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3-(4-Methoxyphenyl)-1-(2-pyrrolyl)prop-2-en-1-one

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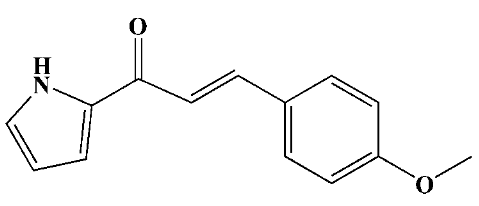
Key indicators: single-crystal X-ray study; *T* = 293 K; mean σ(C–C) = 0.002 Å; *R* factor = 0.048; *wR* factor = 0.125; data-to-parameter ratio = 15.3.

The title molecule, $C_{14}H_{13}NO_2$, is almost flat with a dihedral angle of 8.0 (1)° between the pyrrole and benzene rings. The central C_3O ketone unit has an *s-cis* conformation and is also coplanar with a torsion angle of −0.6 (3) °. An intramolecular C—H···O hydrogen bond generates an *S*(5) ring motif. In addition, the methoxy group is coplanar with the attached benzene ring. In the crystal structure, neighboring molecules are paired through N—H···O hydrogen bonds into centrosymmetric dimers with an $R_2^2(10)$ motif.

Related literature

For the pharmaceutical and biological properties of chalcones, see: Lin *et al.* (2002); Modzelewska *et al.* (2006); Opletalova (2000); Opletalova & Sedivy (1999); Sogawa *et al.* (1994). For chalcones as non-linear optical materials, see: Agrinskaya *et al.* (1999); Indira *et al.* (2002). For related structures, see: Bukhari *et al.* (2008); Fun *et al.* (2008); Gong, *et al.* (2008).



Experimental

Crystal data

$C_{14}H_{13}NO_2$
M_r = 227.25
Monoclinic, $P2_1/c$
a = 5.0815 (7) Å
b = 17.172 (3) Å
c = 13.973 (2) Å
β = 97.878 (3)°
V = 1207.8 (3) Å^3
Z = 4
Mo *K*α radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.40 × 0.24 × 0.20 mm

Data collection

Bruker SMART APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.967, T_{max} = 0.988
5842 measured reflections
2369 independent reflections
1809 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.124
S = 1.05
2369 reflections
155 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O1	0.93	2.52	2.838 (2)	100
N1—H1···O1^{i}	0.86	2.03	2.8314 (17)	155

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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: CS2091).

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supplementary materials

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3-(4-Methoxyphenyl)-1-(2-pyrrolyl)prop-2-en-1-one

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Comment

Chalcone derivatives have recently attracted extensive interest due to possessing a wide variety of pharmaceutical (Lin *et al.*, 2002; Modzelewska *et al.*, 2006; Sogawa *et al.*, 1994) and biological properties (Opletalova, 2000; Opletalova & Sedivy, 1999). Some substituted chalcones also exhibit the potential applications as non-linear optical materials (Agrinskaya *et al.*, 1999; Indira *et al.*, 2002). Considering the importance of these types of compounds, a new chalcone compound was synthesized and its crystal structure is reported here.

The molecular structure of the title molecule (Fig. 1) is almost planar as indicated by a dihedral angle of 8.0 (1) ° between the pyrrole and benzene rings. The central O1/C5/C6/C7 ketone motif exhibits an *s-cis* conformation as usual in other related chalcone derivatives (Bukhari *et al.*, 2008; Fun *et al.*, 2008; Gong, *et al.*, 2008;) and also coplanar with a torsion angle of -0.6 (3) °, meanwhile, O1 atom acts as an acceptor and is involved in an intramolecular C—H···O hydrogen bond (Table 1) to generate an S(5) ring motif. In the crystal packing, the compound can be stabilized by intermolecular N—H···O hydrogen bonds with –NH groups as donors to form centrosymmetric dimers with an $R^2_2(10)$ motif as shown in Fig. 2.

Experimental

The title compound was synthesized by the condensation of 2-acetylpyrrole (1.09 g, 10.0 mmol) and 4-methoxybenzaldehyde (1.06 g, 5.0 mmol) in methanol (30 ml) and ammonia (25%, 25 ml) in the presence of sodium hydroxide (0.56 g, 10 mmol). After refluxed at 358 K for 8 h, the contents of the flask were cooled to give a yellow crude precipitate which was separated by filtration, washed with water and iced ethanol. Recrystallization from ethanol afforded yellow prism-like crystals. Yield: 0.85 g (74.8%).

Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.93 Å, U_{iso}=1.2U_{eq} (C) for aromatic and ethylene; 0.96 Å, U_{iso}= 1.5U_{eq} (C) for CH_3 atoms, and d(N—H) = 0.86 Å, U_{iso}=1.2U_{eq} (N) for pyrrole nitrogen atom.

Figures

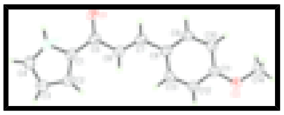

Fig. 1. The molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level and H atoms as spheres of arbitrary radius.

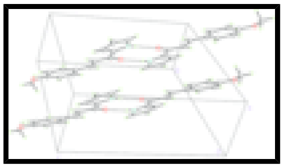

Fig. 2. Packing diagram of the title structure showing the N—H···.O hydrogen bonding interactions.

3-(4-Methoxyphenyl)-1-(2-pyrrolyl)prop-2-en-1-one

Crystal data

$C_{14}H_{13}NO_2$	$F_{000} = 480$
$M_r = 227.25$	$D_x = 1.250$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 1716 reflections
$a = 5.0815$ (7) Å	$\theta = 2.4–25.8°$
$b = 17.172$ (3) Å	$\mu = 0.08$ mm^{-1}
$c = 13.973$ (2) Å	$T = 293$ (2) K
$\beta = 97.878$ (3)°	Prism, yellow
$V = 1207.8$ (3) Å^3	0.40 × 0.24 × 0.20 mm
$Z = 4$	

Data collection

Bruker APEX area-detector diffractometer	2369 independent reflections
Radiation source: fine-focus sealed tube	1809 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.020$
$T = 293(2)$ K	$\theta_{max} = 26.0°$
φ and ω scans	$\theta_{min} = 1.9°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -6 \rightarrow 5$
$T_{min} = 0.967$, $T_{max} = 0.988$	$k = -20 \rightarrow 21$
5842 measured reflections	$l = -14 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H-atom parameters constrained
$wR(F^2) = 0.124$	$w = 1/[\sigma^2(F_o^2) + (0.0557P)^2 + 0.1497P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
2369 reflections	$\Delta\rho_{max} = 0.13$ e Å^{-3}
155 parameters	$\Delta\rho_{min} = -0.13$ e Å^{-3}

Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	−0.2188 (3)	0.56328 (8)	0.38761 (9)	0.0567 (4)
H1	−0.1976	0.5437	0.4448	0.068*
O1	0.1957 (3)	0.45435 (7)	0.40994 (8)	0.0707 (4)
O2	0.9171 (3)	0.29580 (8)	−0.06480 (9)	0.0769 (4)
C1	−0.0745 (3)	0.54326 (9)	0.31541 (10)	0.0520 (4)
C2	−0.1690 (4)	0.58892 (10)	0.23690 (12)	0.0634 (5)
H2	−0.1082	0.5885	0.1771	0.076*
C3	−0.3705 (4)	0.63554 (11)	0.26280 (13)	0.0707 (5)
H3	−0.4688	0.6721	0.2238	0.085*
C4	−0.3978 (3)	0.61792 (11)	0.35599 (12)	0.0634 (5)
H4	−0.5202	0.6401	0.3916	0.076*
C5	0.1294 (3)	0.48406 (9)	0.32984 (11)	0.0535 (4)
C6	0.2491 (3)	0.45958 (10)	0.24510 (11)	0.0570 (4)
H6	0.1913	0.4834	0.1862	0.068*
C7	0.4347 (3)	0.40549 (10)	0.24796 (11)	0.0556 (4)
H7	0.4909	0.3835	0.3081	0.067*
C8	0.5616 (3)	0.37631 (9)	0.16757 (11)	0.0517 (4)
C9	0.7403 (3)	0.31532 (10)	0.17995 (11)	0.0578 (4)
H9	0.7789	0.2930	0.2409	0.069*
C10	0.8645 (3)	0.28594 (10)	0.10527 (12)	0.0586 (4)
H10	0.9827	0.2445	0.1160	0.070*
C11	0.8105 (3)	0.31894 (10)	0.01503 (11)	0.0563 (4)
C12	0.6337 (4)	0.38052 (11)	0.00062 (12)	0.0714 (5)
H12	0.5978	0.4033	−0.0602	0.086*
C13	0.5110 (4)	0.40830 (11)	0.07518 (12)	0.0669 (5)
H13	0.3915	0.4494	0.0639	0.080*
C14	1.0982 (4)	0.23244 (12)	−0.05485 (15)	0.0873 (6)
H14A	1.2445	0.2445	−0.0060	0.131*
H14B	1.1631	0.2235	−0.1153	0.131*
H14C	1.0094	0.1866	−0.0365	0.131*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0611 (8)	0.0626 (9)	0.0479 (7)	−0.0046 (7)	0.0129 (6)	−0.0043 (6)
O1	0.0880 (9)	0.0760 (8)	0.0520 (7)	0.0121 (7)	0.0233 (6)	0.0115 (6)
O2	0.0977 (9)	0.0780 (9)	0.0577 (7)	0.0310 (7)	0.0207 (7)	0.0018 (6)
C1	0.0533 (9)	0.0579 (10)	0.0459 (8)	−0.0089 (7)	0.0107 (7)	−0.0036 (7)
C2	0.0698 (11)	0.0717 (12)	0.0499 (9)	0.0006 (9)	0.0120 (8)	0.0007 (8)
C3	0.0771 (12)	0.0731 (12)	0.0605 (11)	0.0098 (10)	0.0042 (9)	0.0001 (9)
C4	0.0606 (10)	0.0670 (11)	0.0630 (10)	0.0017 (9)	0.0098 (8)	−0.0132 (9)
C5	0.0581 (9)	0.0570 (10)	0.0468 (8)	−0.0110 (8)	0.0120 (7)	0.0004 (7)
C6	0.0610 (10)	0.0631 (10)	0.0480 (8)	−0.0034 (8)	0.0112 (7)	0.0020 (7)

