

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Isopropyl 4-nitrobenzoate

Pei Zou, Min-Hao Xie, Hao Wu, Ya-Ling Liu and Zheng-Ping Chen*

Jiangsu Institute of Nuclear Medicine, Wuxi 214063, People's Republic of China
Correspondence e-mail: wxzoupei@126.com

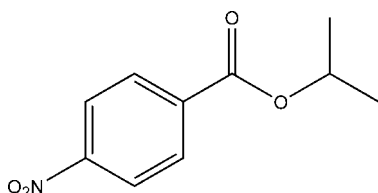
Received 22 September 2011; accepted 26 September 2011

Key indicators: single-crystal X-ray study; $T = 153$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å;
 R factor = 0.046; wR factor = 0.150; data-to-parameter ratio = 20.7.

In the molecule of the title compound, $\text{C}_{10}\text{H}_{11}\text{NO}_4$, the nitro group is approximately coplanar with the benzene ring [dihedral angle = $4.57(10)^\circ$], while the carboxylate group is slightly twisted, making an angle of $12.16(8)^\circ$. In the crystal, weak intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonding and $\pi-\pi$ stacking interactions [centroid-centroid distances = $3.670(2)$ and $3.665(2)$ Å] are observed.

Related literature

For applications of benzoates in the chemistry of pigments and pharmaceuticals, see: Zhang *et al.* (1990, 1995). For a related structure, see: Wu *et al.* (2009).



Experimental

Crystal data

$\text{C}_{10}\text{H}_{11}\text{NO}_4$
 $M_r = 209.20$

Triclinic, $P\bar{1}$
 $a = 6.729(4)$ Å

$b = 7.192(4)$ Å
 $c = 10.388(6)$ Å
 $\alpha = 94.751(9)^\circ$
 $\beta = 92.503(7)^\circ$
 $\gamma = 95.901(10)^\circ$
 $V = 497.6(5)$ Å³

$Z = 2$
Mo $K\alpha$ radiation
 $\mu = 0.11$ mm⁻¹
 $T = 153$ K
 $0.37 \times 0.33 \times 0.10$ mm

Data collection

Rigaku SPIDER diffractometer
6626 measured reflections
2862 independent reflections

1947 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.150$
 $S = 1.00$
2862 reflections

138 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.34$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.29$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C1}-\text{H1}\cdots\text{O4}^i$	0.95	2.46	3.311 (3)	149
$\text{C4}-\text{H4}\cdots\text{O2}^{ii}$	0.95	2.46	3.294 (3)	147

Symmetry codes: (i) $x, y-1, z$; (ii) $x, y+1, z$.

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors acknowledge financial support from Jiangsu Institute of Nuclear Medicine, China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5329).

References

- Rigaku (2004). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Wu, H., Xie, M.-H., Zou, P., Liu, Y.-L. & He, Y.-J. (2009). *Acta Cryst.* **E65**, o3096.
Zhang, A.-Y., Qian, B., Min, J. & Fang, Q.-X. (1995). *J. Shanxi Normal Univ. (Nat. Sci. Ed.)*, **23**, 44–47.
Zhang, Z.-S., Wu, J.-G. & Deng, R.-W. (1990). *J. Lanzhou Univ. (Nat. Sci. Ed.)*, **26**, 69–75.

supplementary materials

Acta Cryst. (2011). E67, o2806 [doi:10.1107/S1600536811039407]

Isopropyl 4-nitrobenzoate

P. Zou, M.-H. Xie, H. Wu, Y.-L. Liu and Z.-P. Chen

Comment

Benzoates are important intermediates in the chemistry of pigments and pharmaceuticals, which are widely used all over the world (Zhang *et al.*, 1995; Zhang *et al.*, 1990). The crystal structure of methyl 4-nitrobenzoate has been reported (Wu *et al.*, 2009). As an extension of our study, we report here the crystal structure of the title compound.

