} \hat{\mathbf{y}} - cz_{26} \sin \beta \hat{\mathbf{z}} &(4e) & \text{N II} \\
\mathbf{B}_{104} &= x_{26} \mathbf{a}_1 - (y_{26} - \frac{1}{2}) \mathbf{a}_2 + (z_{26} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{26} + c(z_{26} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{26} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{26} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4e) & \text{N II} \\
\mathbf{B}_{105} &= x_{27} \mathbf{a}_1 + y_{27} \mathbf{a}_2 + z_{27} \mathbf{a}_3 &= (ax_{27} + cz_{27} \cos \beta) \hat{\mathbf{x}} + by_{27} \hat{\mathbf{y}} + cz_{27} \sin \beta \hat{\mathbf{z}} &(4e) & \text{N III} \\
\mathbf{B}_{106} &= -x_{27} \mathbf{a}_1 + (y_{27} + \frac{1}{2}) \mathbf{a}_2 - (z_{27} - \frac{1}{2}) \mathbf{a}_3 &= - (ax_{27} + c(z_{27} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{27} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{27} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4e) & \text{N III} \\
\mathbf{B}_{107} &= -x_{27} \mathbf{a}_1 - y_{27} \mathbf{a}_2 - z_{27} \mathbf{a}_3 &= - (ax_{27} + cz_{27} \cos \beta) \hat{\mathbf{x}} - by_{27} \hat{\mathbf{y}} - cz_{27} \sin \beta \hat{\mathbf{z}} &(4e) & \text{N III} \\
\mathbf{B}_{108} &= x_{27} \mathbf{a}_1 - (y_{27} - \frac{1}{2}) \mathbf{a}_2 + (z_{27} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{27} + c(z_{27} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{27} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{27} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4e) & \text{N III} \\
\mathbf{B}_{109} &= x_{28} \mathbf{a}_1 + y_{28} \mathbf{a}_2 + z_{28} \mathbf{a}_3 &= (ax_{28} + cz_{28} \cos \beta) \hat{\mathbf{x}} + by_{28} \hat{\mathbf{y}} + cz_{28} \sin \beta \hat{\mathbf{z}} &(4e) & \text{N IV} \\
\mathbf{B}_{110} &= -x_{28} \mathbf{a}_1 + (y_{28} + \frac{1}{2}) \mathbf{a}_2 - (z_{28} - \frac{1}{2}) \mathbf{a}_3 &= - (ax_{28} + c(z_{28} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{28} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{28} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4e) & \text{N IV} \\
\mathbf{B}_{111} &= -x_{28} \mathbf{a}_1 - y_{28} \mathbf{a}_2 - z_{28} \mathbf{a}_3 &= - (ax_{28} + cz_{28} \cos \beta) \hat{\mathbf{x}} - by_{28} \hat{\mathbf{y}} - cz_{28} \sin \beta \hat{\mathbf{z}} &(4e) & \text{N IV} \\
\mathbf{B}_{112} &= x_{28} \mathbf{a}_1 - (y_{28} - \frac{1}{2}) \mathbf{a}_2 + (z_{28} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{28} + c(z_{28} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{28} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{28} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4e) & \text{N IV} \\
\mathbf{B}_{113} &= x_{29} \mathbf{a}_1 + y_{29} \mathbf{a}_2 + z_{29} \mathbf{a}_3 &= (ax_{29} + cz_{29} \cos \beta) \hat{\mathbf{x}} + by_{29} \hat{\mathbf{y}} + cz_{29} \sin \beta \hat{\mathbf{z}} &(4e) & \text{N V} \\
\mathbf{B}_{114} &= -x_{29} \mathbf{a}_1 + (y_{29} + \frac{1}{2}) \mathbf{a}_2 - (z_{29} - \frac{1}{2}) \mathbf{a}_3 &= - (ax_{29} + c(z_{29} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{29} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{29} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4e) & \text{N V} \\
\mathbf{B}_{115} &= -x_{29} \mathbf{a}_1 - y_{29} \mathbf{a}_2 - z_{29} \mathbf{a}_3 &= - (ax_{29} + cz_{29} \cos \beta) \hat{\mathbf{x}} - by_{29} \hat{\mathbf{y}} - cz_{29} \sin \beta \hat{\mathbf{z}} &(4e) & \text{N V} \\
