Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N′-{2-[2-(4-Methoxyphenyl)ethenyl]-phenyl}acetamide

Kartini Ahmad, Noel F. Thomas, Mohd Fadzli Din, Khalijah Awang and Seik Weng Ng*

Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

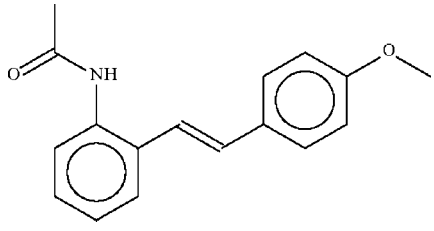
Received 5 May 2009; accepted 8 May 2009

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.033; wR factor = 0.096; data-to-parameter ratio = 8.8.

In the title compound, $C_{17}H_{17}NO_2$, the phenylene rings are nearly coplanar [dihedral angle 7.3 (1)°]. The acetamido group is twisted out of the plane of the aromatic ring in order to form an N–H···O hydrogen bond to the acetamido group of an adjacent molecule, generating a helical chain running along the *b* 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, $P2_1$
a = 5.4225 (1) Å
b = 9.4222 (2) Å
c = 13.5653 (3) Å
β = 98.402 (1)°
V = 685.64 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.25 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
4781 measured reflections
1654 independent reflections
1605 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.096
S = 1.05
1654 reflections
187 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 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)	2.03 (1)	2.895 (2)	169 (2)

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

Data collection: *APEX2* (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: HG2513).

References

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supplementary materials

Acta Cryst. (2009). E**65**, o1289 [**doi:10.1107/S1600536809017395**]

N'-{2-[2-(4-Methoxyphenyl)ethenyl]phenyl}acetamide

K. Ahmad, N. F. Thomas, M. F. Din, K. Awang and S. W. Ng

Comment

(type here to add)

Experimental

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

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. Friedel pairs were merged.

Figures

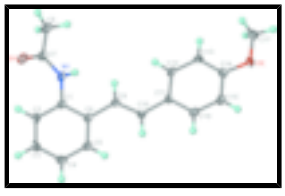

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $C_{17}H_{17}NO_2$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

N'-{2-[2-(4-Methoxyphenyl)ethenyl]phenyl}acetamide

Crystal data

$C_{17}H_{17}NO_2$	F_{000} = 284
M_r = 267.32	D_x = 1.295 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 3188 reflections
a = 5.4225 (1) Å	θ = 2.6–28.3º
b = 9.4222 (2) Å	μ = 0.09 mm^{-1}
c = 13.5653 (3) Å	T = 100 K
β = 98.402 (1)º	Block, colorless
V = 685.64 (2) Å^3	0.25 × 0.20 × 0.20 mm
Z = 2	

Data collection

Bruker SMART APEX diffractometer	1605 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.016$
Monochromator: graphite	$\theta_{max} = 27.5^{o}$
$T = 100$ K	$\theta_{min} = 1.5^{o}$
ω scans	$h = -7\rightarrow6$
Absorption correction: None	$k = -11\rightarrow12$
4781 measured reflections	$l = -17\rightarrow17$
1654 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.033$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.096$	$w = 1/[\sigma^2(F_o^2) + (0.0726P)^2 + 0.080P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
1654 reflections	$\Delta\rho_{max} = 0.25$ e Å^{-3}
187 parameters	$\Delta\rho_{min} = -0.22$ e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.5611 (2)	−0.00004 (14)	0.48762 (9)	0.0210 (3)
O2	0.0298 (2)	0.84291 (14)	0.93515 (9)	0.0198 (3)
N1	0.6516 (3)	0.22034 (16)	0.55197 (10)	0.0142 (3)
H1	0.597 (4)	0.3083 (13)	0.5476 (17)	0.021 (6)*
C1	0.8511 (3)	0.18307 (17)	0.62796 (11)	0.0137 (3)
C2	1.0223 (3)	0.07880 (19)	0.60968 (12)	0.0167 (3)
H2	0.9996	0.0294	0.5480	0.020*
C3	1.2247 (3)	0.0471 (2)	0.68092 (13)	0.0178 (3)
H3	1.3400	−0.0242	0.6683	0.021*
C4	1.2586 (3)	0.12030 (19)	0.77122 (13)	0.0186 (4)
H4	1.3989	0.1001	0.8198	0.022*
C5	1.0881 (3)	0.22226 (19)	0.79020 (12)	0.0163 (3)
H5	1.1130	0.2709	0.8522	0.020*
C6	0.8790 (3)	0.25582 (17)	0.72004 (12)	0.0134 (3)
C7	0.5199 (3)	0.12874 (19)	0.48755 (12)	0.0154 (3)
C8	0.3184 (3)	0.1947 (2)	0.41365 (12)	0.0197 (4)

