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n-Butyl 3,5-dinitrobenzoate

Fen-Fang Li, Xiao Feng-Ping, Long-Fei Jin* and Yong-Fei Wu

College of Chemistry, Central China Normal Univesity, Wuhan 430079, People's Republic of China

Correspondence e-mail: jlf163@public.wh.hb.cn

Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.004 Å
R factor = 0.057
wR factor = 0.177
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.

The molecule of the title compound, $C_{11}H_{12}N_2O_6$, is essentially planar except for the alkyl chain, which has a non-extended conformation.

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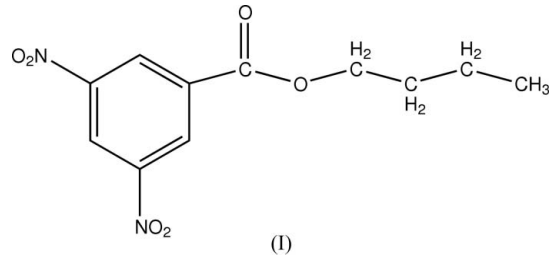
Comment

Ninitrobenzoate derivatives are of interest because of their biological activities. A series of 3,5-dinitrobenzoic acid ester had been synthesized and demonstrated promising anticreatinine effects (Yu & Yang, 2002). Dinitrobenzoic acid derivatives are also effective as radiation sensitizers in tumor 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). As part of our ongoing studies (Jin & Xiao, 2005), we report here the crystal structure of the title compound, (I).



(I)

The bond lengths and angles in (I) show normal values (Table 1). Except for atoms C9, C10 and C11, all non-H atoms lie in a plane with an r.m.s deviation of 0.0792 Å. The alkyl chain lies out of this plane and has a non-extended conformation, with torsion angles of 64.4 (3)° for O1—C8—C9—C10 and 176.2 (3)° for C8—C9—C10—C11. There are no unusual intermolecular interactions.

Experimental

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

Crystal data

$C_{11}H_{12}N_2O_6$
M_r = 268.23
Monoclinic, $P2_1/n$
a = 9.681 (3) Å
b = 5.8632 (17) Å
c = 22.164 (6) Å
β = 90.826 (5)°
V = 1257.9 (6) Å^3
Z = 4
D_x = 1.416 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1716 reflections
θ = 2.3–23.6°
μ = 0.12 mm^{-1}
T = 273 (2) K
Prism, colorless
0.56 × 0.24 × 0.03 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.937, T_{max} = 0.997
6678 measured reflections
2417 independent reflections
1724 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 26.0°
$h = -11 \rightarrow 8$
$k = -7 \rightarrow 7$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.177
S = 1.08
2417 reflections
173 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.086P)^2 + 0.3114P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C7	1.494 (3)	C7—O2	1.205 (3)
C3—N1	1.477 (3)	C7—O1	1.318 (3)
C5—N2	1.461 (3)	C8—O1	1.459 (3)
O2—C7—O1	124.8 (2)	O4—N1—O3	124.6 (2)
O1—C7—C1	113.0 (2)	O6—N2—O5	123.2 (2)
O1—C8—C9	108.0 (2)	C7—O1—C8	115.6 (2)
C2—C1—C7—O2	4.8 (4)	C8—C9—C10—C11	176.2 (3)
C6—C1—C7—O1	6.9 (3)	O2—C7—O1—C8	−2.1 (4)
O1—C8—C9—C10	64.3 (3)	C1—C7—O1—C8	178.9 (2)

All H atoms were included in the riding-model approximation, with C–H distances of 0.93 Å (aromatic), 0.97 Å (CH_2) and 0.96 Å (CH_3) and $U_{iso}(H) = 1.2U_{eq}(C)$ for the aromatic H and CH_2 and $U_{iso}(H) = 1.5U_{eq}(C)$ for CH_3.

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*.

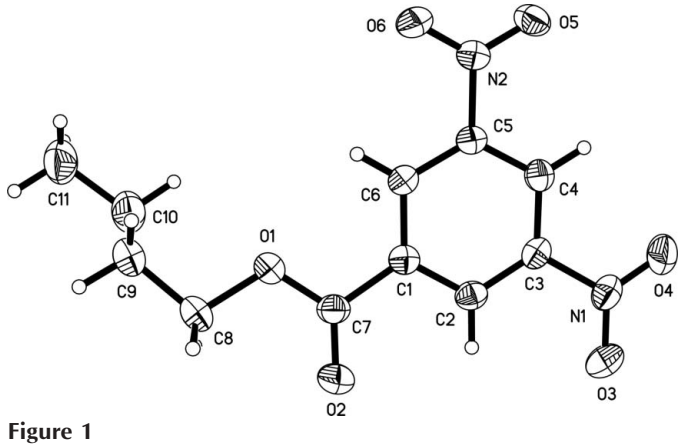


Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 30% probability level.

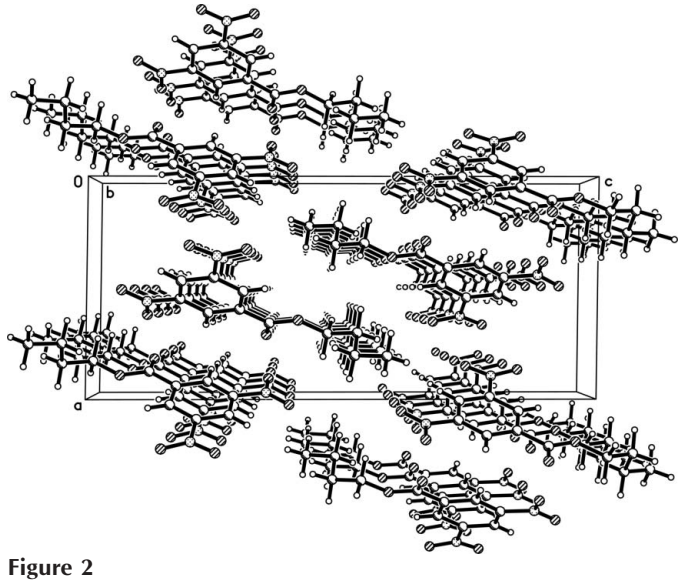


Figure 2
Packing diagram for (I).

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