organic compounds

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(*E*)-2-[2-(3-Fluorophenyl)ethenyl]-quinolin-8-yl acetate

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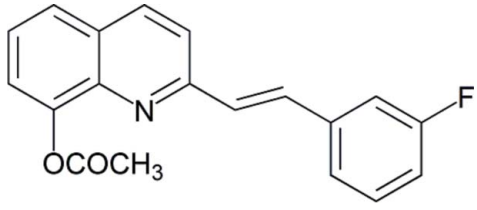
Key indicators: single-crystal X-ray study; T = 110 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.134; data-to-parameter ratio = 15.3.

In the crystal of the title compound, $C_{19}H_{14}FNO_2$, the molecules are linked by C—H···O hydrogen bonds in translational chains along the b axis. The dihedral angles formed by the quinoline system with the fluorobenzene ring and the acetoxy group are 8.15 (3) and 77.42 (4)°, respectively.

Related literature

For the synthetic procedure, see: Zeng *et al.* (2006).



Experimental

Crystal data

$C_{19}H_{14}FNO_2$
M_r = 307.31
Monoclinic, $P2_1/c$
a = 17.628 (3) Å
b = 5.2641 (9) Å
c = 16.062 (3) Å
β = 100.528 (2)°
V = 1465.4 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 110 K
0.35 × 0.24 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.972, T_{max} = 0.982
8139 measured reflections
3177 independent reflections
2663 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.134
S = 1.02
3177 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1D···O2^{i}	0.98 (1)	2.54 (1)	3.495 (2)	166 (2)

Symmetry code: (i) $x, y+1, z$.

Data collection: *SMART* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; 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: LD2060).

References

Bruker (2008). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zeng, H., OuYang, X., Wang, T., Yuan, G., Zhang, G. & Zhang, X. (2006). *Cryst. Growth Des.* **6**, 1697–1702.

supporting information

Acta Cryst. (2012). E**68**, o2420 [https://doi.org/10.1107/S1600536812030255]

(*E*)-2-[2-(3-Fluorophenyl)ethenyl]quinolin-8-yl acetate

Yan-Ping Huo, Xiao-Li Nie and Xiao-Ming Fang

S1. Comment

The (*E*)-2-[2-(3-fluorophenyl)ethenyl]-8-acetoxyquinoline was prepared *via* a reaction of 2-methyl-8-hydroxyquinaldine with 3-fluorobenzaldehyde according to Zeng *et al.* (2006). The molecular structure is shown on Fig. 1. There are non-classical intermolecular hydrogen bonds C–H···O between carbonyl oxygen and the methyl group (C···O = 3.495 (2) Å; C–H···O = 166°) connecting molecules into chains along the *b* axis.

S2. Experimental

The title compound was prepared by a method reported in the literature, see: Zeng *et al.* (2006). The crystals were obtained by dissolving the compound (0.1 g) in dichloromethane (5 ml) and then evaporating the solvent slowly at room temperature for about 3 days.

S3. Refinement

All H atoms were refined as riding atoms with isotropic displacement parameters 1.2 times larger or 1.5 times larger (methyl H) than the corresponding host carbon atoms. The methyl H atoms′ positions were set based using AFIX 33 instruction in *SHELXL97* (Sheldrick, 2008)). The C—H distances were kept at 0.95 Å (0.98 Å for methyl hydrogens).