H8A	0.1965	0.1219	0.3881	0.030*
H8B	0.3925	0.2354	0.3583	0.030*
H8C	0.2351	0.2697	0.4465	0.030*
C9	0.6925 (3)	0.36010 (18)	0.74194 (12)	0.0138 (3)
H9	0.5492	0.3725	0.6934	0.017*
C10	0.7082 (3)	0.43902 (18)	0.82474 (12)	0.0139 (3)
H10	0.8543	0.4281	0.8721	0.017*
C11	0.5219 (3)	0.54060 (17)	0.84945 (12)	0.0133 (3)
C12	0.3218 (3)	0.58920 (19)	0.78032 (12)	0.0167 (3)
H12	0.2993	0.5521	0.7145	0.020*
C13	0.1558 (3)	0.6903 (2)	0.80590 (12)	0.0176 (4)
H13	0.0238	0.7230	0.7574	0.021*
C14	0.1830 (3)	0.74359 (17)	0.90263 (13)	0.0159 (3)
C15	0.3793 (3)	0.6960 (2)	0.97288 (12)	0.0174 (3)
H15	0.3988	0.7316	1.0391	0.021*
C16	0.5455 (3)	0.59685 (19)	0.94598 (12)	0.0166 (3)
H16	0.6794	0.5661	0.9943	0.020*
C17	−0.1752 (3)	0.8937 (2)	0.86533 (13)	0.0195 (4)
H17A	−0.2719	0.9622	0.8983	0.029*
H17B	−0.2822	0.8138	0.8405	0.029*
H17C	−0.1116	0.9399	0.8094	0.029*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0263 (7)	0.0130 (6)	0.0215 (6)	0.0003 (5)	−0.0038 (5)	−0.0027 (5)
O2	0.0180 (6)	0.0207 (7)	0.0199 (6)	0.0059 (5)	0.0003 (4)	−0.0056 (5)
N1	0.0181 (7)	0.0110 (6)	0.0128 (6)	0.0011 (5)	−0.0004 (5)	−0.0001 (5)
C1	0.0146 (7)	0.0124 (8)	0.0138 (7)	−0.0028 (6)	0.0010 (6)	0.0009 (6)
C2	0.0195 (8)	0.0147 (8)	0.0164 (7)	−0.0003 (6)	0.0038 (6)	−0.0019 (6)
C3	0.0163 (7)	0.0163 (8)	0.0214 (8)	0.0033 (7)	0.0051 (6)	0.0014 (7)
C4	0.0145 (7)	0.0181 (8)	0.0221 (8)	0.0011 (7)	−0.0005 (6)	0.0026 (7)
C5	0.0171 (8)	0.0165 (8)	0.0146 (7)	−0.0010 (7)	−0.0002 (6)	−0.0011 (6)
C6	0.0157 (8)	0.0107 (7)	0.0139 (7)	−0.0019 (6)	0.0019 (6)	0.0002 (6)
C7	0.0191 (8)	0.0149 (9)	0.0122 (7)	−0.0011 (6)	0.0021 (6)	−0.0003 (6)
C8	0.0239 (8)	0.0181 (9)	0.0151 (8)	0.0006 (7)	−0.0042 (6)	0.0003 (6)
C9	0.0142 (7)	0.0131 (7)	0.0135 (7)	0.0001 (6)	−0.0003 (5)	0.0003 (6)
C10	0.0160 (7)	0.0115 (7)	0.0139 (7)	0.0002 (6)	0.0014 (5)	0.0020 (6)
C11	0.0153 (7)	0.0108 (8)	0.0140 (7)	−0.0011 (6)	0.0028 (6)	0.0006 (6)
C12	0.0191 (8)	0.0164 (8)	0.0137 (7)	−0.0003 (7)	−0.0004 (6)	−0.0031 (6)
C13	0.0155 (8)	0.0186 (9)	0.0173 (8)	0.0007 (7)	−0.0020 (6)	−0.0021 (7)
C14	0.0151 (7)	0.0126 (8)	0.0203 (8)	−0.0001 (6)	0.0032 (6)	−0.0010 (6)
C15	0.0225 (8)	0.0174 (8)	0.0121 (7)	0.0011 (7)	0.0022 (6)	−0.0019 (6)
C16	0.0194 (8)	0.0161 (8)	0.0134 (7)	0.0015 (7)	−0.0008 (6)	0.0008 (6)
C17	0.0165 (8)	0.0179 (8)	0.0236 (8)	0.0030 (7)	0.0012 (6)	0.0005 (7)

Geometric parameters (Å, °)

