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3-[4-(Dimethylamino)phenyl]-1-(3-pyridyl)prop-2-en-1-one

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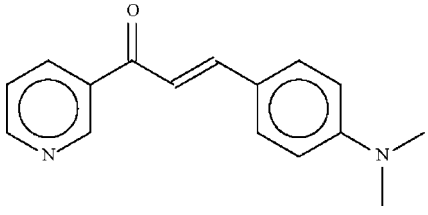
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.055; wR factor = 0.147; data-to-parameter ratio = 17.1.

The pyridyl and aryl rings in the title compound, $C_{16}H_{16}N_2O$, which are located at the ends of the propenone unit, are inclined at an angle of 17.1 (1)° with respect to each other.

Related literature

For 3-(4-chlorophenyl)-1-(3-pyridyl)prop-2-en-1-one, which crystallizes in a non-centrosymmetric space group, see: Uchida *et al.* (1998). For the general synthesis by the Claisen–Schmidt condensation, see: Vogel (1999). For literature on related compounds exhibiting second-harmonic generation activity, see: Gu *et al.* (2008); Ravindra *et al.* (2008*a*,*b*).



Experimental

Crystal data

$C_{16}H_{16}N_2O$
M_r = 252.31
Monoclinic, $C2/c$
a = 14.6672 (6) Å
b = 11.0644 (4) Å
c = 16.7272 (6) Å
β = 107.205 (3)°
V = 2593.1 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 K
0.20 × 0.20 × 0.03 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: none
11747 measured reflections
2976 independent reflections
1817 reflections with $I > 2\sigma(I)$
R_{int} = 0.063

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.147
S = 1.02
2976 reflections
174 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); 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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2931).

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supporting information

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3-[4-(Dimethylamino)phenyl]-1-(3-pyridyl)prop-2-en-1-one

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S1. Comment

Some chalcone derivatives exhibit high second-harmonic generation conversion efficiency (Gu *et al.*, 2008; Ravindra *et al.*, 2008*a*,*b*). The title compound was synthesized for the purpose of examining this property; unfortunately, the compound crystallizes in a centrosymmetric space group.

S2. Experimental

The compound was synthesized by the Claisen–Schmidt condensation (Vogel, 1999). To a mixture of ethanol (20 ml) and 10% sodium hydroxide solution (5 ml) was added an ethanol (15 ml) solution of 3-acetyl pyridine (0.001 mol) and 4-dimethylaminobenzaldehyde (0.001 mol). The temperature of the mixture was maintained at below 298 K for 2 h. The solid product that formed was washed with water. The compound was recrystallized from methanol.

S3. Refinement

H atoms were placed in calculated positions (C—H 0.95 to 0.98 Å) and were included in the refinement in the riding model approximation, with U(H) restrained to 1.2–1.5U_{eq}(C).

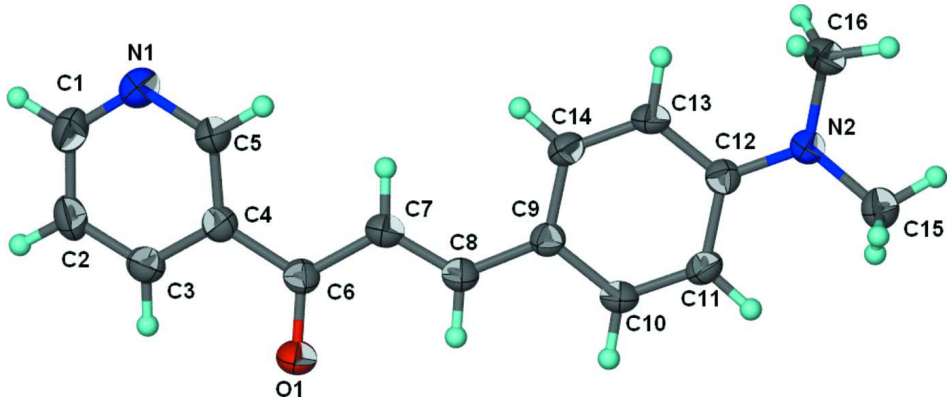

Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of $C_{16}H_{16}N_2O$ at the 70% probability level. H atoms are drawn as spheres of arbitrary radius.

