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2-Methylquinolin-8-yl 2-nitrobenzoate

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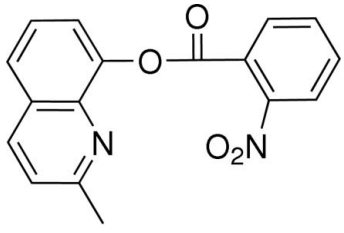
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.103; data-to-parameter ratio = 15.6.

In the title compound, $C_{17}H_{12}N_2O_4$, the quinoline ring system is essentially planar. The ester group is twisted away from the quinoline ring system and nitrobenzene ring by 84.83 (3) and 80.56 (4)°, respectively. The crystal packing is stabilized by C—H···O intermolecular hydrogen bonds, and π–π interactions between the quinoline ring systems of inversion-related molecules, with a centroid–centroid distance of 3.6346 (6) Å.

Related literature

For applications of quinoline benzoate derivatives, see: Zhang *et al.* (2005); Cheng *et al.* (2006).



Experimental

Crystal data

$C_{17}H_{12}N_2O_4$
M_r = 308.29
Triclinic, $P\overline{1}$
a = 7.6661 (4) Å
b = 8.1331 (3) Å
c = 12.3871 (5) Å
α = 95.979 (1)°
β = 105.389 (2)°
γ = 100.749 (1)°
V = 721.88 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 153 (2) K
0.58 × 0.54 × 0.35 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: none
7096 measured reflections
3266 independent reflections
2892 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.103
S = 1.00
3266 reflections
210 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O2^{i}	0.95	2.53	3.3790 (13)	148
C4—H4···O4^{ii}	0.95	2.49	3.4277 (13)	168
C6—H6···O4^{iii}	0.95	2.58	3.4965 (14)	163
C15—H15···O2^{iv}	0.95	2.49	3.2698 (12)	140

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

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2478).

References

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supplementary materials

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2-Methylquinolin-8-yl 2-nitrobenzoate

G. Lei

Comment

8-Hydroxyquinoline benzoate derivatives are a class of chemosensors for metal ions (Zhang *et al.*, 2005; Cheng *et al.*, 2006). We report here the crystal structure of the title compound, (I).

Bond lengths and angles in (I) are normal. The quinoline ring system is planar, with a maximum deviation of 0.019 (4)Å for atom C3. The ester group is twisted away from the planes of the attached rings (Fig. 1). The dihedral angle between the N1/C2—C10 and O1/O2/C12/C13 planes is 84.83 (3)°, and that between O1/O2/C12/C13 and C13—C18 planes is 80.56 (4)°. The C13—C18 and N2/O3/O4/C18 planes form a dihedral angle of 13.18 (4)°. The crystal packing is stabilized by C—H···O hydrogen bonds (Table 1), and π-π interactions between the quinoline ring systems of the inversion-related molecules at (*x*, *y*, *z*) and (1 − *x*, 1 − *y*, −*z*), with a centroid–centroid distance of 3.6346 (6) Å.

Experimental

Compound (I) was prepared according to the procedure of Zhang *et al.* (2005). Colourless single crystals suitable for X-ray diffraction were obtained by recrystallization from ethyl acetate.

Refinement

All H atoms were placed in calculated positions, with C—H = 0.95 or 0.98 Å, and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

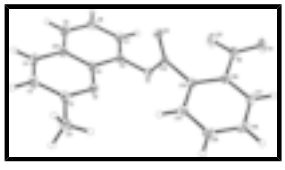


Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids.

