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2,6-Dinitrotoluene

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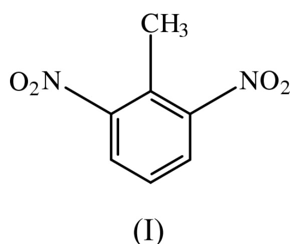
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.046
wR factor = 0.133
Data-to-parameter ratio = 8.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Crystals of 2,6-dinitrotoluene, $C_7H_6N_2O_4$, were obtained from a methanol solution of the mixture of 2,6- and 2,4-dinitrotoluene. The $P2_12_12_1$ space group shows the compound is chiral, but the absolute configuration was not determined reliably. The nitro group planes are inclined to the benzene plane with dihedral angles of 53.1 (1) and 38.1 (1)°, respectively. The repulsion between methyl and nitro groups results in a rather small C—C—C angle of 112.6 (2)° within the benzene ring.



(I)

Experimental

Single crystals of the title chiral compound were obtained from a methanol solution containing 2,6- and 2,4-dinitrotoluene when we tried to separate the isomers.

Crystal data

$C_7H_6N_2O_4$
M_r = 182.14
Orthorhombic, $P2_12_12_1$
a = 7.830 (2) Å
b = 13.683 (3) Å
c = 7.296 (2) Å
V = 781.7 (3) Å^3
Z = 4
D_x = 1.548 Mg m^{-3}
D_m not measured
Mo $K\alpha$ radiation
Cell parameters from 20 reflections
θ = 11.7–21.5°
μ = 0.13 mm^{-1}
T = 293 (2) K
Prismatic, yellow
0.30 × 0.24 × 0.20 mm

Data collection

Rigaku AFC-7R diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.963, T_{max} = 0.974
1061 measured reflections
1061 independent reflections
906 reflections with $I > 2\sigma(I)$
θ_{max} = 27.5°
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 17$
$l = 0 \rightarrow 9$
3 standard reflections every 100 reflections intensity decay: 0.3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.133
S = 1.05
1061 reflections
119 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0748P)^2 + 0.2426P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Extinction correction: *SHELXL*93
Extinction coefficient: 0.0719 (109)

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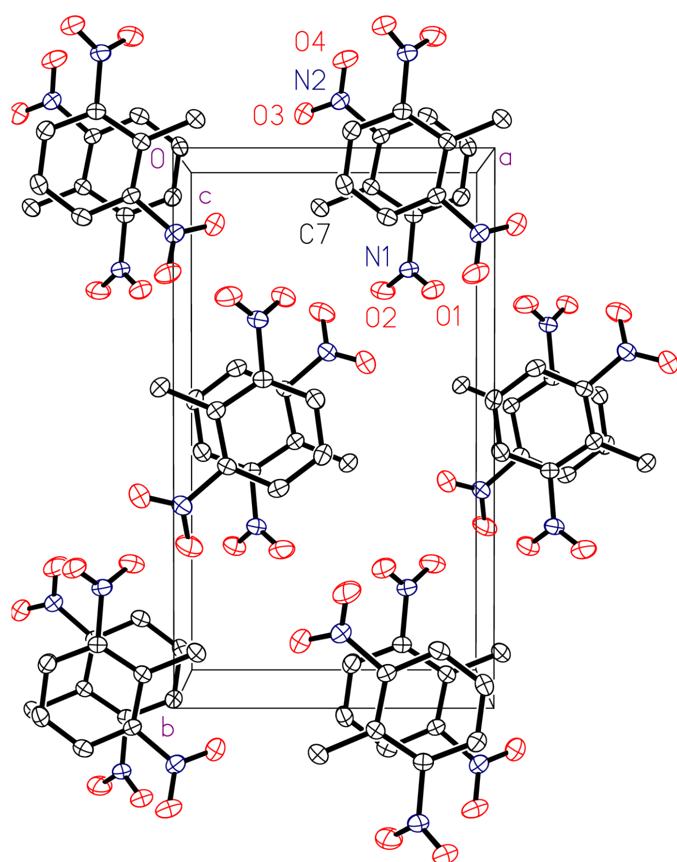

Figure 1
View of the crystal packing of the title compound with 30% probability displacement ellipsoids, showing the overlap of adjacent benzene rings. H atoms have been omitted for clarity.

Table 1
Selected geometric parameters (Å, °).

O1—N1	1.216 (3)	O4—N2	1.206 (4)
O2—N1	1.213 (4)	N1—C2	1.482 (3)
O3—N2	1.221 (3)	N2—C6	1.476 (3)
O1—N1—O2	124.8 (2)	O4—N2—C6	117.4 (3)
O1—N1—C2	117.5 (3)	O3—N2—C6	118.7 (2)
O2—N1—C2	117.6 (3)	C2—C1—C6	112.6 (2)
O4—N2—O3	124.0 (3)		

H atoms were located in calculated positions and constrained to ride on their parent C atoms during refinement. The absolute configuration could not be reliably determined.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1985*a*, 1992*a*); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1985*b*, 1992*b*); program(s) used to solve structure: *SHELXS*93 (Sheldrick, 1993); program(s) used to refine structure: *SHELXL*93; molecular graphics: *XP* (Siemens, 1994).

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