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N′-{2-[2-(3-Methoxyphenyl)ethenyl]-phenyl}acetamide

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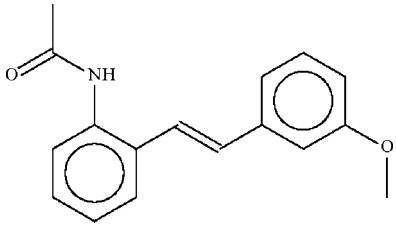
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.052; wR factor = 0.140; data-to-parameter ratio = 17.3.

In the title compound, $C_{17}H_{17}NO_2$, the phenylene rings are bent with respect to the carbon–carbon double bond [dihedral angle between rings = 39.6 (1)°]. The acetamido group is twisted out of the plane of the aromatic ring [dihedral angle = 44.2 (1)°] in order to form an N–H···O hydrogen bond to the acetamido group of an adjacent molecule, generating a zigzag chain running along the *c* axis.

Related literature

The compound was synthesized in a study on indolostilbenes; see: Ahmad *et al.* (2009).



Experimental

Crystal data

$C_{17}H_{17}NO_2$
M_r = 267.32
Monoclinic, $P2_1/c$
a = 14.5588 (5) Å
b = 10.3633 (4) Å
c = 9.3667 (3) Å
β = 90.118 (1)°
V = 1413.22 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 K
0.21 × 0.07 × 0.02 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
12919 measured reflections
3236 independent reflections
2036 reflections with $I > 2\sigma(I)$
R_{int} = 0.069

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.140
S = 1.01
3236 reflections
187 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.88 (1)	1.93 (1)	2.804 (2)	175 (2)

Symmetry code: (i) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

Data collection: *APEX2* software (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: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

We thank the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2514).

References

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Bruker (2008). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
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supporting information

Acta Cryst. (2009). E**65**, o1290 [doi:10.1107/S1600536809017401]

N′-{2-[2-(3-Methoxyphenyl)ethenyl]phenyl}acetamide

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S1. Experimental

The compound was synthesized in a study on indolostilbenes (Ahmad *et al.*, 2009). Crystals were grown from its solution in ethyl acetate.

S2. Refinement

Hydrogen atoms were placed at calculated positions (C–H 0.95–0.98 Å) and were treated as riding on their parent carbon atoms, with *U*(H) set to 1.2–1.5 times *U*~eq~(*C*). The amino H-atom was located in a difference Fourier map, and was refined with a distance restraint of N–H 0.88±0.01 Å; its temperature factor was refined.

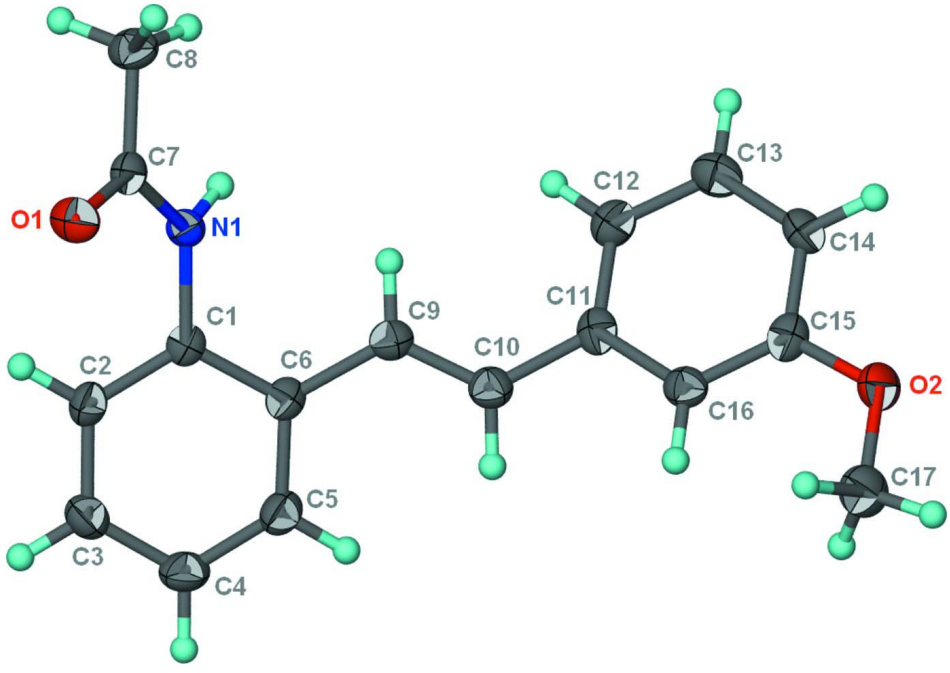

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_{17}H_{17}NO_2$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