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Crystal data

$C_{16}H_{16}N_2O$	a = 14.6672 (6) Å
M_r = 252.31	b = 11.0644 (4) Å
Monoclinic, $C2/c$	c = 16.7272 (6) Å
Hall symbol: -C 2yc	β = 107.205 (3)°

V = 2593.1 (2) Å^3
Z = 8
F(000) = 1072
D_x = 1.293 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1330 reflections

θ = 2.5–24.9°
μ = 0.08 mm^{-1}
T = 100 K
Plate, orange
0.20 × 0.20 × 0.03 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
11747 measured reflections
2976 independent reflections

1817 reflections with $I > 2\sigma(I)$
R_{int} = 0.063
θ_{max} = 27.5°, θ_{min} = 2.4°
h = −19→18
k = −14→14
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.147
S = 1.02
2976 reflections
174 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
$w = 1/[\sigma^2(F_o^2) + (0.0648P)^2 + 0.8849P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
O1	0.70214 (10)	0.23165 (12)	0.74962 (8)	0.0328 (4)
N1	0.60015 (14)	0.57819 (16)	0.86721 (11)	0.0408 (5)
N2	0.89331 (12)	0.58854 (14)	0.38128 (10)	0.0270 (4)
C1	0.55057 (16)	0.5062 (2)	0.90340 (14)	0.0394 (6)
H1	0.5185	0.5423	0.9390	0.047*
C2	0.54329 (15)	0.3828 (2)	0.89203 (13)	0.0314 (5)
H2	0.5073	0.3354	0.9192	0.038*
C3	0.58905 (14)	0.33046 (18)	0.84076 (12)	0.0273 (5)
H3	0.5855	0.2455	0.8322	0.033*
C4	0.64088 (13)	0.40126 (16)	0.80103 (11)	0.0242 (4)
C5	0.64452 (15)	0.52517 (17)	0.81678 (12)	0.0292 (5)
H5	0.6802	0.5746	0.7905	0.035*
C6	0.69040 (13)	0.34254 (16)	0.74515 (12)	0.0240 (4)
C7	0.72162 (14)	0.41654 (17)	0.68607 (12)	0.0268 (5)
H7	0.7108	0.5013	0.6846	0.032*
C8	0.76531 (13)	0.36800 (17)	0.63362 (11)	0.0250 (4)
H8	0.7750	0.2831	0.6380	0.030*
C9	0.79945 (13)	0.42798 (16)	0.57141 (11)	0.0226 (4)
C10	0.83957 (14)	0.35986 (17)	0.51975 (12)	0.0259 (5)
H10	0.8451	0.2748	0.5277	0.031*
C11	0.87122 (14)	0.41098 (16)	0.45818 (12)	0.0254 (4)

