Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Methyl 4-nitrobenzoate

Hao Wu,* Min-Hao Xie, Pei Zou, Ya-Ling Liu and Yong-Jun He

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

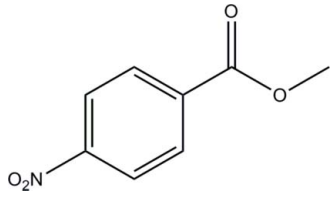
Received 4 November 2009; accepted 10 November 2009

Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.002 Å; R factor = 0.034; wR factor = 0.080; data-to-parameter ratio = 15.0.

In the molecule of the title compound, $C_8H_7NO_4$, the nitro group is approximately coplanar with the benzene ring [dihedral angle = 0.6 (1)°], while the dihedral angle between the methoxycarbonyl group and the benzene ring is 8.8 (1)°. In the crystal structure, weak intermolecular aromatic C—H···$O_{carboxyl}$ and C—H···O_{nitro} hydrogen-bonding interactions are present.

Related literature

For related literature on benzoates, see: Zhang (1992); Zhang *et al.* (1990); Zhang *et al.* (1995).



Experimental

Crystal data

$C_8H_7NO_4$
M_r = 181.15
Monoclinic, $P2_1/c$
a = 7.109 (3) Å
b = 17.092 (6) Å
c = 7.193 (3) Å
β = 116.292 (4)°
V = 783.6 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 93 K
0.43 × 0.40 × 0.10 mm

Data collection

Rigaku SPIDER CCD-detector diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.948, T_{max} = 0.988
6176 measured reflections
1787 independent reflections
1445 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.080
S = 1.00
1787 reflections
119 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O2^{i}	0.95	2.59	3.384 (2)	141
C5—H5···O4^{ii}	0.95	2.58	3.378 (2)	142

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

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.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2018).

References

North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Rigaku (2004). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhang, S. G. (1992). *Technical Book of Fine Chemicals*. Beijing: Science Publishing.
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.

supporting information

Acta Cryst. (2009). E**65**, o3096 [doi:10.1107/S160053680904745X]

Methyl 4-nitrobenzoate

Hao Wu, Min-Hao Xie, Pei Zou, Ya-Ling Liu and Yong-Jun He

S1. Comment

Benzoates are important intermediates in the chemistry of pigments and pharmaceuticals, which are used worldwide (Zhang, 1992; Zhang *et al.*, 1990; Zhang *et al.*, 1995). We report here the crystal structure of methyl 4-nitrobenzoate, $C_8H_7NO_4$ (I). 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, 0.6 (1)°], while the methoxycarbonyl group forms a dihedral angle of 8.8 (1)° with the benzene ring. In the crystal structure, adjacent molecules are linked by weak intermolecular aromatic C—H···$O_{carboxyl}$ and O_{nitro} hydrogen bonds (Table 1).

S2. Experimental

4-Nitrobenzoic acid (5.0 g, 30 mmol) was dissolved in hot methanol (10 ml), then six drops of concentrated sulfuric acid were added. The mixture was stirred at 353 K for 4 h, poured into ice water and stirred for 3 min. After filtering, washing with water and drying in vacuum, a white powder was then obtained (yield: 73%). The crude product was purified by recrystallization from methanol (yield: 51%). Colourless plate-shaped crystals [m.p. 369 (2) K] were obtained after several days, by slow evaporation of a 1:1 (*v*/*v*) methanol-water solution. .

S3. Refinement

Positional parameters of all H atoms were calculated geometrically and were allowed to ride on the C atoms to which they are bonded, with C_{aryl}—H = 0.95 Å, and C_{methyl}—H = 0.98 Å, and with U_{iso}(H) = 1.2U_{eq}(C)

