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

Zhen-Qi Gong[a]* and You-Liang Shen[b]

[a]Department of Chemistry, Jiangxi Science and Technology Normal University, Jiangxi 330013, People's Republic of China, and [b]Jiangxi Key Laboratory of Surface Engineering, Jiangxi Science and Technology Normal University, Jiangxi 330013, People's Republic of China
Correspondence e-mail: zhqgong@126.com

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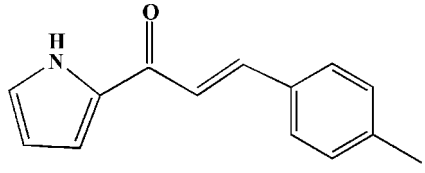
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.051; wR factor = 0.145; data-to-parameter ratio = 15.3.

In the title compound, $C_4H_{13}NO$, the pyrrole and benzene rings are almost coplanar, with a dihedral angle of 2.90 (1)° between them. In the crystal structure, molecules form centrosymmetric dimers through N—H···O hydrogen-bonding interactions. Neighbouring molecular pairs are held together by face-to-face π–π stacking interactions between adjacent pyrrole rings [perpendicular interplanar distance = 3.3948 (3) Å and centroid-to-centroid distance = 3.723 (2) Å], forming one-dimensional chains along the b axis.

Related literature

For details of the biological properties of chalcones, see: Dimmock *et al.* (1999); Go *et al.* (2005); Opletalova (2000); Opletalova & Sedivy (1999). For related structures, see: Kumaran *et al.* (1996); Shanmuga Sundara Raj *et al.*, (1997, 1998).



Experimental

Crystal data

$C_{14}H_{13}NO$
M_r = 211.25
Monoclinic, $P2_1/c$
a = 8.6236 (11) Å
b = 5.6273 (7) Å
c = 23.958 (3) Å
β = 97.305 (2)°
V = 1153.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295 (2) K
0.43 × 0.22 × 0.18 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.892, T_{max} = 0.985
6514 measured reflections
2241 independent reflections
1757 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.145
S = 1.05
2241 reflections
146 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 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}	0.86	2.07	2.8525 (19)	151

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); 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: SJ2339).

References

Bruker (2002). *SMART* (Version 6.36A), *SAINT* (Version 6.36A) and *SHELXTL* (Version 6.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Dimmock, J. R., Elias, D. W., Beazely, M. A. & Kandepu, N. (1999). *Curr. Med. Chem.* **6**, 1125–1149.
Go, M. L., Wu, X. & Liu, X.-L. (2005). *Curr. Med. Chem.* **12**, 481–499.
Kumaran, D., Eswaramoorthy, S., Ponnuswamy, M. N., Raju, K. S. & Nanjundan, S. (1996). *Acta Cryst.* C**52**, 2543–2545.
Opletalova, V. (2000). *Ceska Slov. Farm.* **49**, 278–284.
Opletalova, V. & Sedivy, D. (1999). *Ceska Slov. Farm.* **48**, 252–255.
Shanmuga Sundara Raj, S., Ponnuswamy, M. N., Shanmugam, G. & Nanjundan, S. (1997). *Acta Cryst.* C**53**, 917–918.
Shanmuga Sundara Raj, S., Ponnuswamy, M. N., Shanmugam, G. & Nanjundan, S. (1998). *Acta Cryst.* C**54**, 541–542.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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supplementary materials

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

Z.-Q. Gong and Y.-L. Shen

Comment

Chalcones have attracted considerable interest as a template in the development of biology. The anticancer, antibacterial, antiviral, antiprotozoal, insecticidal and enzyme-inhibitory properties of a number of chalcones have been reviewed (Dimmock *et al.*, 1999; Go *et al.*, 2005; Opletalova, 2000; Opletalova & Sedivy, 1999). The objective of this study therefore synthesize and elucidate the crystal structure of a new chalcone compound, (I), Fig. 1.

The pyrrole ring, benzene ring and the enone group of the molecule containing atoms O1, C5, C6 and C7, are almost co-planar with the maximum deviation 0.0702 Å for C7. The short H6···H9 (2.25 Å) contact causes the bond angles C7—C8—C9 [123.1 (2)°] C6—C7—C8 [127.7 (1)°] to deviate significantly from 120°.

In the crystal, molecules form inversion related dimers through N—H···O hydrogen bonds. Neighboring pairs are further linked by face-to-face π–π stacking interactions between adjacent pyrrole rings [perpendicular interplanar distance 3.3948 (3) Å and centroid-to-centroid distance 3.723 (2) Å], forming one-dimensional chains, Fig. 2.