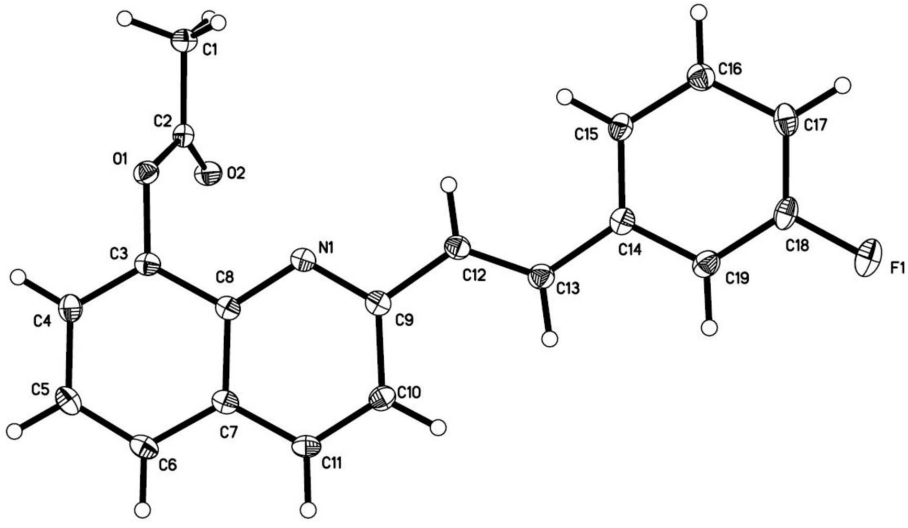

Figure 1

The asymmetric unit of the title compound.

(*E*)-2-[2-(3-Fluorophenyl)ethenyl]quinolin-8-yl acetate

Crystal data

$C_{19}H_{14}FNO_2$
$M_r = 307.31$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 17.628$ (3) Å
$b = 5.2641$ (9) Å
$c = 16.062$ (3) Å
$\beta = 100.528$ (2)°
$V = 1465.4$ (4) Å^3
$Z = 4$
$F(000) = 640$
$D_x = 1.393$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8139 reflections
$\theta = 2.4$–$27.1°$
$\mu = 0.10$ mm^{-1}
$T = 110$ K
Plate, colorless
0.35 × 0.24 × 0.18 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.972$, $T_{max} = 0.982$
8139 measured reflections
3177 independent reflections
2663 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 27.1°$, $\theta_{min} = 2.4°$
$h = -22 \rightarrow 22$
$k = -6 \rightarrow 6$
$l = -20 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.134$
$S = 1.02$
3177 reflections
208 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
$w = 1/[\sigma^2(F_o^2) + (0.0792P)^2 + 0.6625P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.67$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ 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	0.34904 (6)	0.31492 (19)	0.74280 (6)	0.0242 (2)
N1	0.26746 (7)	−0.0961 (2)	0.66528 (7)	0.0220 (3)
F1	−0.13987 (6)	−0.95702 (19)	0.54984 (6)	0.0398 (3)
O2	0.36690 (7)	0.0337 (2)	0.85047 (7)	0.0308 (3)