N′-{2-[2-(3-Methoxyphenyl)ethenyl]phenyl}acetamide

Crystal data

$C_{17}H_{17}NO_2$
M_r = 267.32

Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc

a = 14.5588 (5) Å
b = 10.3633 (4) Å
c = 9.3667 (3) Å
β = 90.118 (1)°
V = 1413.22 (9) Å^3
Z = 4
F(000) = 568
D_x = 1.256 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1682 reflections
θ = 2.4–27.7°
μ = 0.08 mm^{-1}
T = 100 K
Plate, colorless
0.21 × 0.07 × 0.02 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
12919 measured reflections
3236 independent reflections

2036 reflections with $I > 2\sigma(I)$
R_{int} = 0.069
θ_{max} = 27.5°, θ_{min} = 1.4°
h = −18→18
k = −13→13
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.140
S = 1.01
3236 reflections
187 parameters
1 restraint
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0657P)^2 + 0.3754P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
O1	0.11400 (10)	0.71029 (14)	0.73510 (14)	0.0246 (4)
O2	0.65965 (10)	0.58338 (15)	0.10659 (16)	0.0273 (4)
N1	0.12402 (11)	0.66372 (17)	0.49961 (17)	0.0177 (4)
H1	0.1185 (16)	0.699 (2)	0.4151 (15)	0.032 (7)*
C1	0.14037 (13)	0.5285 (2)	0.5123 (2)	0.0172 (4)
C2	0.08867 (14)	0.4550 (2)	0.6068 (2)	0.0204 (5)
H2	0.0432	0.4955	0.6639	0.024*
C3	0.10283 (14)	0.3241 (2)	0.6183 (2)	0.0243 (5)
H3	0.0686	0.2749	0.6853	0.029*
C4	0.16751 (15)	0.2639 (2)	0.5315 (2)	0.0269 (5)
H4	0.1771	0.1734	0.5382	0.032*
C5	0.21760 (14)	0.3364 (2)	0.4357 (2)	0.0236 (5)
H5	0.2601	0.2941	0.3746	0.028*
C6	0.20754 (13)	0.4707 (2)	0.4259 (2)	0.0185 (4)
C7	0.10934 (13)	0.7448 (2)	0.6095 (2)	0.0187 (4)
C8	0.08548 (16)	0.8812 (2)	0.5694 (2)	0.0257 (5)
H8A	0.1255	0.9410	0.6216	0.038*
H8B	0.0213	0.8985	0.5941	0.038*