O1—C7	1.234 (2)	C8—H8B	0.9800

O2—C14	1.367 (2)	C8—H8C	0.9800
O2—C17	1.433 (2)	C9—C10	1.339 (2)
N1—C7	1.355 (2)	C9—H9	0.9500
N1—C1	1.425 (2)	C10—C11	1.465 (2)
N1—H1	0.879 (10)	C10—H10	0.9500
C1—C2	1.398 (2)	C11—C16	1.401 (2)
C1—C6	1.413 (2)	C11—C12	1.403 (2)
C2—C3	1.385 (2)	C12—C13	1.389 (2)
C2—H2	0.9500	C12—H12	0.9500
C3—C4	1.394 (3)	C13—C14	1.393 (2)
C3—H3	0.9500	C13—H13	0.9500
C4—C5	1.383 (2)	C14—C15	1.395 (2)
C4—H4	0.9500	C15—C16	1.384 (2)
C5—C6	1.406 (2)	C15—H15	0.9500
C5—H5	0.9500	C16—H16	0.9500
C6—C9	1.471 (2)	C17—H17A	0.9800
C7—C8	1.505 (2)	C17—H17B	0.9800
C8—H8A	0.9800	C17—H17C	0.9800
C14—O2—C17	117.70 (13)	C10—C9—C6	125.37 (14)
C7—N1—C1	125.62 (15)	C10—C9—H9	117.3
C7—N1—H1	114.7 (15)	C6—C9—H9	117.3
C1—N1—H1	119.5 (15)	C9—C10—C11	126.38 (15)
C2—C1—C6	120.61 (15)	C9—C10—H10	116.8
C2—C1—N1	119.89 (14)	C11—C10—H10	116.8
C6—C1—N1	119.45 (14)	C16—C11—C12	117.21 (15)
C3—C2—C1	120.45 (15)	C16—C11—C10	119.28 (15)
C3—C2—H2	119.8	C12—C11—C10	123.48 (14)
C1—C2—H2	119.8	C13—C12—C11	121.52 (15)
C2—C3—C4	119.71 (16)	C13—C12—H12	119.2
C2—C3—H3	120.1	C11—C12—H12	119.2
C4—C3—H3	120.1	C12—C13—C14	119.98 (15)
C5—C4—C3	120.08 (16)	C12—C13—H13	120.0
C5—C4—H4	120.0	C14—C13—H13	120.0
C3—C4—H4	120.0	O2—C14—C13	124.45 (15)
C4—C5—C6	121.68 (15)	O2—C14—C15	116.02 (14)
C4—C5—H5	119.2	C13—C14—C15	119.53 (15)
C6—C5—H5	119.2	C16—C15—C14	119.89 (15)
C5—C6—C1	117.44 (15)	C16—C15—H15	120.1
C5—C6—C9	121.59 (14)	C14—C15—H15	120.1
C1—C6—C9	120.95 (14)	C15—C16—C11	121.86 (15)
O1—C7—N1	123.22 (16)	C15—C16—H16	119.1
O1—C7—C8	121.35 (16)	C11—C16—H16	119.1
N1—C7—C8	115.43 (16)	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	38.5 (2)	C1—C6—C9—C10	−176.68 (16)
C7—N1—C1—C6	−143.74 (16)	C6—C9—C10—C11	−178.20 (15)
C6—C1—C2—C3	−1.2 (2)	C9—C10—C11—C16	169.14 (16)
N1—C1—C2—C3	176.45 (14)	C9—C10—C11—C12	−12.9 (3)
C1—C2—C3—C4	−0.4 (3)	C16—C11—C12—C13	0.9 (2)
C2—C3—C4—C5	1.2 (3)	C10—C11—C12—C13	−177.13 (16)
C3—C4—C5—C6	−0.4 (3)	C11—C12—C13—C14	−1.3 (3)
C4—C5—C6—C1	−1.1 (2)	C17—O2—C14—C13	1.1 (2)
C4—C5—C6—C9	177.47 (16)	C17—O2—C14—C15	−179.56 (15)
C2—C1—C6—C5	2.0 (2)	C12—C13—C14—O2	−179.96 (16)
N1—C1—C6—C5	−175.74 (15)	C12—C13—C14—C15	0.8 (3)
C2—C1—C6—C9	−176.66 (14)	O2—C14—C15—C16	−179.11 (15)
N1—C1—C6—C9	5.6 (2)	C13—C14—C15—C16	0.2 (3)
C1—N1—C7—O1	−0.4 (3)	C14—C15—C16—C11	−0.7 (3)
C1—N1—C7—C8	−179.72 (14)	C12—C11—C16—C15	0.1 (2)
C5—C6—C9—C10	4.8 (3)	C10—C11—C16—C15	178.23 (16)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.88 (1)	2.03 (1)	2.895 (2)	169 (2)

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+1.

Fig. 1