Trinitrobenzene

(Last updated 17 December 2024)



Figure . The molecular diagram of trinitrobenzene.

# CSP studies

A lot of the stored crystal structures are bad structures, with molecules too close to symmetry elements and clashing. Since there are 180 problematic structures, these have been ignored rather than manually checked.

A total of 135 structures matched form III across the 9 searches. Matches to forms I and II could only be achieved by increasing the tolerances in Compack.

For all searches, a single CrystalPredictor search was carried out, followed by DMACRYS optimization with the appropriate potential.

|  |  |
| --- | --- |
| REFCODE | TNBENZ |
| Formula | C6 H3 N3 O6 |
| Common Name | Trinitrobenzene |
| IUPAC Systematic Name | 1,3,5-trinitrobenzene |
| CSD Refcodes | TNBENZ11, TNBENZ12, TNBENZ13 |
|  |  |
| Search Identifier | A |
| Scientist | Alex Aina |
| Date | 2020 |
| Publication | Aina AA, Misquitta, AJ, Price SL, J Chem Phys 2021, 154(9) 094123 |
| Programs | Rigid CrystalPredictor (2.0.1), DMACRYS (2.2.1.1) |
| Energy Model | 1 |
| Study\_ID | 23 |
| Location on S Drive | \CHEMISTRY\_CPOSS\Trinitrobenzene\DIFF |
| Potential Description | ISA-DMA(PBE0/augA-sadlej) + non-empirical potential with an anisotropic repulsion fit to 2nd order dimer energies and a C10 damped isotropic dispersion, and rank 1 anisotropic polarization model |
| Energy Model | 2 |
| Study\_ID | 24 |
| Location on S Drive | \CHEMISTRY\_CPOSS\Trinitrobenzene\DIFF\_no\_pol |
| Potential Description | ISA-DMA(PBE0/augA-sadlej) + non-empirical potential with an anisotropic repulsion fit to 2nd order dimer energies and a C10 damped isotropic dispersion, with no polarization model |
| Energy Model | 3 |
| Study\_ID | 30 |
| Location on S Drive | \CHEMISTRY\_CPOSS\Trinitrobenzene\diff+e\_3 |
| Potential Description | ISA-DMA(PBE0/augA-sadlej) under polarizable continuum model with a dielectric constant of 3 + non-empirical potential with an anisotropic repulsion fit to 2nd order dimer energies and a C10 damped isotropic dispersio |
| Energy Model | 4 |
| Study\_ID | 31 |
| Location on S Drive | \CHEMISTRY\_CPOSS\Trinitrobenzene\diff+e\_7 |
| Potential Description | ISA-DMA(PBE0/augA-sadlej) under polarizable continuum model with a dielectric constant of 7 + non-empirical potential with an anisotropic repulsion fit to 2nd order dimer energies and a C10 damped isotropic dispersio |
| Energy Model | 5 |
| Study\_ID | 32 |
| Location on S Drive | \CHEMISTRY\_CPOSS\Trinitrobenzene\diff+e\_11 |
| Potential Description | ISA-DMA(PBE0/augA-sadlej) under polarizable continuum model with a dielectric constant of 11 + non-empirical potential with an anisotropic repulsion fit to 2nd order dimer energies and a C10 damped isotropic dispersio |
| Energy Model | 6 |
| Study\_ID | 22 |
| Location on S Drive | \CHEMISTRY\_CPOSS\Trinitrobenzene\Model0\_Aniso |
| Potential Description | ISA-DMA(PBE0/augA-sadlej) + non-empirical potential with an anisotropic repulsion fit to 1st order dimer energies and a C10 damped isotropic dispersion, and rank 1 anisotropic polarization model |
| Energy Model | 7 |
| Study\_ID | 21 |
| Location on S Drive | \CHEMISTRY\_CPOSS\Trinitrobenzene\Model0\_Iso |
| Potential Description | ISA-DMA(PBE0/augA-sadlej) + non-empirical potential with an isotropic repulsion fit to 1st order dimer energies and a C10 damped isotropic dispersion, and rank 1 anisotropic polarization model. |
| Energy Model | 8 |
| Study\_ID | 20 |
| Location on S Drive | \CHEMISTRY\_CPOSS\Trinitrobenzene\FIT+ISA |
| Potential Description | ISA-DMA(PBE0/augA-sadlej) + FIT |
| Energy Model | 9 |
| Study\_ID | 25 |
| Location on S Drive | \CHEMISTRY\_CPOSS\Trinitrobenzene\FIT+GDMA |
| Potential Description | GDMA(PBE0/6-31(d,p)) + FIT |

A screen shot of a graph

Description automatically generated

Figure . Crystal energy landscape of trinitrobenzene with the DIFF potential.

# CSD structures (CSD version 5.43 with Mar, Jun, Sep and Nov 2022 updates)

Table . Crystallographic information for CSD entries for trinitrobenzene. Different polymorphs are coloured differently.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| REFCODE | space group | Z’ | a / Å | b / Å | c / Å | α / ° | β / ° | γ / ° | density / g cm-3 | Form |
| TNBENZ10 | Pbca | 2 | 9.78 | 26.94 | 12.82 | 90 | 90 | 90 | 1.676 | I |
| TNBENZ11 | Pbca | 2 | 12.587 | 9.684 | 26.86 | 90 | 90 | 90 | 1.729 | I |
| TNBENZ12 | Pca21 | 2 | 9.297 | 18.73 | 9.633 | 90 | 90 | 90 | 1.688 | II |
| TNBENZ13 | P21/c | 1 | 12.896 | 5.723 | 11.287 | 90 | 98.19 | 90 | 1.717 | III |
| TNBENZ14 | Pbca | 2 | 12.6388 | 9.6357 | 26.7738 | 90 | 90 | 90 | 1.736 | I |

Table . Experimental information for CSD entries for trinitrobenzene.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| REFCODE | space group | R factor | T / K | Year | Comments |
| TNBENZ10 | Pbca | 4.6 | 295 | 1972 | Grown from the melt1 |
| TNBENZ11 | Pbca | 4.5 | 183 | 2004 | Not specified2 |
| TNBENZ12 | Pca21 | 3.97 | 120 | 2004 | Failed cocrystallization2 |
| TNBENZ13 | P21/c | 6.09 | 183 | 2004 | In the presence of an additive2 |
| TNBENZ14 | Pbca | 3.73 | 130 | 2020 | Not recorded (cocrystallization paper)3 |

1. C. S. Choi and J. E. Abel, *Acta Crystallographica Section B*, 1972, **28**, 193-201.

2. P. K. Thallapally, R. K. R. Jetti, A. K. Katz, H. L. Carrell, K. Singh, K. Lahiri, S. Kotha, R. Boese and G. R. Desiraju, *Angewandte Chemie-International Edition*, 2004, **43**, 1149-1155.

3. Z. Yang, H. Wang, J. Zhang, Y. Ma, Y. Tan, F. Nie, J. Zhang and H. Li, *Crystal Growth & Design*, 2020, **20**, 2129-2134.