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Methyl 3,5-dinitrobenzoate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.061
wR factor = 0.169
Data-to-parameter ratio = 14.0

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

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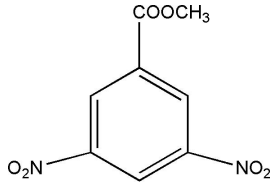
The structure of the title compound, $C_8H_6N_2O_6$, is essentially planar, except for the methyl H atoms. In the crystal structure, the molecules are stacked along the *a* axis with π–π interactions.

Comment

Dinitrobenzoate compounds are of interest for their biological activities. Among them, a series of 3,5-dinitrobenzoic acid esters have been synthesized which have anti-creatinine properties (Yu & Yang, 2002). Moreover, dinitrobenzoic acid derivatives have been found to be effective as radiation sensitizers in tumour treatment (Kagitani *et al.*, 1984). Furthermore, some synthetic dinitrobenzoate compounds have shown useful properties in DNA and oligosaccharide synthesis (Olive, 1979; Huang *et al.*, 2004). To study their structures and activities, we report here the crystal structure of the title compound, (I). .



(I)

In compound (I) (Fig. 1), the bond lengths and angles are within expected ranges. The molecule is essentially planar: the

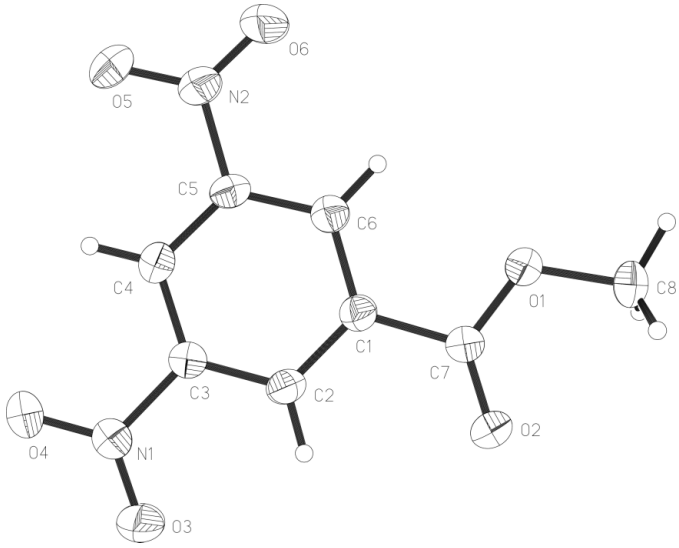


Figure 1
A view of the molecular structure of (I), showing 30% probability displacement ellipsoids.

maximum deviations from the weighted least-squares plane calculated through all the non-H atoms are −0.090 (3), 0.074 (3) and 0.054 (2) Å for atoms O3, O4 and O2, respectively.

Molecules translated one unit cell along [100] are stacked via π–π interactions, with minimum short contacts for C4···C2^{i} [3.440 (4) Å], C5···C1^{i} [3.461 (4) Å] and C5···C7^{i} [3.481 (4) Å] [symmetry code (i): $1 + x, y, z$].

Experimental

Compound (I) was prepared as described previously by Bartlett & Trachtenberg (1958). Crystals suitable for X-ray analysis were obtained by slow evaporation of a methanol solution.

Crystal data

$C_8H_6N_2O_6$
$M_r = 226.15$
Monoclinic, $P2_1/c$
$a = 4.5833$ (15) Å
$b = 18.843$ (6) Å
$c = 11.112$ (4) Å
$\beta = 100.738$ (7)°
$V = 942.8$ (5) Å^3
$Z = 4$
$D_x = 1.593$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 733 reflections
$\theta = 2.9$–$23.1°$
$\mu = 0.14$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.25 × 0.20 × 0.06 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.966$, $T_{max} = 0.992$
5458 measured reflections
2050 independent reflections
1112 reflections with $I > 2\sigma(I)$
$R_{int} = 0.038$
$\theta_{max} = 27.0°$
$h = -5 \rightarrow 5$
$k = -12 \rightarrow 24$
$l = -13 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.170$
$S = 1.03$
2050 reflections
146 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0662P)^2 + 0.0259P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C7	1.495 (3)	C8—O1	1.457 (3)
C3—N1	1.473 (3)	N1—O4	1.207 (3)
C5—N2	1.475 (3)	N1—O3	1.207 (3)
C7—O2	1.199 (3)	N2—O6	1.205 (3)
C7—O1	1.312 (3)	N2—O5	1.217 (3)
C6—C1—C7	122.3 (2)	O6—N2—O5	124.0 (2)
O2—C7—O1	125.6 (2)	C7—O1—C8	118.0 (2)
O4—N1—O3	124.3 (3)		
C6—C1—C7—O2	179.2 (3)	C4—C3—N1—O3	175.0 (2)
C2—C1—C7—O1	177.8 (2)	C6—C5—N2—O5	−178.8 (2)
C2—C3—N1—O4	175.7 (2)	C1—C7—O1—C8	179.5 (2)

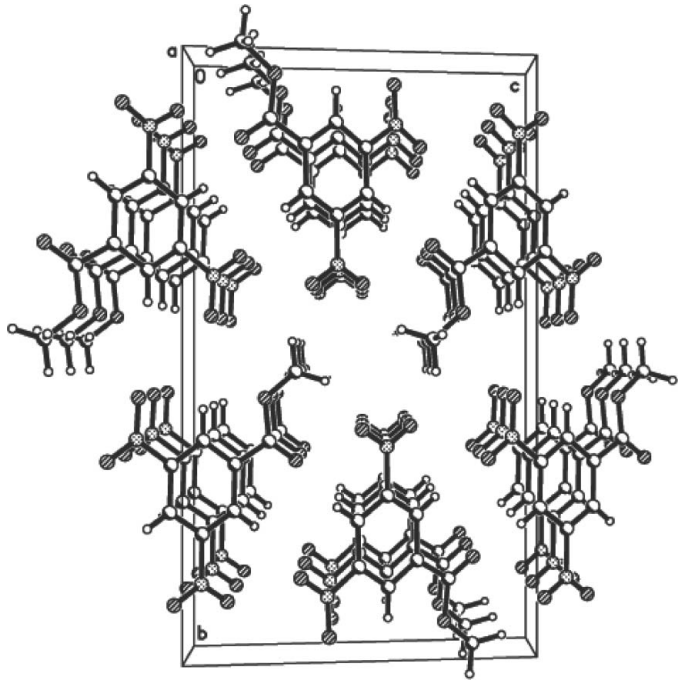


Figure 2
A packing diagram for (I), viewed along the *a* axis.

H atoms were positioned geometrically and refined with a riding model, with C—H = 0.93–0.96 Å and with U_{iso} constrained to 1.2 (1.5 for the methyl group) times U_{eq} of the carrier atom.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-NT* (Bruker, 2001); software used to prepare material for publication: *SHELXTL-NT*.

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