C7	0.0607 (10)	0.0594 (10)	0.0473 (8)	−0.0088 (8)	0.0097 (7)	0.0029 (7)
C8	0.0562 (9)	0.0501 (9)	0.0492 (8)	−0.0053 (7)	0.0084 (7)	0.0006 (7)
C9	0.0609 (10)	0.0617 (11)	0.0499 (9)	0.0015 (8)	0.0049 (8)	0.0112 (7)
C10	0.0583 (10)	0.0567 (10)	0.0604 (10)	0.0089 (8)	0.0062 (8)	0.0056 (8)
C11	0.0636 (10)	0.0549 (10)	0.0507 (9)	0.0046 (8)	0.0096 (8)	−0.0014 (7)
C12	0.0972 (14)	0.0701 (12)	0.0473 (9)	0.0254 (11)	0.0115 (9)	0.0082 (8)
C13	0.0855 (13)	0.0608 (11)	0.0553 (10)	0.0232 (9)	0.0137 (9)	0.0050 (8)
C14	0.1013 (15)	0.0851 (14)	0.0779 (13)	0.0345 (13)	0.0212 (11)	−0.0047 (11)

Geometric parameters (Å, °)

N1—C4	1.339 (2)	C7—C8	1.459 (2)
N1—C1	1.3699 (19)	C7—H7	0.9300
N1—H1	0.8600	C8—C9	1.382 (2)
O1—C5	1.2342 (18)	C8—C13	1.394 (2)
O2—C11	1.3644 (19)	C9—C10	1.386 (2)
O2—C14	1.419 (2)	C9—H9	0.9300
C1—C2	1.380 (2)	C10—C11	1.375 (2)
C1—C5	1.446 (2)	C10—H10	0.9300
C2—C3	1.386 (2)	C11—C12	1.384 (2)
C2—H2	0.9300	C12—C13	1.371 (2)
C3—C4	1.362 (2)	C12—H12	0.9300
C3—H3	0.9300	C13—H13	0.9300
C4—H4	0.9300	C14—H14A	0.9600
C5—C6	1.465 (2)	C14—H14B	0.9600
C6—C7	1.320 (2)	C14—H14C	0.9600
C6—H6	0.9300		
C4—N1—C1	109.93 (14)	C9—C8—C13	116.70 (15)
C4—N1—H1	125.0	C9—C8—C7	121.10 (14)
C1—N1—H1	125.0	C13—C8—C7	122.20 (15)
C11—O2—C14	117.91 (14)	C8—C9—C10	122.74 (15)
N1—C1—C2	106.24 (15)	C8—C9—H9	118.6
N1—C1—C5	121.30 (14)	C10—C9—H9	118.6
C2—C1—C5	132.46 (15)	C11—C10—C9	119.07 (15)
C1—C2—C3	108.04 (15)	C11—C10—H10	120.5
C1—C2—H2	126.0	C9—C10—H10	120.5