Experimental

2-Acetylpyrrole (4.36 g, 40.0 mmol) was added to a solution of *p*-tolualdehyde (2.42 g, 20.0 mmol) in methanol (130 ml). Potassium hydroxide (2.24 g, 40 mmol) and ammonia (25%, 100 ml) were then added to the solution and refluxed for 36 h. The yellow precipitate that formed was removed by vacuum filtration, washed with water to neutral pH. The product was recrystallized from chloroform/ethanol (3:1) to yield 2.10 g (49%) of the title compound.

Refinement

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

Figures

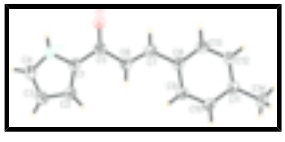

Fig. 1. The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level, and H atoms as spheres of arbitrary radius.

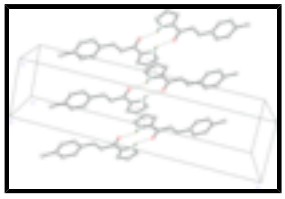

Fig. 2. Packing diagram showing the N—H···O hydrogen bonding and face-to-face π–π stacking interactions interactions (dashed lines). H atoms not involved in hydrogen bonding have been omitted for clarity.

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

Crystal data

$C_{14}H_{13}NO$	$F_{000} = 448$
$M_r = 211.25$	$D_x = 1.217$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P2ybc	Cell parameters from 1908 reflections
$a = 8.6236$ (11) Å	$\theta = 2.4$–26.2^o
$b = 5.6273$ (7) Å	$\mu = 0.08$ mm^{-1}
$c = 23.958$ (3) Å	$T = 295$ (2) K
$\beta = 97.305$ (2)^o	Prism, yellow
$V = 1153.2$ (3) Å^3	0.43 × 0.22 × 0.18 mm
$Z = 4$	