2-Methylquinolin-8-yl 2-nitrobenzoate

Crystal data

$C_{17}H_{12}N_2O_4$	$Z = 2$
$M_r = 308.29$	$F_{000} = 320$
Triclinic, $P\overline{1}$	$D_x = 1.418$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å

a = 7.6661 (4) Å	Cell parameters from 6275 reflections
b = 8.1331 (3) Å	θ = 3.3–27.5º
c = 12.3871 (5) Å	μ = 0.10 mm^{-1}
α = 95.979 (1)º	T = 153 (2) K
β = 105.389 (2)º	Block, colourless
γ = 100.749 (1)º	0.58 × 0.54 × 0.35 mm
V = 721.88 (6) $Å^3$	

Data collection

Rigaku R-AXIS RAPID diffractometer	2892 reflections with $I > 2\sigma(I)$
Radiation source: Rotating Anode	R_{int} = 0.019
Monochromator: graphite	θ_{max} = 27.5º
T = 153(2) K	θ_{min} = 3.3º
ω scans	h = −9→9
Absorption correction: none	k = −9→10
7096 measured reflections	l = −16→13
3266 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.035	$w = 1/[\sigma^2(F_o^2) + (0.0656P)^2 + 0.1316P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.103	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.00	$\Delta\rho_{max}$ = 0.30 e $Å^{-3}$
3266 reflections	$\Delta\rho_{min}$ = −0.21 e $Å^{-3}$
210 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.081 (8)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.73507 (9)	0.38524 (8)	0.30774 (6)	0.02379 (18)
O2	0.60868 (9)	0.12003 (9)	0.32654 (6)	0.02626 (18)
O3	0.77544 (12)	0.34184 (12)	0.55498 (7)	0.0408 (2)
O4	0.96676 (13)	0.26474 (12)	0.69219 (6)	0.0402 (2)
N1	0.66377 (12)	0.25217 (10)	0.08459 (7)	0.0239 (2)
N2	0.91199 (12)	0.28391 (11)	0.59306 (7)	0.0267 (2)
C2	0.62798 (15)	0.18862 (12)	−0.02351 (9)	0.0274 (2)
C3	0.46019 (17)	0.19190 (14)	−0.10690 (9)	0.0332 (3)
H3	0.4387	0.1427	−0.1836	0.040*
C4	0.33156 (16)	0.26503 (14)	−0.07696 (9)	0.0321 (3)
H4	0.2204	0.2687	−0.1325	0.038*
C5	0.23707 (15)	0.41284 (14)	0.07774 (10)	0.0313 (2)
H5	0.1245	0.4210	0.0255	0.038*
C6	0.27352 (15)	0.47534 (14)	0.19005 (10)	0.0319 (2)
H6	0.1864	0.5261	0.2154	0.038*
C7	0.44085 (15)	0.46453 (13)	0.26868 (9)	0.0273 (2)
H7	0.4665	0.5073	0.3469	0.033*
C8	0.56502 (13)	0.39205 (12)	0.23104 (8)	0.0226 (2)
C9	0.53342 (13)	0.32493 (11)	0.11554 (8)	0.0221 (2)
C10	0.36400 (14)	0.33626 (12)	0.03803 (9)	0.0261 (2)
C11	0.77083 (18)	0.11101 (14)	−0.05889 (10)	0.0357 (3)
H11A	0.8732	0.1112	0.0083	0.043*
H11B	0.8185	0.1769	−0.1109	0.043*
H11C	0.7143	−0.0059	−0.0972	0.043*
C12	0.74052 (13)	0.23497 (12)	0.34368 (7)	0.0198 (2)
C13	0.93617 (13)	0.22311 (12)	0.39880 (8)	0.0209 (2)
C14	1.03825 (14)	0.18029 (14)	0.32710 (9)	0.0286 (2)
H14	0.9882	0.1720	0.2474	0.034*
C15	1.21351 (15)	0.14958 (15)	0.37172 (11)	0.0338 (3)
H15	1.2825	0.1204	0.3222	0.041*
C16	1.28816 (14)	0.16115 (14)	0.48743 (11)	0.0340 (3)
H16	1.4079	0.1396	0.5170	0.041*
C17	1.18880 (14)	0.20419 (13)	0.56056 (9)	0.0290 (2)
H17	1.2391	0.2122	0.6403	0.035*
C18	1.01464 (13)	0.23525 (12)	0.51498 (8)	0.0224 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0232 (4)	0.0227 (4)	0.0204 (3)	0.0044 (3)	−0.0019 (3)	0.0041 (2)
O2	0.0197 (3)	0.0278 (4)	0.0308 (4)	0.0054 (3)	0.0051 (3)	0.0086 (3)
O3	0.0394 (5)	0.0640 (6)	0.0249 (4)	0.0296 (4)	0.0077 (3)	0.0043 (4)
O4	0.0487 (5)	0.0538 (5)	0.0171 (4)	0.0174 (4)	0.0036 (3)	0.0056 (3)
N1	0.0266 (4)	0.0210 (4)	0.0224 (4)	0.0047 (3)	0.0040 (3)	0.0048 (3)