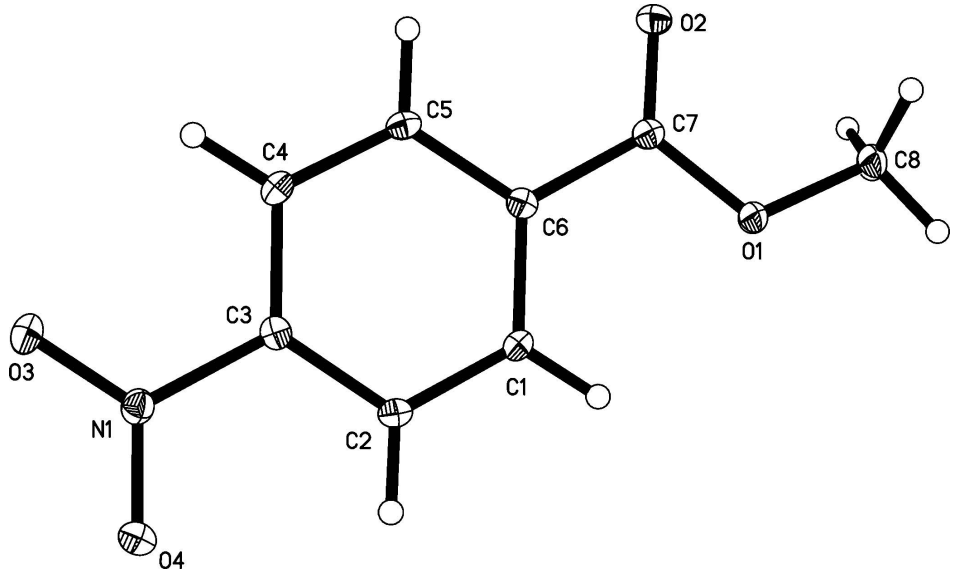


Figure 1

Atom numbering scheme for the title compound (I) with the displacement ellipsoids drawn at the 30% probability level.

Methyl 4-nitrobenzoate

Crystal data

$C_8H_7NO_4$
M_r = 181.15
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 7.109 (3) Å
b = 17.092 (6) Å
c = 7.193 (3) Å
β = 116.292 (4)°
V = 783.6 (5) Å^3
Z = 4
$F(000)$ = 376
D_x = 1.536 Mg m^{-3}
Melting point: 369(2) K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2257 reflections
θ = 3.2–27.4°
μ = 0.13 mm^{-1}
T = 93 K
Plate, colorless
0.43 × 0.40 × 0.10 mm

Data collection

Rigaku SPIDER CCD-detector diffractometer
Radiation source: rotating anode
Graphite monochromator
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.948, T_{max} = 0.988
6176 measured reflections
1787 independent reflections
1445 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.5°, θ_{min} = 3.2°
h = −9→9
k = −20→22
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.080
S = 1.00
1787 reflections
119 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0303P)^2 + 0.336P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.35100 (15)	0.66883 (5)	0.67509 (14)	0.0205 (2)
O2	0.30933 (15)	0.59510 (5)	0.91414 (14)	0.0216 (2)
O3	0.14128 (16)	0.28185 (5)	0.23700 (16)	0.0265 (2)
O4	0.14076 (17)	0.36321 (6)	0.00524 (15)	0.0275 (2)
N1	0.15702 (17)	0.34819 (6)	0.17881 (17)	0.0185 (2)
C1	0.25319 (19)	0.54972 (7)	0.39808 (19)	0.0155 (3)
H1	0.2638	0.6016	0.3563	0.019*
C2	0.21513 (19)	0.48826 (7)	0.2601 (2)	0.0160 (3)
H2	0.2007	0.4971	0.1240	0.019*
C3	0.19872 (19)	0.41347 (7)	0.3264 (2)	0.0155 (3)
C4	0.21927 (19)	0.39748 (7)	0.5240 (2)	0.0167 (3)
H4	0.2065	0.3456	0.5643	0.020*
C5	0.25907 (19)	0.45958 (7)	0.6606 (2)	0.0160 (3)
H5	0.2749	0.4503	0.7970	0.019*
C6	0.27592 (18)	0.53560 (7)	0.59852 (19)	0.0149 (3)
C7	0.31372 (19)	0.60132 (7)	0.7484 (2)	0.0162 (3)
C8	0.3760 (2)	0.73724 (8)	0.8036 (2)	0.0239 (3)
H8A	0.2532	0.7425	0.8310	0.029*
H8B	0.3890	0.7840	0.7313	0.029*
H8C	0.5025	0.7314	0.9351	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0302 (5)	0.0155 (5)	0.0190 (5)	−0.0039 (4)	0.0139 (4)	−0.0029 (4)
O2	0.0259 (5)	0.0241 (5)	0.0167 (5)	−0.0026 (4)	0.0111 (4)	−0.0005 (4)
O3	0.0390 (6)	0.0150 (5)	0.0290 (6)	−0.0025 (4)	0.0182 (5)	0.0006 (4)
O4	0.0437 (6)	0.0225 (5)	0.0202 (5)	−0.0009 (5)	0.0177 (5)	−0.0016 (4)
N1	0.0196 (5)	0.0163 (5)	0.0211 (6)	0.0005 (4)	0.0102 (5)	0.0002 (4)
C1	0.0151 (6)	0.0144 (6)	0.0172 (7)	−0.0002 (5)	0.0075 (5)	0.0022 (5)
C2	0.0152 (6)	0.0189 (6)	0.0142 (6)	0.0007 (5)	0.0067 (5)	0.0024 (5)
C3	0.0132 (6)	0.0160 (6)	0.0172 (6)	0.0011 (5)	0.0066 (5)	−0.0008 (5)