H8C	0.0941	0.8931	0.4665	0.038*
C9	0.26855 (14)	0.5474 (2)	0.3343 (2)	0.0208 (5)
H9	0.2507	0.6338	0.3145	0.025*
C10	0.34701 (14)	0.5057 (2)	0.2767 (2)	0.0222 (5)
H10	0.3623	0.4177	0.2919	0.027*
C11	0.41182 (14)	0.5822 (2)	0.1925 (2)	0.0206 (5)
C12	0.38525 (15)	0.6915 (2)	0.1148 (2)	0.0242 (5)
H12	0.3230	0.7191	0.1156	0.029*
C13	0.45036 (16)	0.7595 (2)	0.0361 (2)	0.0261 (5)
H13	0.4322	0.8334	−0.0168	0.031*
C14	0.54070 (15)	0.7208 (2)	0.0343 (2)	0.0223 (5)
H14	0.5844	0.7671	−0.0208	0.027*
C15	0.56799 (14)	0.6138 (2)	0.1129 (2)	0.0218 (5)
C16	0.50366 (14)	0.5444 (2)	0.1902 (2)	0.0212 (5)
H16	0.5224	0.4701	0.2421	0.025*
C17	0.69172 (16)	0.4821 (2)	0.1966 (2)	0.0302 (5)
H17A	0.7586	0.4749	0.1882	0.045*
H17B	0.6631	0.4005	0.1677	0.045*
H17C	0.6755	0.5012	0.2959	0.045*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0362 (9)	0.0232 (8)	0.0144 (7)	0.0009 (7)	0.0007 (6)	−0.0012 (6)
O2	0.0182 (8)	0.0272 (9)	0.0366 (9)	−0.0019 (6)	0.0023 (6)	0.0044 (7)
N1	0.0207 (9)	0.0181 (9)	0.0144 (8)	0.0017 (7)	0.0011 (7)	0.0019 (7)
C1	0.0157 (10)	0.0204 (11)	0.0156 (9)	0.0000 (8)	−0.0024 (8)	−0.0020 (8)
C2	0.0162 (10)	0.0245 (11)	0.0203 (10)	0.0016 (9)	0.0011 (8)	0.0000 (9)
C3	0.0232 (12)	0.0231 (12)	0.0266 (11)	−0.0028 (9)	0.0005 (9)	0.0043 (9)
C4	0.0252 (12)	0.0170 (11)	0.0387 (13)	−0.0006 (9)	−0.0006 (10)	−0.0002 (10)
C5	0.0186 (11)	0.0227 (12)	0.0296 (11)	0.0013 (9)	0.0017 (9)	−0.0028 (10)
C6	0.0150 (10)	0.0210 (11)	0.0195 (10)	−0.0009 (8)	−0.0022 (8)	−0.0026 (9)
C7	0.0150 (10)	0.0214 (11)	0.0196 (10)	−0.0007 (8)	0.0010 (8)	−0.0007 (8)
C8	0.0349 (13)	0.0208 (12)	0.0213 (10)	0.0048 (9)	0.0023 (9)	−0.0014 (9)
C9	0.0212 (11)	0.0190 (11)	0.0220 (10)	0.0008 (9)	−0.0011 (8)	−0.0008 (9)
C10	0.0247 (12)	0.0197 (11)	0.0222 (10)	0.0001 (9)	0.0010 (9)	−0.0009 (9)
C11	0.0225 (11)	0.0233 (11)	0.0160 (9)	−0.0030 (9)	0.0018 (8)	−0.0051 (9)
C12	0.0220 (11)	0.0268 (12)	0.0238 (11)	0.0020 (9)	−0.0007 (9)	−0.0017 (10)
C13	0.0313 (13)	0.0237 (12)	0.0234 (11)	−0.0005 (10)	−0.0024 (9)	0.0028 (9)
C14	0.0241 (12)	0.0215 (11)	0.0213 (10)	−0.0055 (9)	0.0013 (8)	0.0016 (9)
C15	0.0182 (11)	0.0254 (12)	0.0218 (10)	−0.0016 (9)	−0.0005 (8)	−0.0055 (9)
C16	0.0238 (11)	0.0194 (11)	0.0203 (10)	0.0004 (9)	−0.0001 (8)	−0.0007 (9)
C17	0.0205 (12)	0.0338 (14)	0.0361 (13)	−0.0009 (10)	−0.0031 (10)	0.0052 (11)

Geometric parameters (Å, º)

O1—C7	1.231 (2)	C8—H8B	0.9800
O2—C15	1.373 (2)	C8—H8C	0.9800

O2—C17	1.424 (3)	C9—C10	1.336 (3)
N1—C7	1.346 (3)	C9—H9	0.9500
N1—C1	1.426 (3)	C10—C11	1.464 (3)
N1—H1	0.877 (10)	C10—H10	0.9500
C1—C2	1.391 (3)	C11—C16	1.394 (3)
C1—C6	1.405 (3)	C11—C12	1.400 (3)
C2—C3	1.376 (3)	C12—C13	1.393 (3)
C2—H2	0.9500	C12—H12	0.9500
C3—C4	1.393 (3)	C13—C14	1.375 (3)
C3—H3	0.9500	C13—H13	0.9500
C4—C5	1.380 (3)	C14—C15	1.388 (3)
C4—H4	0.9500	C14—H14	0.9500
C5—C6	1.402 (3)	C15—C16	1.386 (3)
C5—H5	0.9500	C16—H16	0.9500
C6—C9	1.470 (3)	C17—H17A	0.9800
C7—C8	1.504 (3)	C17—H17B	0.9800
C8—H8A	0.9800	C17—H17C	0.9800