N2	0.0285 (4)	0.0304 (5)	0.0180 (4)	0.0073 (3)	0.0019 (3)	0.0014 (3)
C2	0.0351 (6)	0.0203 (5)	0.0246 (5)	0.0027 (4)	0.0068 (4)	0.0044 (4)
C3	0.0446 (6)	0.0275 (5)	0.0196 (5)	0.0020 (4)	0.0007 (4)	0.0022 (4)
C4	0.0330 (6)	0.0306 (5)	0.0228 (5)	0.0026 (4)	−0.0061 (4)	0.0067 (4)
C5	0.0231 (5)	0.0299 (5)	0.0377 (6)	0.0082 (4)	−0.0005 (4)	0.0115 (4)
C6	0.0282 (5)	0.0299 (5)	0.0410 (6)	0.0122 (4)	0.0099 (5)	0.0108 (4)
C7	0.0308 (5)	0.0247 (5)	0.0266 (5)	0.0074 (4)	0.0070 (4)	0.0056 (4)
C8	0.0220 (5)	0.0202 (4)	0.0219 (5)	0.0041 (3)	−0.0001 (4)	0.0059 (3)
C9	0.0228 (5)	0.0188 (4)	0.0218 (5)	0.0035 (3)	0.0012 (4)	0.0057 (3)
C10	0.0257 (5)	0.0223 (5)	0.0249 (5)	0.0033 (4)	−0.0016 (4)	0.0076 (4)
C11	0.0462 (7)	0.0295 (6)	0.0336 (6)	0.0074 (5)	0.0171 (5)	0.0029 (4)
C12	0.0217 (4)	0.0241 (5)	0.0143 (4)	0.0074 (3)	0.0050 (3)	0.0025 (3)
C13	0.0188 (4)	0.0215 (4)	0.0215 (5)	0.0040 (3)	0.0040 (3)	0.0049 (3)
C14	0.0258 (5)	0.0352 (6)	0.0278 (5)	0.0077 (4)	0.0111 (4)	0.0079 (4)
C15	0.0251 (5)	0.0378 (6)	0.0451 (7)	0.0098 (4)	0.0179 (5)	0.0104 (5)
C16	0.0174 (5)	0.0335 (6)	0.0502 (7)	0.0077 (4)	0.0051 (4)	0.0110 (5)
C17	0.0225 (5)	0.0284 (5)	0.0299 (5)	0.0040 (4)	−0.0021 (4)	0.0061 (4)
C18	0.0208 (5)	0.0218 (5)	0.0212 (5)	0.0033 (3)	0.0020 (4)	0.0026 (3)

Geometric parameters (Å, °)