In the structure of the title compound (Fig. 1) the bond lengths and angles are within expected ranges. The nitro substituent group is nearly coplanar with the benzene ring (dihedral angle, $4.57 (10)^\circ$), while the ester group forms a dihedral angle of $12.16 (8)^\circ$ with the benzene ring. In the crystal structure, adjacent molecules are linked together by weak C—H \cdots O hydrogen bonds (Table 1). π - π stacking is observed between parallel benzene rings, centroids distances being $3.670 (2)$ [symmetry code $-x, 1-y, 1-z$] and $3.665 (2)$ Å [symmetry code $1-x, 1-y, 1-z$].

Experimental

A sample of commercial isopropyl 4-nitrobenzoate was crystallized by slow evaporation of a solution in methanol, colorless platelet-shaped crystals were formed after several days.

Refinement

Positional parameters of all the H atoms bonds to C atoms were calculated geometrically and were allowed to ride on the C atoms to which they are bonded, with $C_{\text{aromatic}}\text{—H} = 0.95$ Å, $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(C_{\text{aromatic}})$; $C_{\text{methyl}}\text{—H} = 0.98$ Å, $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(C_{\text{methyl}})$ and $C_{\text{methylidyne}}\text{—H} = 1.00$ Å, $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(C_{\text{methylidyne}})$.

Figures

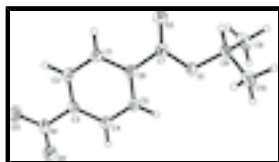


Fig. 1. A view of the title compound with the atomic numbering scheme. Displacement ellipsoids were drawn at the 50% probability level.

Isopropyl 4-nitrobenzoate

Crystal data

$C_{10}H_{11}NO_4$

$M_r = 209.20$

Triclinic, $P\bar{1}$

Hall symbol: $-P 1$

$Z = 2$

$F(000) = 220$

$D_x = 1.396$ Mg m $^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

supplementary materials

$a = 6.729 (4) \text{ \AA}$	Cell parameters from 1490 reflections
$b = 7.192 (4) \text{ \AA}$	$\theta = 2.9\text{--}30.0^\circ$
$c = 10.388 (6) \text{ \AA}$	$\mu = 0.11 \text{ mm}^{-1}$
$\alpha = 94.751 (9)^\circ$	$T = 153 \text{ K}$
$\beta = 92.503 (7)^\circ$	Platelet, colorless
$\gamma = 95.901 (10)^\circ$	$0.37 \times 0.33 \times 0.10 \text{ mm}$
$V = 497.6 (5) \text{ \AA}^3$	

Data collection

Rigaku SPIDER diffractometer	1947 reflections with $I > 2\sigma(I)$
Radiation source: Rotating Anode graphite	$R_{\text{int}} = 0.023$
ω scans	$\theta_{\text{max}} = 30.0^\circ$, $\theta_{\text{min}} = 2.0^\circ$
6626 measured reflections	$h = -9 \rightarrow 9$
2862 independent reflections	$k = -10 \rightarrow 9$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.046$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.150$	H-atom parameters constrained
$S = 1.00$	$w = 1/[\sigma^2(F_o^2) + (0.071P)^2 + 0.196P]$
2862 reflections	where $P = (F_o^2 + 2F_c^2)/3$
138 parameters	$(\Delta/\sigma)_{\text{max}} < 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.34 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.29 \text{ e \AA}^{-3}$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.24504 (18)	0.35230 (15)	0.12880 (10)	0.0258 (3)