\mathbf{B}_{116} &= x_{29} \mathbf{a}_1 - (y_{29} - \frac{1}{2}) \mathbf{a}_2 + (z_{29} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{29} + c(z_{29} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{29} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{29} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4e) & \text{N V} \\
\mathbf{B}_{117} &= x_{30} \mathbf{a}_1 + y_{30} \mathbf{a}_2 + z_{30} \mathbf{a}_3 &= (ax_{30} + cz_{30} \cos \beta) \hat{\mathbf{x}} + by_{30} \hat{\mathbf{y}} + cz_{30} \sin \beta \hat{\mathbf{z}} &(4e) & \text{N VI} \\
\mathbf{B}_{118} &= -x_{30} \mathbf{a}_1 + (y_{30} + \frac{1}{2}) \mathbf{a}_2 - (z_{30} - \frac{1}{2}) \mathbf{a}_3 &= - (ax_{30} + c(z_{30} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{30} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{30} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4e) & \text{N VI} \\
\mathbf{B}_{119} &= -x_{30} \mathbf{a}_1 - y_{30} \mathbf{a}_2 - z_{30} \mathbf{a}_3 &= - (ax_{30} + cz_{30} \cos \beta) \hat{\mathbf{x}} - by_{30} \hat{\mathbf{y}} - cz_{30} \sin \beta \hat{\mathbf{z}} &(4e) & \text{N VI} \\
\mathbf{B}_{120} &= x_{30} \mathbf{a}_1 - (y_{30} - \frac{1}{2}) \mathbf{a}_2 + (z_{30} + \frac{1}{2}) \mathbf{a}_3 &= (ax_{30} + c(z_{30} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{30} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{30} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} &(4e) & \text{N VI}
\end{aligned}$$

$$\begin{aligned}
\mathbf{B}_{147} &= -x_{37} \mathbf{a}_1 - y_{37} \mathbf{a}_2 - z_{37} \mathbf{a}_3 &= & - (ax_{37} + cz_{37} \cos \beta) \hat{\mathbf{x}} - by_{37} \hat{\mathbf{y}} - cz_{37} \sin \beta \hat{\mathbf{z}} & (4e) & \text{O VII} \\
\mathbf{B}_{148} &= x_{37} \mathbf{a}_1 - (y_{37} - \frac{1}{2}) \mathbf{a}_2 + (z_{37} + \frac{1}{2}) \mathbf{a}_3 &= & (ax_{37} + c(z_{37} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{37} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{37} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (4e) & \text{O VII} \\
\mathbf{B}_{149} &= x_{38} \mathbf{a}_1 + y_{38} \mathbf{a}_2 + z_{38} \mathbf{a}_3 &= & (ax_{38} + cz_{38} \cos \beta) \hat{\mathbf{x}} + by_{38} \hat{\mathbf{y}} + cz_{38} \sin \beta \hat{\mathbf{z}} & (4e) & \text{O VIII} \\
\mathbf{B}_{150} &= -x_{38} \mathbf{a}_1 + (y_{38} + \frac{1}{2}) \mathbf{a}_2 - (z_{38} - \frac{1}{2}) \mathbf{a}_3 &= & - (ax_{38} + c(z_{38} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{38} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{38} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (4e) & \text{O VIII} \\
\mathbf{B}_{151} &= -x_{38} \mathbf{a}_1 - y_{38} \mathbf{a}_2 - z_{38} \mathbf{a}_3 &= & - (ax_{38} + cz_{38} \cos \beta) \hat{\mathbf{x}} - by_{38} \hat{\mathbf{y}} - cz_{38} \sin \beta \hat{\mathbf{z}} & (4e) & \text{O VIII} \\
\mathbf{B}_{152} &= x_{38} \mathbf{a}_1 - (y_{38} - \frac{1}{2}) \mathbf{a}_2 + (z_{38} + \frac{1}{2}) \mathbf{a}_3 &= & (ax_{38} + c(z_{38} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{38} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{38} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (4e) & \text{O VIII} \\
\mathbf{B}_{153} &= 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}} & (4e) & \text{O IX} \\
