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# Isopropyl 4-nitrobenzoate

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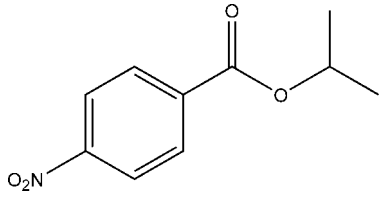
Key indicators: single-crystal X-ray study; $T$ = 153 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.046; $wR$ factor = 0.150; data-to-parameter ratio = 20.7.

In the molecule of the title compound, $C_{10}H_{11}NO_4$, the nitro group is approximately coplanar with the benzene ring [dihedral angle = 4.57 (10)°], while the carboxylate group is slightly twisted, making an angle of 12.16 (8)°. In the crystal, weak intermolecular C—H···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

$C_{10}H_{11}NO_4$
$M_r$ = 209.20
Triclinic, $P\overline{1}$
$a$ = 6.729 (4) Å
$b$ = 7.192 (4) Å
$c$ = 10.388 (6) Å
$\alpha$ = 94.751 (9)°
$\beta$ = 92.503 (7)°
$\gamma$ = 95.901 (10)°
$V$ = 497.6 (5) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.11 mm$^{-1}$
$T$ = 153 K
0.37 × 0.33 × 0.10 mm

### Data collection

Rigaku SPIDER diffractometer
6626 measured reflections
2862 independent reflections
1947 reflections with $I > 2\sigma(I)$
$R_{int}$ = 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
$\Delta\rho_{max}$ = 0.34 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C1—H1···O4$^{i}$ | 0.95 | 2.46 | 3.311 (3) | 149 |
| C4—H4···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*.

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

## References

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Zhang, Z.-S., Wu, J.-G. & Deng, R.-W. (1990). *J. Lanzhou Univ. (Nat. Sci. Ed.)*, **26**, 69–75.

# supporting information

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## Isopropyl 4-nitrobenzoate

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

### S1. 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)°), while the ester group forms a dihedral angle of 12.16 (8)° with the benzene ring. In the crystal structure, adjacent molecules are linked together by weak C—H···O hydrogen bonds (Table 1). $\pi$-$\pi$ 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].

### S2. 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.

### S3. 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 $C_{aromatic}$—H = 0.95 Å, $U_{iso}(H) = 1.2U_{eq}(C_{aromatic})$; $C_{methyl}$—H = 0.98 Å, $U_{iso}(H) = 1.5U_{eq}(C_{methyl})$ and $C_{methylidyne}$—H = 1.00 Å, $U_{iso}(H) = 1.2U_{eq}(C_{methylidyne})$.

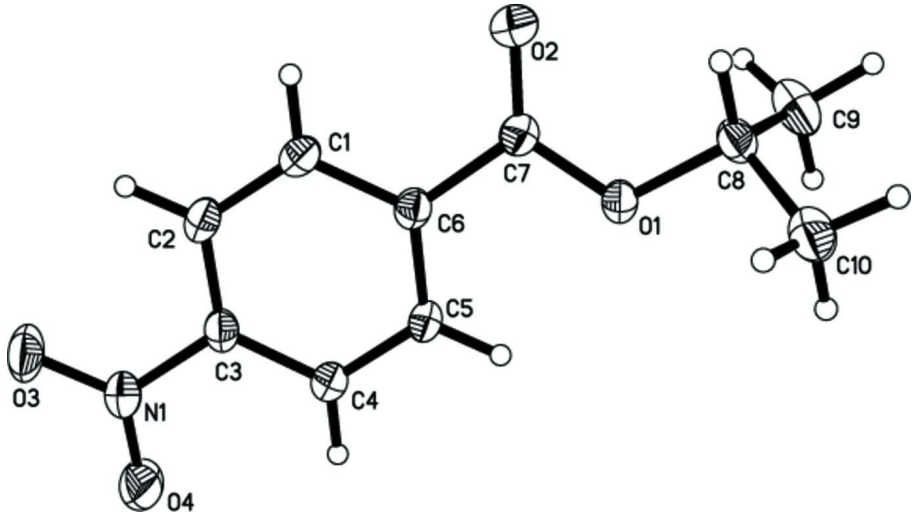


**Figure 1**

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, $P\overline{1}$
Hall symbol: -P 1
$a = 6.729$ (4) Å
$b = 7.192$ (4) Å
$c = 10.388$ (6) Å
$\alpha = 94.751$ (9)°
$\beta = 92.503$ (7)°
$\gamma = 95.901$ (10)°
$V = 497.6$ (5) Å$^3$
$Z = 2$
$F(000) = 220$
$D_x = 1.396$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1490 reflections
$\theta = 2.9$–30.0°
$\mu = 0.11$ mm$^{-1}$
$T = 153$ K
Platelet, colorless
0.37 × 0.33 × 0.10 mm

*Data collection*

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

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.150$
$S = 1.00$
2862 reflections
138 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

$w = 1/[\sigma^2(F_o^2) + (0.071P)^2 + 0.196P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.34$ e Å$^{-3}$
$\Delta\rho_{min} = -0.29$ 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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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 (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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 (Å, º)*

| | | | |
|---|---|---|---|
| O1—C7 | 1.3309 (18) | C4—H4 | 0.9500 |
| O1—C8 | 1.4741 (18) | C5—C6 | 1.390 (2) |
| 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 (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C1—H1···O4$^{i}$ | 0.95 | 2.46 | 3.311 (3) | 149 |
| C4—H4···O2$^{ii}$ | 0.95 | 2.46 | 3.294 (3) | 147 |

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