O2	0.3016 (2)	0.12996 (17)	0.26213 (12)	0.0375 (3)
O3	0.2023 (2)	0.79014 (18)	0.77175 (11)	0.0381 (3)
O4	0.2382 (3)	1.00939 (19)	0.64283 (13)	0.0513 (4)
N1	0.2278 (2)	0.8444 (2)	0.66434 (13)	0.0288 (3)
C1	0.2535 (2)	0.3845 (2)	0.47750 (14)	0.0226 (3)
H1	0.2540	0.2559	0.4922	0.027*
C2	0.2421 (2)	0.5176 (2)	0.58075 (14)	0.0233 (3)
H2	0.2325	0.4818	0.6665	0.028*
C3	0.2450 (2)	0.7032 (2)	0.55569 (14)	0.0221 (3)
C4	0.2586 (2)	0.7627 (2)	0.43241 (14)	0.0234 (3)
H4	0.2618	0.8919	0.4186	0.028*
C5	0.2672 (2)	0.6275 (2)	0.32976 (14)	0.0223 (3)
H5	0.2752	0.6638	0.2441	0.027*
C6	0.2642 (2)	0.4393 (2)	0.35198 (14)	0.0207 (3)
C7	0.2732 (2)	0.2890 (2)	0.24432 (14)	0.0225 (3)
C8	0.2391 (2)	0.2167 (2)	0.01385 (15)	0.0252 (3)
H8	0.2027	0.0870	0.0392	0.030*
C9	0.4432 (3)	0.2293 (3)	-0.04028 (18)	0.0374 (4)
H9A	0.4766	0.3551	-0.0682	0.056*
H9B	0.4435	0.1358	-0.1145	0.056*
H9C	0.5424	0.2052	0.0265	0.056*
C10	0.0769 (3)	0.2689 (3)	-0.07652 (17)	0.0376 (4)
H10A	-0.0497	0.2638	-0.0331	0.056*
H10B	0.0624	0.1806	-0.1543	0.056*
H10C	0.1125	0.3963	-0.1010	0.056*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0401 (7)	0.0214 (5)	0.0164 (5)	0.0043 (4)	0.0039 (4)	0.0014 (4)
O2	0.0614 (9)	0.0256 (6)	0.0276 (6)	0.0129 (6)	0.0017 (6)	0.0047 (5)
O3	0.0533 (8)	0.0423 (7)	0.0184 (6)	0.0022 (6)	0.0076 (5)	0.0014 (5)
O4	0.0989 (13)	0.0302 (7)	0.0272 (7)	0.0169 (7)	0.0103 (7)	0.0003 (5)
N1	0.0359 (8)	0.0324 (7)	0.0185 (6)	0.0060 (6)	0.0028 (5)	0.0004 (5)
C1	0.0229 (7)	0.0240 (7)	0.0218 (7)	0.0027 (6)	0.0012 (5)	0.0071 (5)
C2	0.0234 (7)	0.0296 (8)	0.0174 (6)	0.0024 (6)	0.0014 (5)	0.0061 (5)
C3	0.0223 (7)	0.0275 (7)	0.0165 (6)	0.0035 (6)	0.0021 (5)	0.0006 (5)
C4	0.0290 (8)	0.0229 (7)	0.0191 (7)	0.0046 (6)	0.0025 (6)	0.0035 (5)
C5	0.0265 (8)	0.0257 (7)	0.0158 (6)	0.0043 (6)	0.0036 (5)	0.0047 (5)
C6	0.0197 (7)	0.0245 (7)	0.0183 (6)	0.0030 (5)	0.0021 (5)	0.0034 (5)
C7	0.0245 (7)	0.0234 (7)	0.0201 (7)	0.0030 (6)	0.0030 (5)	0.0041 (5)
C8	0.0341 (9)	0.0198 (7)	0.0209 (7)	0.0016 (6)	0.0039 (6)	-0.0021 (5)
C9	0.0406 (10)	0.0350 (9)	0.0352 (9)	0.0023 (7)	0.0103 (8)	-0.0087 (7)
C10	0.0462 (11)	0.0389 (10)	0.0276 (8)	0.0134 (8)	-0.0034 (7)	-0.0064 (7)

Geometric parameters (\AA , $^\circ$)

