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Methyl 3-nitrobenzoate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.046
wR factor = 0.132
Data-to-parameter ratio = 15.9

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

In the title molecule, $C_8H_7NO_4$, the non-H atoms are essentially coplanar. In the crystal structure, short intermolecular O···C (3.21 Å) and O···N (3.17 Å) contacts indicate the presence of π–π interactions.

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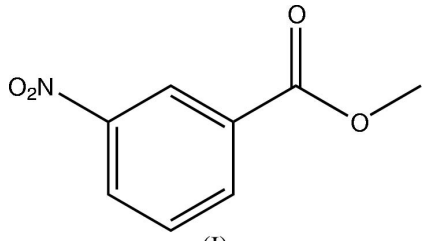
Comment

Benzoates are important intermediates in the chemistry of pigments and pharmaceuticals (Zhang, 1992; Zhang *et al.*, 1990; Zhang *et al.*, 1995). As a part of our work on the characterization of benzoate derivatives, we report here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. All bond lengths and angles in the molecule show normal values (Table 1). The non-H atoms of the molecule lie in a plane, with an r.m.s deviation of 0.019 Å.

As seen in the packing diagram (Fig. 2), there are short intermolecular contacts, namely O3···C7^{i} (3.21 Å) and O2···N1^{i} (3.17 Å) [symmetry code: (i) $1-x, 2-y, 1-z$]. These contacts may indicate the presence of π–π interactions.

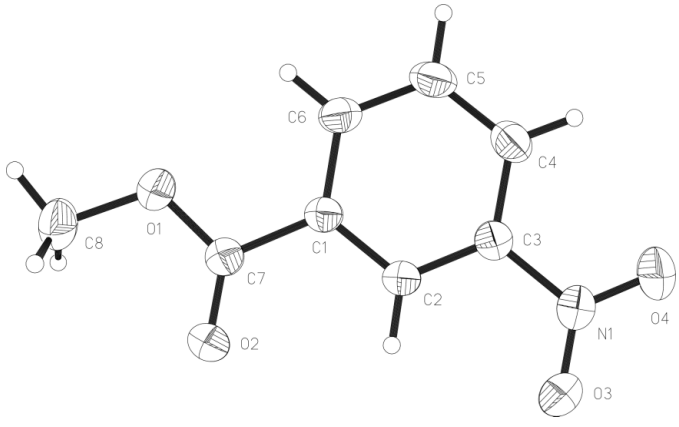


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

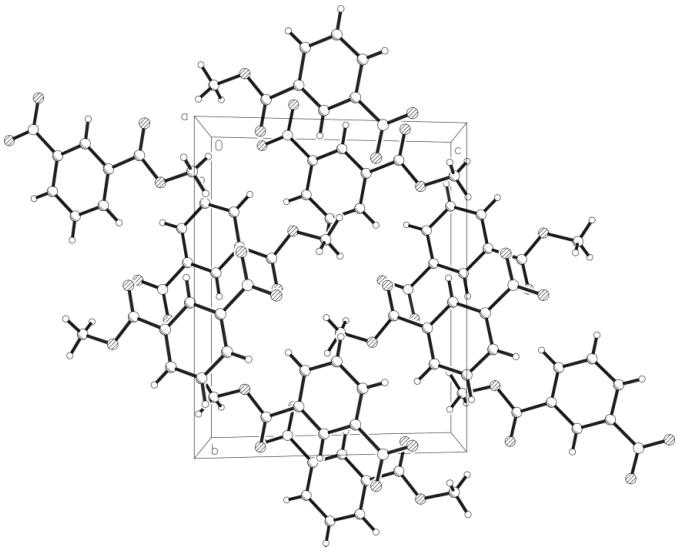


Figure 2
A packing diagram for (I), viewed along the *a* axis.

Experimental

Compound (I) was synthesized according to the literature procedure of Zhou & Li (2004). A crystal of (I) suitable for X-ray analysis was grown from a solution in methanol at room temperature by slow evaporation.

Crystal data

$C_8H_7NO_4$
M_r = 181.15
Monoclinic, $P2_1/c$
a = 7.4937 (19) Å
b = 11.764 (3) Å
c = 9.778 (2) Å
β = 102.784 (4)°
V = 840.6 (3) Å^3
Z = 4
D_x = 1.431 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1544 reflections
θ = 2.8–26.0°
μ = 0.12 mm^{-1}
T = 293 (2) K
Block, colourless
0.30 × 0.30 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
4948 measured reflections
1907 independent reflections
1394 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 27.5°
$h = -6 \rightarrow 9$
$k = -14 \rightarrow 15$
$l = -12 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.132
S = 1.04
1907 reflections
120 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0691P)^2 + 0.0488P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.040 (6)

Table 1
Selected geometric parameters (Å, °).

C1—C7	1.488 (2)	C8—O1	1.4376 (18)
C3—N1	1.469 (2)	N1—O4	1.2124 (16)
C7—O2	1.1988 (17)	N1—O3	1.2146 (18)
C7—O1	1.3245 (18)		
C6—C1—C7	122.43 (13)	O2—C7—C1	123.56 (13)
C2—C1—C7	117.84 (12)	O4—N1—O3	123.24 (14)
O2—C7—O1	123.90 (14)	C7—O1—C8	116.01 (13)
C7—C1—C6—C5	−179.85 (14)	C4—C3—N1—O4	−1.7 (2)
C6—C1—C7—O2	179.35 (15)	C4—C3—N1—O3	178.45 (14)
C2—C1—C7—O1	−179.65 (12)	C1—C7—O1—C8	−179.95 (13)

All H atoms were geometrically positioned and refined using a riding-model approximation, with C—H distances of 0.93 Å (aromatic H atoms) and 0.96 Å (methyl atoms), and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C) for aromatic and methyl H atoms, respectively.

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

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