H11	0.8973	0.3610	0.4243	0.030*
C12	0.86545 (13)	0.53701 (16)	0.44457 (11)	0.0225 (4)
C13	0.82739 (14)	0.60643 (17)	0.49786 (12)	0.0258 (5)
H13	0.8240	0.6918	0.4916	0.031*
C14	0.79515 (14)	0.55355 (17)	0.55848 (12)	0.0258 (4)
H14	0.7692	0.6032	0.5927	0.031*
C15	0.93708 (15)	0.51553 (18)	0.33043 (13)	0.0316 (5)
H15A	0.8972	0.4445	0.3097	0.047*
H15B	1.0006	0.4894	0.3644	0.047*
H15C	0.9429	0.5635	0.2829	0.047*
C16	0.91164 (16)	0.71857 (17)	0.38199 (13)	0.0332 (5)
H16A	0.8521	0.7627	0.3761	0.050*
H16B	0.9364	0.7392	0.3353	0.050*
H16C	0.9587	0.7409	0.4350	0.050*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0461 (9)	0.0199 (7)	0.0374 (8)	−0.0033 (6)	0.0201 (7)	−0.0016 (6)
N1	0.0568 (13)	0.0308 (10)	0.0438 (11)	0.0060 (9)	0.0286 (10)	0.0004 (8)
N2	0.0349 (10)	0.0210 (8)	0.0292 (9)	0.0003 (7)	0.0159 (8)	0.0011 (7)
C1	0.0485 (15)	0.0406 (13)	0.0372 (13)	0.0114 (11)	0.0252 (12)	0.0032 (10)
C2	0.0320 (12)	0.0370 (12)	0.0291 (11)	−0.0004 (9)	0.0152 (9)	0.0073 (9)
C3	0.0316 (11)	0.0232 (10)	0.0268 (11)	−0.0005 (9)	0.0083 (9)	0.0011 (8)
C4	0.0254 (10)	0.0241 (10)	0.0228 (10)	0.0011 (8)	0.0069 (8)	0.0009 (8)
C5	0.0373 (12)	0.0242 (10)	0.0307 (11)	0.0013 (9)	0.0170 (10)	0.0012 (8)
C6	0.0268 (11)	0.0210 (10)	0.0245 (10)	−0.0036 (8)	0.0079 (9)	−0.0016 (8)
C7	0.0311 (11)	0.0207 (10)	0.0295 (11)	0.0012 (8)	0.0105 (9)	0.0016 (8)
C8	0.0302 (11)	0.0196 (9)	0.0262 (10)	−0.0024 (8)	0.0099 (9)	−0.0016 (8)
C9	0.0231 (10)	0.0207 (9)	0.0248 (10)	−0.0010 (8)	0.0084 (8)	−0.0013 (8)
C10	0.0318 (11)	0.0179 (9)	0.0289 (11)	−0.0004 (8)	0.0106 (9)	−0.0005 (8)
C11	0.0292 (11)	0.0211 (10)	0.0281 (10)	0.0001 (8)	0.0119 (9)	−0.0046 (8)
C12	0.0216 (10)	0.0226 (10)	0.0231 (10)	−0.0014 (8)	0.0065 (8)	−0.0003 (8)
C13	0.0315 (11)	0.0163 (9)	0.0311 (11)	0.0000 (8)	0.0115 (9)	−0.0004 (8)
C14	0.0285 (11)	0.0216 (9)	0.0302 (11)	0.0024 (8)	0.0130 (9)	−0.0023 (8)
C15	0.0349 (12)	0.0307 (11)	0.0335 (11)	−0.0019 (9)	0.0164 (10)	0.0003 (9)
C16	0.0405 (13)	0.0233 (10)	0.0394 (12)	−0.0023 (9)	0.0174 (10)	0.0045 (9)

Geometric parameters (Å, º)

O1—C6	1.238 (2)	C8—C9	1.443 (2)
N1—C1	1.338 (3)	C8—H8	0.9500
N1—C5	1.343 (2)	C9—C10	1.401 (2)
N2—C12	1.367 (2)	C9—C14	1.405 (3)
N2—C15	1.453 (2)	C10—C11	1.371 (3)
N2—C16	1.463 (2)	C10—H10	0.9500
C1—C2	1.378 (3)	C11—C12	1.411 (2)
C1—H1	0.9500	C11—H11	0.9500

C2—C3	1.365 (3)	C12—C13	1.411 (3)
C2—H2	0.9500	C13—C14	1.370 (3)
C3—C4	1.390 (3)	C13—H13	0.9500
C3—H3	0.9500	C14—H14	0.9500
C4—C5	1.394 (3)	C15—H15A	0.9800
C4—C6	1.492 (2)	C15—H15B	0.9800
C5—H5	0.9500	C15—H15C	0.9800
C6—C7	1.458 (3)	C16—H16A	0.9800
C7—C8	1.342 (2)	C16—H16B	0.9800
C7—H7	0.9500	C16—H16C	0.9800