C4	0.0152 (6)	0.0153 (6)	0.0204 (7)	0.0008 (5)	0.0088 (5)	0.0033 (5)
C5	0.0143 (6)	0.0196 (6)	0.0150 (6)	0.0012 (5)	0.0071 (5)	0.0036 (5)
C6	0.0115 (5)	0.0175 (6)	0.0152 (6)	0.0003 (5)	0.0055 (5)	−0.0002 (5)
C7	0.0134 (6)	0.0181 (6)	0.0162 (6)	0.0005 (5)	0.0059 (5)	0.0017 (5)
C8	0.0339 (8)	0.0176 (6)	0.0243 (7)	−0.0055 (6)	0.0167 (6)	−0.0060 (5)

Geometric parameters (Å, º)

O1—C7	1.3429 (15)	C2—H2	0.9500
O1—C8	1.4517 (15)	C3—C4	1.3901 (18)
O2—C7	1.2111 (16)	C4—C5	1.3880 (18)
O3—N1	1.2308 (14)	C4—H4	0.9500
O4—N1	1.2290 (15)	C5—C6	1.3962 (18)
N1—C3	1.4770 (16)	C5—H5	0.9500
C1—C2	1.3872 (18)	C6—C7	1.4965 (18)
C1—C6	1.3988 (18)	C8—H8A	0.9800
C1—H1	0.9500	C8—H8B	0.9800
C2—C3	1.3873 (17)	C8—H8C	0.9800
C7—O1—C8	115.59 (10)	C4—C5—C6	120.30 (12)
O4—N1—O3	123.79 (11)	C4—C5—H5	119.8
O4—N1—C3	118.11 (10)	C6—C5—H5	119.8
O3—N1—C3	118.10 (11)	C5—C6—C1	120.22 (12)
C2—C1—C6	120.25 (12)	C5—C6—C7	118.78 (11)
C2—C1—H1	119.9	C1—C6—C7	120.98 (11)
C6—C1—H1	119.9	O2—C7—O1	123.89 (12)
C1—C2—C3	118.10 (12)	O2—C7—C6	124.65 (11)
C1—C2—H2	121.0	O1—C7—C6	111.46 (11)
C3—C2—H2	121.0	O1—C8—H8A	109.5
C2—C3—C4	123.11 (12)	O1—C8—H8B	109.5
C2—C3—N1	118.00 (11)	H8A—C8—H8B	109.5
C4—C3—N1	118.89 (11)	O1—C8—H8C	109.5
C5—C4—C3	118.01 (12)	H8A—C8—H8C	109.5
C5—C4—H4	121.0	H8B—C8—H8C	109.5
C3—C4—H4	121.0		
C6—C1—C2—C3	0.59 (18)	C4—C5—C6—C1	−0.12 (18)
C1—C2—C3—C4	−0.22 (18)	C4—C5—C6—C7	178.53 (11)
C1—C2—C3—N1	179.66 (11)	C2—C1—C6—C5	−0.43 (18)
O4—N1—C3—C2	0.62 (17)	C2—C1—C6—C7	−179.05 (11)
O3—N1—C3—C2	−179.62 (11)	C8—O1—C7—O2	−3.17 (18)
O4—N1—C3—C4	−179.49 (12)	C8—O1—C7—C6	176.11 (10)
O3—N1—C3—C4	0.27 (17)	C5—C6—C7—O2	−8.15 (19)
C2—C3—C4—C5	−0.31 (18)	C1—C6—C7—O2	170.48 (12)
N1—C3—C4—C5	179.80 (11)	C5—C6—C7—O1	172.58 (11)
C3—C4—C5—C6	0.48 (18)	C1—C6—C7—O1	−8.78 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O1	0.95	2.39	2.7149 (19)	100
C2—H2···O2^{i}	0.95	2.59	3.384 (2)	141
C5—H5···O4^{ii}	0.95	2.58	3.378 (2)	142

Symmetry codes: (i) *x*, *y*, *z*−1; (ii) *x*, *y*, *z*+1.