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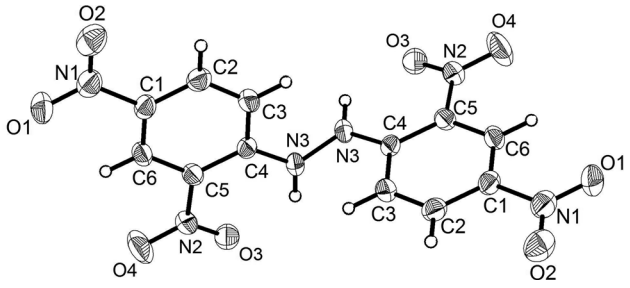
# The crystal structure of 1,2-bis(2,4-dinitrophenyl) hydrazine, $C_{12}H_8N_6O_8$

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**Abstract**

$C_{12}H_8N_6O_8$, orthorhombic, *Pbcn* (no. 60), $a$ = 11.9333(5) Å, $b$ = 9.2524(4) Å, $c$ = 12.8675(7) Å, $V$ = 1420.72(12) Å$^3$, $Z$ = 8, $R_{gt}(F)$ = 0.0468, $wR_{ref}(F^2)$ = 0.1159, $T$ = 170 K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Yellow block |
| Size: | 0.19 × 0.15 × 0.11 mm |
| Wavelength: | Mo *K*α radiation (0.71073 Å) |
| $\mu$: | 0.15 mm$^{-1}$ |
| Diffractometer, scan mode: | D8 VENTURE, $\varphi$ and $\omega$ |
| $\theta_{max}$, completeness: | 26.4°, >99 % |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 9122, 1447, 0.063 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 1059 |
| $N(param)_{refined}$: | 118 |
| Programs: | Bruker [1], Olex2 [2], SHELX [3, 4] |

**Table 2:** Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$).

| Atom | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.29715 (18) | 0.2884 (2) | 0.61255 (17) | 0.0304 (5) |
| C2 | 0.18472 (18) | 0.2660 (2) | 0.59053 (17) | 0.0317 (5) |
| H2 | 0.162967 | 0.198093 | 0.538948 | 0.038* |
| C3 | 0.10582 (18) | 0.3425 (2) | 0.64375 (16) | 0.0306 (5) |
| H3A | 0.028833 | 0.326896 | 0.628683 | 0.037* |
| C4 | 0.13538 (17) | 0.4442 (2) | 0.72054 (16) | 0.0263 (5) |
| C5 | 0.25063 (17) | 0.4585 (2) | 0.74341 (16) | 0.0276 (5) |
| C6 | 0.33110 (17) | 0.3831 (2) | 0.68820 (17) | 0.0307 (5) |
| H6 | 0.408495 | 0.396618 | 0.702460 | 0.037* |
| N1 | 0.38210 (17) | 0.2101 (2) | 0.55410 (15) | 0.0383 (5) |
| N2 | 0.29160 (15) | 0.5562 (2) | 0.82333 (15) | 0.0341 (5) |
| N3 | 0.05447 (13) | 0.5232 (2) | 0.76880 (14) | 0.0318 (5) |
| H3 | 0.071376 | 0.574629 | 0.824172 | 0.038* |
| O1 | 0.48168 (14) | 0.2355 (2) | 0.57332 (14) | 0.0492 (5) |
| O2 | 0.35144 (15) | 0.12157 (19) | 0.48924 (14) | 0.0479 (5) |
| O3 | 0.22502 (13) | 0.63891 (18) | 0.86549 (12) | 0.0402 (4) |
| O4 | 0.39136 (14) | 0.5542 (2) | 0.84564 (16) | 0.0628 (6) |

## 1 Source of materials

Using methanol as solvent, 2,4-dichloro-1,3,5-trinitrobenzene (0.70 g, 2.5 mmol) was mixed with 80 % hydrazine hydrate (0.75 mL, 18.8 mmol) at low temperature and continued to react at room temperature for 2 days. The reaction mixture was filtered, and the resulting filtrate was distilled under vacuum to obtain a yellow solid. The obtained solid was purified by silica gel column chromatography with ethyl acetate/petroleum ether mixture as eluent, and the yellow title compound crystals were obtained by slowly evaporating at room temperature.

## 2 Experimental details

The hydrogen atoms were placed in geometrically idealized positions riding on attached atoms. Their $U_{iso}$(H) values were constrained to 1.2$U_{eq}$.

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## 3 Comment

Nitrophenylhydrazine compounds are important fine organic chemical raw materials and intermediates, which can be used in dyes, medicine and the preparation of benzidine, azobenzene compounds, etc. [5–9] The title compound (*cf*. the figure) presents a centrosymmetric structure with the center point of the N–N bond as the center of symmetry. Its molecular structure contains two benzene rings, four nitro groups, and one hydrazine group. Each nitro group is in the same plane as their attached benzene rings for their dihedral angles to the attached benzene ring are 2.78° (O2, N1, C1) and 8.09° (O3, N2, C5), respectively. The hydrazine group and benzene ring are also approximately coplanar (dihedral Angle 11.73°), while the dihedral angle of the two benzene rings is 86.49°. All bond angles and lengths are within the normal range. And the structural characteristics of the title compound are similar to those of (2,4-dinitrophenyl) hydrazine [10], 1,2-diphenylhydrazine [11] and 1,2-diethyl-1,2-bis(2-nitrophenyl)hydrazine [12].

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