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Propyl 3,5-dinitrobenzoate

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The title compound, $C_{10}H_{10}N_2O_6$, has two independent molecules in the asymmetric unit. All bond lengths and angles in the molecules are in normal ranges. The crystal packing is stabilized by van der Waals forces and π–π stacking interactions.

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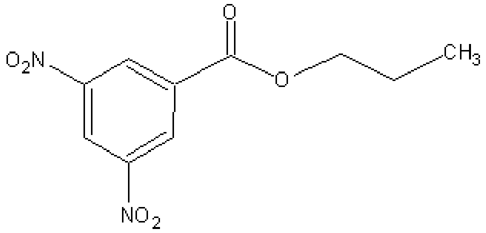
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.056
wR factor = 0.152
Data-to-parameter ratio = 14.8

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

Comment

Due to their biological activities, dinitrobenzoate derivatives are widely used in pharmacology. It is known (Olive, 1979; Huang *et al.*, 2004) that synthetic dinitrobenzoate compounds are useful in the synthesis of DNA and oligosaccharides. Dinitrobenzoic acid derivatives are effective in tumour treatment as radiation sensitizers (Kagitani *et al.*, 1984). Furthermore, a recently synthesized series of 3,5-dinitrobenzoic acid esters has demonstrated promising anticreatinine effects (Yu & Yang, 2002). As part of an ongoing study of dinitrobenzoate derivatives, we report here the crystal structure of the title compound, (I).



(I)

All bond lengths and angles in the two independent molecules of (I) (Fig. 1) are normal (Table 1). Except for methyl atoms C10 and C20, all non-H atoms of each molecule lie in a plane (r.m.s deviations = 0.037 and 0.094 Å, respectively). The

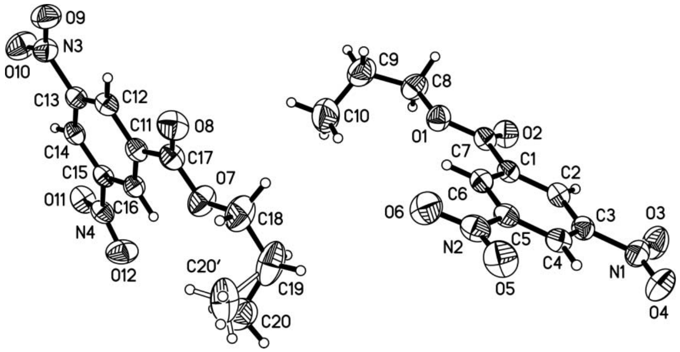


Figure 1
The two independent molecules of (I) with the disordered methyl group in one (both components shown). Displacement ellipsoids are drawn at the 30% probability level.

crystal packing is stabilized by van der Waals forces and π–π stacking interactions, evidenced by the short intermolecular contacts N3···O8^{i} [3.045 (3) Å; symmetry code (i): $2-x$, $2-y$, $1-z$], C12···C12^{i} [3.436 (3) Å] and C17···O9^{i} [3.104 (3) Å].

Experimental

The title compound, (I), was synthesized according to the literature procedure of Bartlett & Trachtenberg (1958). Crystals suitable for X-ray analysis were grown from a solution in methanol at room temperature by slow evaporation.

Crystal data

$C_{10}H_{10}N_2O_6$
$M_r = 254.20$
Triclinic, $P\overline{1}$
$a = 11.0566$ (16) Å
$b = 11.3596$ (17) Å
$c = 11.4916$ (17) Å
$\alpha = 117.554$ (2)°
$\beta = 99.937$ (3)°
$\gamma = 102.830$ (2)°
$V = 1182.7$ (3) Å^3
$Z = 4$
$D_x = 1.428$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2196 reflections
$\theta = 2.2$–25.6°
$\mu = 0.12$ mm^{-1}
$T = 292$ (2) K
Block, colourless
0.60 × 0.50 × 0.30 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.931$, $T_{\max} = 0.965$
7233 measured reflections
4995 independent reflections
3237 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.044$
$\theta_{\max} = 27.0°$
$h = -14 \rightarrow 12$
$k = -14 \rightarrow 13$
$l = -13 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.152$
$S = 0.97$
4995 reflections
338 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0774P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.17$ e Å^{-3}
$\Delta\rho_{\min} = -0.21$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C7	1.490 (2)	C11—C17	1.492 (3)
C7—O2	1.197 (2)	C17—O8	1.199 (2)
C7—O1	1.327 (2)	C17—O7	1.320 (2)
C8—O1	1.458 (2)	C18—O7	1.465 (2)
C2—C1—C7	117.62 (16)	O8—C17—O7	125.14 (18)
O2—C7—O1	125.02 (17)	O8—C17—C11	123.25 (19)
O2—C7—C1	123.28 (17)	C7—O1—C8	116.43 (15)
C12—C11—C17	117.89 (17)	C17—O7—C18	115.95 (17)
C6—C1—C7—O2	−175.97 (18)	C12—C13—N3—O9	−1.2 (3)
C16—C11—C17—O8	−175.27 (19)	C14—C15—N4—O11	10.9 (2)
C2—C3—N1—O3	−0.1 (3)	C9—C8—O1—C7	174.60 (18)
C4—C5—N2—O5	4.9 (3)	C19—C18—O7—C17	−178.0 (2)

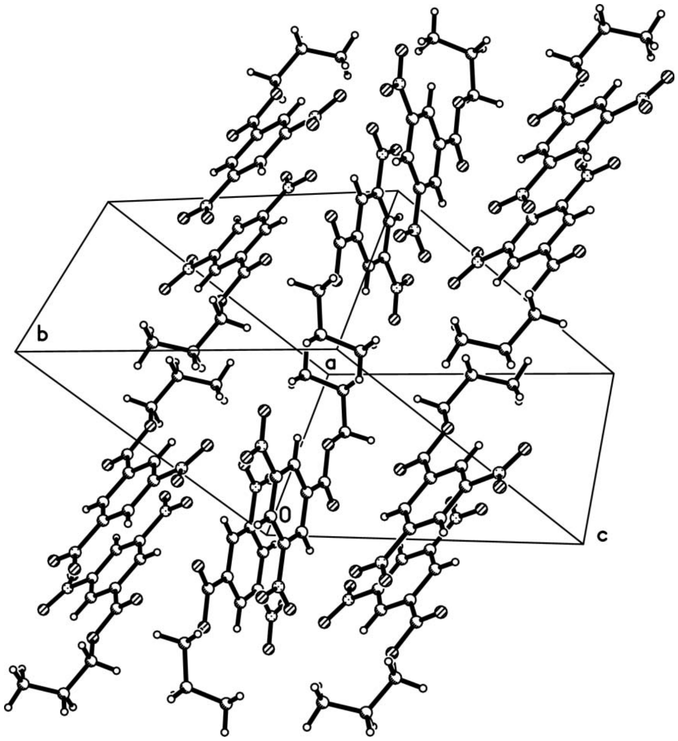


Figure 2
Packing diagram for (I). Only the major component of the disordered methyl group is shown.

H atoms were positioned geometrically and refined as riding, with C—H = 0.93–0.97 Å and $U_{\rm iso}$(H) = 1.2–1.5$U_{\rm eq}$(C). The methyl group attached to C20 was treated as disordered over two positions; the refined occupancies were 0.83 (2) and 0.17 (2).

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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