C15—O2—C17	117.48 (17)	C10—C9—C6	125.4 (2)
C7—N1—C1	125.17 (17)	C10—C9—H9	117.3
C7—N1—H1	114.4 (16)	C6—C9—H9	117.3
C1—N1—H1	120.2 (16)	C9—C10—C11	126.5 (2)
C2—C1—C6	120.73 (19)	C9—C10—H10	116.7
C2—C1—N1	120.06 (18)	C11—C10—H10	116.7
C6—C1—N1	119.19 (18)	C16—C11—C12	118.93 (19)
C3—C2—C1	120.6 (2)	C16—C11—C10	118.36 (19)
C3—C2—H2	119.7	C12—C11—C10	122.71 (19)
C1—C2—H2	119.7	C13—C12—C11	119.8 (2)
C2—C3—C4	119.8 (2)	C13—C12—H12	120.1
C2—C3—H3	120.1	C11—C12—H12	120.1
C4—C3—H3	120.1	C14—C13—C12	120.7 (2)
C5—C4—C3	119.6 (2)	C14—C13—H13	119.6
C5—C4—H4	120.2	C12—C13—H13	119.6
C3—C4—H4	120.2	C13—C14—C15	119.9 (2)
C4—C5—C6	121.8 (2)	C13—C14—H14	120.0
C4—C5—H5	119.1	C15—C14—H14	120.0
C6—C5—H5	119.1	O2—C15—C16	124.12 (19)
C5—C6—C1	117.31 (19)	O2—C15—C14	115.96 (18)
C5—C6—C9	120.78 (19)	C16—C15—C14	119.9 (2)
C1—C6—C9	121.83 (19)	C15—C16—C11	120.7 (2)
O1—C7—N1	122.77 (19)	C15—C16—H16	119.6
O1—C7—C8	121.59 (18)	C11—C16—H16	119.6
N1—C7—C8	115.64 (17)	O2—C17—H17A	109.5
C7—C8—H8A	109.5	O2—C17—H17B	109.5
C7—C8—H8B	109.5	H17A—C17—H17B	109.5
H8A—C8—H8B	109.5	O2—C17—H17C	109.5
C7—C8—H8C	109.5	H17A—C17—H17C	109.5
H8A—C8—H8C	109.5	H17B—C17—H17C	109.5

H8B—C8—H8C	109.5		
C7—N1—C1—C2	42.6 (3)	C1—C6—C9—C10	162.9 (2)
C7—N1—C1—C6	−138.9 (2)	C6—C9—C10—C11	−175.99 (18)
C6—C1—C2—C3	0.5 (3)	C9—C10—C11—C16	154.0 (2)
N1—C1—C2—C3	178.97 (18)	C9—C10—C11—C12	−25.9 (3)
C1—C2—C3—C4	−2.0 (3)	C16—C11—C12—C13	0.5 (3)
C2—C3—C4—C5	0.7 (3)	C10—C11—C12—C13	−179.63 (19)
C3—C4—C5—C6	2.1 (3)	C11—C12—C13—C14	−0.2 (3)
C4—C5—C6—C1	−3.5 (3)	C12—C13—C14—C15	−0.9 (3)
C4—C5—C6—C9	173.33 (19)	C17—O2—C15—C16	−6.6 (3)
C2—C1—C6—C5	2.2 (3)	C17—O2—C15—C14	174.07 (18)
N1—C1—C6—C5	−176.28 (18)	C13—C14—C15—O2	−179.00 (19)
C2—C1—C6—C9	−174.62 (18)	C13—C14—C15—C16	1.7 (3)
N1—C1—C6—C9	6.9 (3)	O2—C15—C16—C11	179.34 (19)
C1—N1—C7—O1	4.4 (3)	C14—C15—C16—C11	−1.4 (3)
C1—N1—C7—C8	−174.86 (18)	C12—C11—C16—C15	0.3 (3)
C5—C6—C9—C10	−13.8 (3)	C10—C11—C16—C15	−179.58 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.88 (1)	1.93 (1)	2.804 (2)	175 (2)

Symmetry code: (i) x, $-y+3/2$, $z-1/2$.