C9	0.22819 (8)	−0.2876 (3)	0.62482 (8)	0.0225 (3)
C8	0.34042 (8)	−0.0532 (3)	0.65088 (8)	0.0213 (3)
C19	−0.02215 (9)	−0.7381 (3)	0.58416 (9)	0.0279 (3)
H19A	0.0009	−0.8581	0.5523	0.033*
C7	0.37520 (8)	−0.2014 (3)	0.59403 (8)	0.0225 (3)
C14	0.02131 (8)	−0.5360 (3)	0.62403 (9)	0.0236 (3)
C17	−0.13480 (8)	−0.5983 (3)	0.63768 (9)	0.0279 (3)
H17A	−0.1874	−0.6201	0.6420	0.033*
C3	0.38386 (8)	0.1525 (3)	0.69226 (8)	0.0224 (3)
C12	0.14966 (8)	−0.3207 (3)	0.64139 (9)	0.0239 (3)
H12A	0.1314	−0.1968	0.6760	0.029*
C11	0.33106 (8)	−0.4031 (3)	0.55183 (8)	0.0248 (3)
H11A	0.3517	−0.5070	0.5131	0.030*
C4	0.45559 (8)	0.2107 (3)	0.67758 (9)	0.0254 (3)
H4A	0.4828	0.3519	0.7053	0.031*
C6	0.45038 (8)	−0.1410 (3)	0.58087 (9)	0.0263 (3)
H6A	0.4739	−0.2420	0.5436	0.032*
C5	0.48937 (8)	0.0617 (3)	0.62139 (9)	0.0277 (3)
H5A	0.5395	0.1021	0.6116	0.033*
C10	0.25884 (8)	−0.4474 (3)	0.56703 (9)	0.0248 (3)
H10A	0.2289	−0.5835	0.5394	0.030*
C16	−0.09130 (8)	−0.3979 (3)	0.67832 (9)	0.0279 (3)
H16A	−0.1146	−0.2810	0.7110	0.033*
C18	−0.09877 (9)	−0.7629 (3)	0.59126 (9)	0.0275 (3)
C15	−0.01447 (8)	−0.3665 (3)	0.67175 (9)	0.0252 (3)
H15A	0.0141	−0.2287	0.6999	0.030*
C13	0.10159 (8)	−0.5092 (3)	0.61214 (9)	0.0262 (3)
H13A	0.1211	−0.6386	0.5806	0.031*
C2	0.34043 (8)	0.2298 (3)	0.82022 (9)	0.0241 (3)
C1	0.29471 (9)	0.4184 (3)	0.86069 (11)	0.0334 (4)
H1B	0.2887	0.3564	0.9166	0.050*
H1C	0.2437	0.4403	0.8251	0.050*
H1D	0.3218	0.5818	0.8668	0.050*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0275 (5)	0.0202 (5)	0.0253 (5)	0.0016 (4)	0.0058 (4)	−0.0001 (4)
N1	0.0229 (6)	0.0225 (6)	0.0209 (6)	0.0027 (4)	0.0049 (4)	0.0021 (4)
F1	0.0423 (6)	0.0331 (5)	0.0408 (6)	−0.0137 (4)	−0.0008 (4)	−0.0013 (4)
O2	0.0405 (6)	0.0254 (6)	0.0286 (5)	0.0033 (5)	0.0118 (5)	0.0030 (4)
C9	0.0236 (6)	0.0245 (7)	0.0190 (6)	0.0022 (5)	0.0028 (5)	0.0035 (5)
C8	0.0225 (6)	0.0221 (7)	0.0192 (6)	0.0030 (5)	0.0039 (5)	0.0043 (5)
C19	0.0344 (8)	0.0259 (7)	0.0238 (7)	−0.0037 (6)	0.0065 (6)	−0.0017 (6)
C7	0.0245 (7)	0.0250 (7)	0.0183 (6)	0.0044 (5)	0.0044 (5)	0.0046 (5)
C14	0.0273 (7)	0.0232 (7)	0.0198 (6)	−0.0022 (5)	0.0029 (5)	0.0034 (5)
C17	0.0227 (7)	0.0292 (8)	0.0302 (7)	−0.0035 (6)	0.0007 (6)	0.0087 (6)
C3	0.0254 (7)	0.0213 (7)	0.0207 (6)	0.0044 (5)	0.0050 (5)	0.0031 (5)

C12	0.0245 (7)	0.0261 (7)	0.0213 (6)	0.0015 (6)	0.0050 (5)	0.0006 (5)
C11	0.0297 (7)	0.0269 (7)	0.0184 (6)	0.0051 (6)	0.0061 (5)	−0.0002 (5)
C4	0.0250 (7)	0.0252 (7)	0.0253 (7)	−0.0018 (5)	0.0025 (5)	0.0044 (5)
C6	0.0266 (7)	0.0313 (8)	0.0227 (7)	0.0052 (6)	0.0089 (5)	0.0040 (6)
C5	0.0232 (7)	0.0348 (8)	0.0259 (7)	0.0002 (6)	0.0065 (6)	0.0070 (6)
C10	0.0275 (7)	0.0252 (7)	0.0208 (6)	0.0009 (6)	0.0017 (5)	−0.0011 (5)
C16	0.0265 (7)	0.0267 (8)	0.0301 (7)	0.0028 (6)	0.0042 (6)	0.0021 (6)
C18	0.0319 (7)	0.0233 (7)	0.0244 (7)	−0.0082 (6)	−0.0025 (6)	0.0044 (5)
C15	0.0256 (7)	0.0220 (7)	0.0266 (7)	−0.0016 (5)	0.0015 (6)	0.0011 (5)
C13	0.0288 (7)	0.0260 (7)	0.0245 (7)	−0.0007 (6)	0.0070 (6)	−0.0008 (5)
C2	0.0239 (6)	0.0222 (7)	0.0272 (7)	−0.0039 (5)	0.0070 (5)	−0.0016 (5)
C1	0.0351 (8)	0.0267 (8)	0.0424 (9)	0.0000 (6)	0.0177 (7)	−0.0047 (7)