C1—N1—C5	116.96 (18)	C10—C9—C8	119.74 (17)
C12—N2—C15	120.43 (15)	C14—C9—C8	123.82 (17)
C12—N2—C16	120.01 (16)	C11—C10—C9	122.61 (17)
C15—N2—C16	116.07 (16)	C11—C10—H10	118.7
N1—C1—C2	123.9 (2)	C9—C10—H10	118.7
N1—C1—H1	118.1	C10—C11—C12	120.76 (18)
C2—C1—H1	118.1	C10—C11—H11	119.6
C3—C2—C1	118.4 (2)	C12—C11—H11	119.6
C3—C2—H2	120.8	N2—C12—C13	121.80 (16)
C1—C2—H2	120.8	N2—C12—C11	121.30 (17)
C2—C3—C4	120.10 (18)	C13—C12—C11	116.87 (17)
C2—C3—H3	120.0	C14—C13—C12	121.51 (17)
C4—C3—H3	120.0	C14—C13—H13	119.2
C3—C4—C5	117.36 (18)	C12—C13—H13	119.2
C3—C4—C6	119.39 (17)	C13—C14—C9	121.77 (18)
C5—C4—C6	123.24 (17)	C13—C14—H14	119.1
N1—C5—C4	123.34 (19)	C9—C14—H14	119.1
N1—C5—H5	118.3	N2—C15—H15A	109.5
C4—C5—H5	118.3	N2—C15—H15B	109.5
O1—C6—C7	122.12 (17)	H15A—C15—H15B	109.5
O1—C6—C4	118.59 (17)	N2—C15—H15C	109.5
C7—C6—C4	119.28 (16)	H15A—C15—H15C	109.5
C8—C7—C6	121.66 (17)	H15B—C15—H15C	109.5
C8—C7—H7	119.2	N2—C16—H16A	109.5
C6—C7—H7	119.2	N2—C16—H16B	109.5
C7—C8—C9	128.46 (18)	H16A—C16—H16B	109.5
C7—C8—H8	115.8	N2—C16—H16C	109.5
C9—C8—H8	115.8	H16A—C16—H16C	109.5
C10—C9—C14	116.44 (17)	H16B—C16—H16C	109.5

C5—N1—C1—C2	0.3 (3)	C7—C8—C9—C14	2.9 (3)
N1—C1—C2—C3	−0.1 (3)	C14—C9—C10—C11	−1.5 (3)
C1—C2—C3—C4	−0.4 (3)	C8—C9—C10—C11	178.42 (18)
C2—C3—C4—C5	0.8 (3)	C9—C10—C11—C12	0.6 (3)
C2—C3—C4—C6	−179.95 (18)	C15—N2—C12—C13	176.60 (17)
C1—N1—C5—C4	0.1 (3)	C16—N2—C12—C13	18.5 (3)
C3—C4—C5—N1	−0.6 (3)	C15—N2—C12—C11	−5.1 (3)

C6—C4—C5—N1	−179.85 (19)	C16—N2—C12—C11	−163.19 (18)
C3—C4—C6—O1	−15.8 (3)	C10—C11—C12—N2	−177.40 (18)
C5—C4—C6—O1	163.44 (19)	C10—C11—C12—C13	1.0 (3)
C3—C4—C6—C7	162.98 (18)	N2—C12—C13—C14	176.66 (18)
C5—C4—C6—C7	−17.8 (3)	C11—C12—C13—C14	−1.7 (3)
O1—C6—C7—C8	−0.4 (3)	C12—C13—C14—C9	0.8 (3)
C4—C6—C7—C8	−179.08 (18)	C10—C9—C14—C13	0.8 (3)
C6—C7—C8—C9	179.34 (18)	C8—C9—C14—C13	−179.16 (18)
C7—C8—C9—C10	−177.03 (19)		