O1—C7	1.3309 (18)	C4—H4	0.9500
O1—C8	1.4741 (18)	C5—C6	1.390 (2)

supplementary materials

O2—C7	1.2067 (19)	C5—H5	0.9500
O3—N1	1.2255 (18)	C6—C7	1.497 (2)
O4—N1	1.221 (2)	C8—C9	1.503 (2)
N1—C3	1.471 (2)	C8—C10	1.506 (2)
C1—C2	1.387 (2)	C8—H8	1.0000
C1—C6	1.396 (2)	C9—H9A	0.9800
C1—H1	0.9500	C9—H9B	0.9800
C2—C3	1.380 (2)	C9—H9C	0.9800
C2—H2	0.9500	C10—H10A	0.9800
C3—C4	1.387 (2)	C10—H10B	0.9800
C4—C5	1.390 (2)	C10—H10C	0.9800
C7—O1—C8	117.82 (12)	O2—C7—O1	124.91 (14)
O4—N1—O3	123.35 (14)	O2—C7—C6	123.18 (14)
O4—N1—C3	118.42 (13)	O1—C7—C6	111.91 (13)
O3—N1—C3	118.23 (14)	O1—C8—C9	108.43 (13)
C2—C1—C6	120.08 (14)	O1—C8—C10	105.50 (13)
C2—C1—H1	120.0	C9—C8—C10	114.14 (15)
C6—C1—H1	120.0	O1—C8—H8	109.5
C3—C2—C1	118.24 (14)	C9—C8—H8	109.5
C3—C2—H2	120.9	C10—C8—H8	109.5
C1—C2—H2	120.9	C8—C9—H9A	109.5
C2—C3—C4	123.15 (14)	C8—C9—H9B	109.5
C2—C3—N1	118.50 (13)	H9A—C9—H9B	109.5
C4—C3—N1	118.34 (14)	C8—C9—H9C	109.5
C3—C4—C5	117.92 (14)	H9A—C9—H9C	109.5
C3—C4—H4	121.0	H9B—C9—H9C	109.5
C5—C4—H4	121.0	C8—C10—H10A	109.5
C4—C5—C6	120.24 (13)	C8—C10—H10B	109.5
C4—C5—H5	119.9	H10A—C10—H10B	109.5
C6—C5—H5	119.9	C8—C10—H10C	109.5
C5—C6—C1	120.35 (13)	H10A—C10—H10C	109.5
C5—C6—C7	122.02 (13)	H10B—C10—H10C	109.5
C1—C6—C7	117.62 (14)		
C6—C1—C2—C3	-1.0 (2)	C4—C5—C6—C7	179.97 (14)
C1—C2—C3—C4	0.1 (2)	C2—C1—C6—C5	1.2 (2)
C1—C2—C3—N1	178.46 (13)	C2—C1—C6—C7	-179.10 (14)
O4—N1—C3—C2	177.20 (16)	C8—O1—C7—O2	2.8 (2)
O3—N1—C3—C2	-3.3 (2)	C8—O1—C7—C6	-176.78 (12)
O4—N1—C3—C4	-4.3 (2)	C5—C6—C7—O2	168.27 (16)
O3—N1—C3—C4	175.17 (15)	C1—C6—C7—O2	-11.5 (2)
C2—C3—C4—C5	0.8 (2)	C5—C6—C7—O1	-12.1 (2)
N1—C3—C4—C5	-177.64 (14)	C1—C6—C7—O1	168.17 (13)
C3—C4—C5—C6	-0.6 (2)	C7—O1—C8—C9	-96.71 (16)
C4—C5—C6—C1	-0.3 (2)	C7—O1—C8—C10	140.63 (15)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
---------------	-------	-------------	-------------	---------------

C1—H1 \cdots O4 ⁱ	0.95	2.46	3.311 (3)	149
C4—H4 \cdots O2 ⁱⁱ	0.95	2.46	3.294 (3)	147

Symmetry codes: (i) $x, y-1, z$; (ii) $x, y+1, z$.

Fig. 1