O1—C12	1.3476 (11)	C7—C8	1.3633 (14)
O1—C8	1.4091 (11)	C7—H7	0.95
O2—C12	1.1970 (12)	C8—C9	1.4169 (13)
O3—N2	1.2282 (11)	C9—C10	1.4208 (13)
O4—N2	1.2244 (11)	C11—H11A	0.98
N1—C2	1.3203 (13)	C11—H11B	0.98
N1—C9	1.3683 (13)	C11—H11C	0.98
N2—C18	1.4669 (13)	C12—C13	1.4998 (12)
C2—C3	1.4268 (15)	C13—C14	1.3887 (14)
C2—C11	1.4982 (16)	C13—C18	1.3898 (13)
C3—C4	1.3530 (17)	C14—C15	1.3903 (15)
C3—H3	0.95	C14—H14	0.95
C4—C10	1.4187 (15)	C15—C16	1.3811 (17)
C4—H4	0.95	C15—H15	0.95
C5—C6	1.3658 (17)	C16—C17	1.3868 (16)
C5—C10	1.4117 (16)	C16—H16	0.95
C5—H5	0.95	C17—C18	1.3859 (13)
C6—C7	1.4138 (14)	C17—H17	0.95
C6—H6	0.95		
C12—O1—C8	114.97 (7)	C5—C10—C9	119.76 (9)
C2—N1—C9	117.53 (9)	C4—C10—C9	116.60 (10)
O4—N2—O3	123.68 (9)	C2—C11—H11A	109.5
O4—N2—C18	118.44 (8)	C2—C11—H11B	109.5
O3—N2—C18	117.88 (8)	H11A—C11—H11B	109.5
N1—C2—C3	122.62 (10)	C2—C11—H11C	109.5
N1—C2—C11	118.09 (10)	H11A—C11—H11C	109.5
C3—C2—C11	119.29 (10)	H11B—C11—H11C	109.5
C4—C3—C2	120.10 (10)	O2—C12—O1	124.81 (8)

C4—C3—H3	120.0	O2—C12—C13	123.67 (8)
C2—C3—H3	120.0	O1—C12—C13	111.29 (8)
C3—C4—C10	119.46 (10)	C14—C13—C18	118.23 (9)
C3—C4—H4	120.3	C14—C13—C12	116.83 (8)
C10—C4—H4	120.3	C18—C13—C12	124.62 (8)
C6—C5—C10	121.08 (9)	C13—C14—C15	120.16 (10)
C6—C5—H5	119.5	C13—C14—H14	119.9
C10—C5—H5	119.5	C15—C14—H14	119.9
C5—C6—C7	120.06 (10)	C16—C15—C14	120.61 (10)
C5—C6—H6	120.0	C16—C15—H15	119.7
C7—C6—H6	120.0	C14—C15—H15	119.7
C8—C7—C6	119.32 (10)	C15—C16—C17	120.17 (9)
C8—C7—H7	120.3	C15—C16—H16	119.9
C6—C7—H7	120.3	C17—C16—H16	119.9
C7—C8—O1	120.01 (9)	C18—C17—C16	118.62 (10)
C7—C8—C9	122.77 (9)	C18—C17—H17	120.7
O1—C8—C9	117.21 (8)	C16—C17—H17	120.7
N1—C9—C8	119.31 (8)	C17—C18—C13	122.21 (9)
N1—C9—C10	123.67 (9)	C17—C18—N2	118.26 (9)
C8—C9—C10	117.01 (9)	C13—C18—N2	119.52 (8)
C5—C10—C4	123.62 (10)		
C9—N1—C2—C3	−0.68 (15)	N1—C9—C10—C4	0.80 (14)
C9—N1—C2—C11	179.05 (9)	C8—C9—C10—C4	−178.51 (9)
N1—C2—C3—C4	1.30 (16)	C8—O1—C12—O2	−9.72 (13)
C11—C2—C3—C4	−178.44 (10)	C8—O1—C12—C13	164.90 (8)
C2—C3—C4—C10	−0.80 (16)	O2—C12—C13—C14	93.64 (11)
C10—C5—C6—C7	0.22 (16)	O1—C12—C13—C14	−81.05 (10)
C5—C6—C7—C8	0.32 (15)	O2—C12—C13—C18	−79.68 (13)
C6—C7—C8—O1	177.95 (8)	O1—C12—C13—C18	105.63 (10)
C6—C7—C8—C9	−0.53 (15)	C18—C13—C14—C15	0.46 (15)
C12—O1—C8—C7	99.86 (10)	C12—C13—C14—C15	−173.31 (9)
C12—O1—C8—C9	−81.58 (10)	C13—C14—C15—C16	0.01 (16)
C2—N1—C9—C8	178.93 (8)	C14—C15—C16—C17	−0.19 (17)
C2—N1—C9—C10	−0.37 (14)	C15—C16—C17—C18	−0.11 (16)
C7—C8—C9—N1	−179.16 (9)	C16—C17—C18—C13	0.61 (15)
O1—C8—C9—N1	2.33 (13)	C16—C17—C18—N2	−178.83 (9)
C7—C8—C9—C10	0.19 (14)	C14—C13—C18—C17	−0.78 (14)
O1—C8—C9—C10	−178.32 (8)	C12—C13—C18—C17	172.46 (9)
C6—C5—C10—C4	178.22 (10)	C14—C13—C18—N2	178.66 (9)
C6—C5—C10—C9	−0.55 (16)	C12—C13—C18—N2	−8.10 (14)
C3—C4—C10—C5	−178.99 (10)	O4—N2—C18—C17	−13.43 (14)
C3—C4—C10—C9	−0.18 (15)	O3—N2—C18—C17	166.56 (9)
N1—C9—C10—C5	179.66 (9)	O4—N2—C18—C13	167.11 (9)
C8—C9—C10—C5	0.35 (14)	O3—N2—C18—C13	−12.90 (14)