\mathbf{B}_{154} &= -x_{39} \mathbf{a}_1 + (y_{39} + \frac{1}{2}) \mathbf{a}_2 - (z_{39} - \frac{1}{2}) \mathbf{a}_3 &= & - (ax_{39} + c(z_{39} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{39} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{39} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (4e) & \text{O IX} \\
\mathbf{B}_{155} &= -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}} & (4e) & \text{O IX} \\
\mathbf{B}_{156} &= x_{39} \mathbf{a}_1 - (y_{39} - \frac{1}{2}) \mathbf{a}_2 + (z_{39} + \frac{1}{2}) \mathbf{a}_3 &= & (ax_{39} + c(z_{39} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{39} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{39} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (4e) & \text{O IX} \\
\mathbf{B}_{157} &= 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}} & (4e) & \text{O X} \\
\mathbf{B}_{158} &= -x_{40} \mathbf{a}_1 + (y_{40} + \frac{1}{2}) \mathbf{a}_2 - (z_{40} - \frac{1}{2}) \mathbf{a}_3 &= & - (ax_{40} + c(z_{40} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{40} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{40} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (4e) & \text{O X} \\
\mathbf{B}_{159} &= -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}} & (4e) & \text{O X} \\
\mathbf{B}_{160} &= x_{40} \mathbf{a}_1 - (y_{40} - \frac{1}{2}) \mathbf{a}_2 + (z_{40} + \frac{1}{2}) \mathbf{a}_3 &= & (ax_{40} + c(z_{40} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{40} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{40} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (4e) & \text{O X} \\
\mathbf{B}_{161} &= 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}} & (4e) & \text{O XI} \\
\mathbf{B}_{162} &= -x_{41} \mathbf{a}_1 + (y_{41} + \frac{1}{2}) \mathbf{a}_2 - (z_{41} - \frac{1}{2}) \mathbf{a}_3 &= & - (ax_{41} + c(z_{41} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{41} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{41} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (4e) & \text{O XI} \\
\mathbf{B}_{163} &= -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}} & (4e) & \text{O XI} \\
\mathbf{B}_{164} &= x_{41} \mathbf{a}_1 - (y_{41} - \frac{1}{2}) \mathbf{a}_2 + (z_{41} + \frac{1}{2}) \mathbf{a}_3 &= & (ax_{41} + c(z_{41} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{41} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{41} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (4e) & \text{O XI} \\
\mathbf{B}_{165} &= 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}} & (4e) & \text{O XII} \\
\mathbf{B}_{166} &= -x_{42} \mathbf{a}_1 + (y_{42} + \frac{1}{2}) \mathbf{a}_2 - (z_{42} - \frac{1}{2}) \mathbf{a}_3 &= & - (ax_{42} + c(z_{42} - \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} + b(y_{42} + \frac{1}{2}) \hat{\mathbf{y}} - c(z_{42} - \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (4e) & \text{O XII} \\
\mathbf{B}_{167} &= -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}} & (4e) & \text{O XII} \\
\mathbf{B}_{168} &= x_{42} \mathbf{a}_1 - (y_{42} - \frac{1}{2}) \mathbf{a}_2 + (z_{42} + \frac{1}{2}) \mathbf{a}_3 &= & (ax_{42} + c(z_{42} + \frac{1}{2}) \cos \beta) \hat{\mathbf{x}} - b(y_{42} - \frac{1}{2}) \hat{\mathbf{y}} + c(z_{42} + \frac{1}{2}) \sin \beta \hat{\mathbf{z}} & (4e) & \text{O XII}
\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.