C3—C2—H2	126.0	O2—C11—C10	125.29 (15)
C4—C3—C2	107.26 (17)	O2—C11—C12	115.23 (14)
C4—C3—H3	126.4	C10—C11—C12	119.48 (15)
C2—C3—H3	126.4	C13—C12—C11	120.59 (16)
N1—C4—C3	108.52 (15)	C13—C12—H12	119.7
N1—C4—H4	125.7	C11—C12—H12	119.7
C3—C4—H4	125.7	C12—C13—C8	121.42 (16)
O1—C5—C1	121.24 (14)	C12—C13—H13	119.3
O1—C5—C6	121.48 (16)	C8—C13—H13	119.3
C1—C5—C6	117.27 (14)	O2—C14—H14A	109.5
C7—C6—C5	123.47 (15)	O2—C14—H14B	109.5
C7—C6—H6	118.3	H14A—C14—H14B	109.5
C5—C6—H6	118.3	O2—C14—H14C	109.5

C6—C7—C8	127.43 (15)	H14A—C14—H14C	109.5
C6—C7—H7	116.3	H14B—C14—H14C	109.5
C8—C7—H7	116.3		

C4—N1—C1—C2	0.86 (18)	C6—C7—C8—C9	−175.31 (17)
C4—N1—C1—C5	−178.71 (14)	C6—C7—C8—C13	5.0 (3)
N1—C1—C2—C3	−0.38 (19)	C13—C8—C9—C10	−0.4 (3)
C5—C1—C2—C3	179.11 (17)	C7—C8—C9—C10	179.89 (15)
C1—C2—C3—C4	−0.2 (2)	C8—C9—C10—C11	0.6 (3)
C1—N1—C4—C3	−1.01 (19)	C14—O2—C11—C10	0.2 (3)
C2—C3—C4—N1	0.7 (2)	C14—O2—C11—C12	−179.46 (18)
N1—C1—C5—O1	−6.2 (2)	C9—C10—C11—O2	−179.72 (16)
C2—C1—C5—O1	174.32 (17)	C9—C10—C11—C12	−0.1 (3)
N1—C1—C5—C6	172.35 (14)	O2—C11—C12—C13	179.16 (17)
C2—C1—C5—C6	−7.1 (3)	C10—C11—C12—C13	−0.5 (3)
O1—C5—C6—C7	−0.6 (3)	C11—C12—C13—C8	0.6 (3)
C1—C5—C6—C7	−179.16 (15)	C9—C8—C13—C12	−0.2 (3)
C5—C6—C7—C8	178.75 (15)	C7—C8—C13—C12	179.49 (16)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O1	0.93	2.52	2.838 (2)	100
N1—H1···O1^{i}	0.86	2.03	2.8314 (17)	155

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

Fig. 1

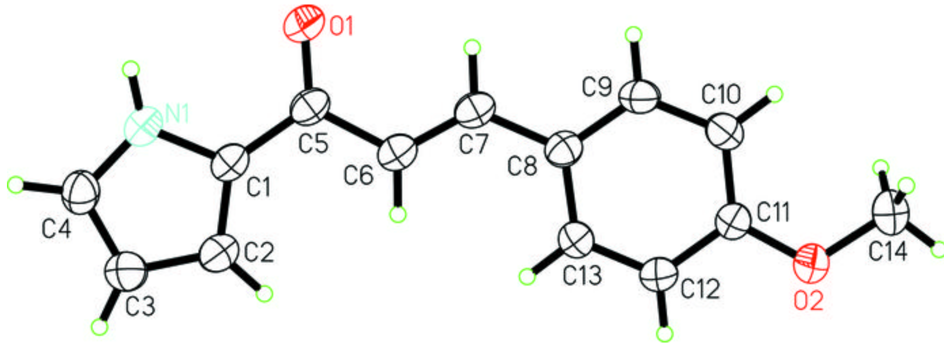

Fig. 2