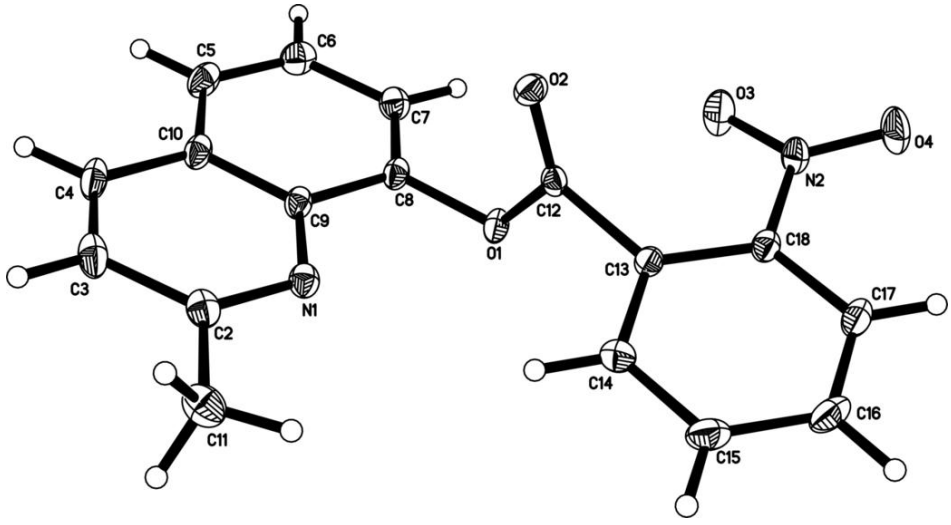
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O2^{i}	0.95	2.53	3.3790 (13)	148

C4—H4···O4^{ii}	0.95	2.49	3.4277 (13)	168
C6—H6···O4^{iii}	0.95	2.58	3.4965 (14)	163
C15—H15···O2^{iv}	0.95	2.49	3.2698 (12)	140

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

Fig. 1


C5
C6
C7
O2
O3
O4
C10
N2
C4
C8
C12
C9
O1
C18
C13
C3
N1
C17
C2
C14
C16
C11
C15