Geometric parameters (Å, º)

O1—C2	1.3561 (17)	C3—C4	1.3627 (19)
O1—C3	1.3962 (17)	C12—C13	1.334 (2)
N1—C9	1.3241 (19)	C12—H12A	0.9500
N1—C8	1.3667 (17)	C11—C10	1.360 (2)
F1—C18	1.3550 (17)	C11—H11A	0.9500
O2—C2	1.1986 (18)	C4—C5	1.407 (2)
C9—C10	1.430 (2)	C4—H4A	0.9500
C9—C12	1.4669 (19)	C6—C5	1.368 (2)
C8—C3	1.419 (2)	C6—H6A	0.9500
C8—C7	1.4221 (19)	C5—H5A	0.9500
C19—C18	1.382 (2)	C10—H10A	0.9500
C19—C14	1.396 (2)	C16—C15	1.387 (2)
C19—H19A	0.9500	C16—H16A	0.9500
C7—C11	1.414 (2)	C15—H15A	0.9500
C7—C6	1.4157 (19)	C13—H13A	0.9500
C14—C15	1.399 (2)	C2—C1	1.500 (2)
C14—C13	1.469 (2)	C1—H1B	0.9800
C17—C18	1.372 (2)	C1—H1C	0.9800
C17—C16	1.394 (2)	C1—H1D	0.9800
C17—H17A	0.9500		
C2—O1—C3	117.75 (11)	C5—C4—H4A	120.0
C9—N1—C8	117.80 (12)	C5—C6—C7	120.43 (13)
N1—C9—C10	122.74 (13)	C5—C6—H6A	119.8
N1—C9—C12	115.29 (12)	C7—C6—H6A	119.8
C10—C9—C12	121.95 (13)	C6—C5—C4	120.35 (13)
N1—C8—C3	119.39 (12)	C6—C5—H5A	119.8
N1—C8—C7	123.20 (13)	C4—C5—H5A	119.8
C3—C8—C7	117.39 (12)	C11—C10—C9	119.54 (13)
C18—C19—C14	119.78 (14)	C11—C10—H10A	120.2
C18—C19—H19A	120.1	C9—C10—H10A	120.2
C14—C19—H19A	120.1	C15—C16—C17	121.03 (14)
C11—C7—C6	123.02 (13)	C15—C16—H16A	119.5

C11—C7—C8	117.10 (12)	C17—C16—H16A	119.5
C6—C7—C8	119.87 (13)	F1—C18—C17	118.95 (14)
C19—C14—C15	118.19 (13)	F1—C18—C19	118.26 (14)
C19—C14—C13	118.33 (13)	C17—C18—C19	122.79 (14)
C15—C14—C13	123.46 (13)	C16—C15—C14	120.65 (14)
C18—C17—C16	117.54 (14)	C16—C15—H15A	119.7
C18—C17—H17A	121.2	C14—C15—H15A	119.7
C16—C17—H17A	121.2	C12—C13—C14	126.22 (14)
C4—C3—O1	118.91 (13)	C12—C13—H13A	116.9
C4—C3—C8	121.92 (13)	C14—C13—H13A	116.9
O1—C3—C8	118.86 (12)	O2—C2—O1	123.76 (13)
C13—C12—C9	125.75 (14)	O2—C2—C1	126.49 (14)
C13—C12—H12A	117.1	O1—C2—C1	109.74 (12)
C9—C12—H12A	117.1	C2—C1—H1B	109.5
C10—C11—C7	119.61 (13)	C2—C1—H1C	109.5
C10—C11—H11A	120.2	H1B—C1—H1C	109.5
C7—C11—H11A	120.2	C2—C1—H1D	109.5
C3—C4—C5	120.02 (14)	H1B—C1—H1D	109.5
C3—C4—H4A	120.0	H1C—C1—H1D	109.5

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*D*···O2^{i}	0.98 (1)	2.54 (1)	3.495 (2)	166 (2)

Symmetry code: (i) *x*, *y*+1, *z*.