Data collection

Bruker APEX area-detector diffractometer	2241 independent reflections
Radiation source: fine-focus sealed tube	1757 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.022$
$T = 295$(2) K	$\theta_{max} = 26.0^o$
φ and ω scans	$\theta_{min} = 2.4^o$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -10 \rightarrow 10$
$T_{min} = 0.892$, $T_{max} = 0.985$	$k = -6 \rightarrow 6$
6514 measured reflections	$l = -29 \rightarrow 29$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.051$	H-atom parameters constrained
$wR(F^2) = 0.145$	$w = 1/[\sigma^2(F_o^2) + (0.0733P)^2 + 0.198P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
2241 reflections	$\Delta\rho_{max} = 0.22$ e Å^{-3}
146 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.41397 (15)	0.4506 (2)	0.42156 (5)	0.0652 (4)
N1	0.65056 (16)	0.2223 (3)	0.49341 (6)	0.0550 (4)
H1	0.6209	0.3507	0.5084	0.066*
C1	0.10198 (19)	−0.0007 (3)	0.15386 (7)	0.0524 (4)
C2	0.2228 (2)	−0.1227 (3)	0.18472 (8)	0.0610 (5)
H2	0.2580	−0.2638	0.1705	0.073*
C3	0.2927 (2)	−0.0405 (3)	0.23608 (8)	0.0628 (5)
H3	0.3739	−0.1269	0.2558	0.075*
C4	0.24344 (18)	0.1698 (3)	0.25891 (7)	0.0500 (4)
C5	0.1241 (2)	0.2946 (3)	0.22729 (7)	0.0565 (5)
H5	0.0903	0.4378	0.2409	0.068*
C6	0.0545 (2)	0.2104 (3)	0.17596 (7)	0.0587 (5)
H6	−0.0257	0.2973	0.1559	0.070*
C7	0.0241 (2)	−0.0992 (4)	0.09886 (8)	0.0699 (6)
H7A	0.0887	−0.0688	0.0698	0.105*
H7B	−0.0757	−0.0241	0.0893	0.105*
H7C	0.0098	−0.2674	0.1024	0.105*
C8	0.30938 (19)	0.2592 (3)	0.31416 (7)	0.0532 (4)
H8	0.2768	0.4098	0.3237	0.064*
C9	0.40985 (19)	0.1515 (3)	0.35225 (7)	0.0566 (5)
H9	0.4450	0.0004	0.3443	0.068*
C10	0.46818 (18)	0.2609 (3)	0.40658 (7)	0.0521 (4)
C11	0.59111 (18)	0.1372 (3)	0.44173 (7)	0.0495 (4)
C12	0.6710 (2)	−0.0694 (3)	0.43344 (8)	0.0589 (5)
H12	0.6556	−0.1664	0.4018	0.071*
C13	0.7789 (2)	−0.1066 (4)	0.48098 (8)	0.0669 (5)
H13	0.8493	−0.2320	0.4869	0.080*
C14	0.7621 (2)	0.0753 (3)	0.51726 (8)	0.0627 (5)
H14	0.8186	0.0943	0.5527	0.075*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0716 (8)	0.0628 (8)	0.0578 (8)	0.0086 (6)	−0.0054 (6)	−0.0152 (6)
N1	0.0557 (8)	0.0583 (8)	0.0494 (8)	0.0015 (7)	0.0008 (6)	−0.0053 (7)
C1	0.0536 (9)	0.0589 (10)	0.0450 (9)	−0.0076 (8)	0.0074 (7)	−0.0022 (8)
C2	0.0626 (10)	0.0620 (11)	0.0579 (11)	0.0063 (9)	0.0055 (8)	−0.0173 (9)
C3	0.0562 (9)	0.0701 (12)	0.0590 (11)	0.0146 (9)	−0.0041 (8)	−0.0137 (9)
C4	0.0478 (8)	0.0540 (10)	0.0478 (9)	−0.0044 (7)	0.0048 (7)	−0.0057 (7)
C5	0.0698 (11)	0.0469 (9)	0.0520 (10)	0.0039 (8)	0.0050 (8)	−0.0030 (8)
C6	0.0656 (10)	0.0595 (10)	0.0483 (10)	0.0061 (8)	−0.0025 (8)	0.0035 (8)
C7	0.0754 (12)	0.0805 (14)	0.0513 (10)	−0.0049 (10)	−0.0013 (9)	−0.0107 (9)
C8	0.0524 (9)	0.0557 (10)	0.0517 (10)	−0.0034 (7)	0.0072 (8)	−0.0099 (8)
C9	0.0536 (9)	0.0600 (10)	0.0544 (10)	0.0008 (8)	−0.0001 (8)	−0.0125 (8)
C10	0.0473 (8)	0.0564 (10)	0.0523 (10)	−0.0052 (7)	0.0055 (7)	−0.0071 (8)
C11	0.0468 (8)	0.0562 (10)	0.0454 (9)	−0.0066 (7)	0.0044 (7)	−0.0045 (7)
C12	0.0599 (10)	0.0595 (11)	0.0576 (10)	−0.0013 (8)	0.0093 (8)	−0.0070 (9)
C13	0.0639 (11)	0.0679 (12)	0.0676 (12)	0.0120 (9)	0.0033 (9)	0.0052 (10)
C14	0.0601 (10)	0.0723 (12)	0.0531 (10)	0.0000 (9)	−0.0025 (8)	0.0044 (9)

Geometric parameters (Å, °)

O1—C10	1.237 (2)	C6—H6	0.9300
N1—C14	1.340 (2)	C7—H7A	0.9600
N1—C11	1.365 (2)	C7—H7B	0.9600
N1—H1	0.8600	C7—H7C	0.9600
C1—C2	1.382 (2)	C8—C9	1.323 (2)
C1—C6	1.384 (2)	C8—H8	0.9300
C1—C7	1.506 (2)	C9—C10	1.470 (2)
C2—C3	1.379 (2)	C9—H9	0.9300
C2—H2	0.9300	C10—C11	1.446 (2)
C3—C4	1.393 (2)	C11—C12	1.379 (2)
C3—H3	0.9300	C12—C13	1.392 (2)
C4—C5	1.389 (2)	C12—H12	0.9300
C4—C8	1.462 (2)	C13—C14	1.362 (3)
C5—C6	1.381 (2)	C13—H13	0.9300
C5—H5	0.9300	C14—H14	0.9300
C14—N1—C11	109.67 (15)	C1—C7—H7C	109.5
C14—N1—H1	125.2	H7A—C7—H7C	109.5
C11—N1—H1	125.2	H7B—C7—H7C	109.5
C2—C1—C6	117.49 (15)	C9—C8—C4	127.73 (17)
C2—C1—C7	120.48 (17)	C9—C8—H8	116.1
C6—C1—C7	122.02 (16)	C4—C8—H8	116.1
C3—C2—C1	121.66 (17)	C8—C9—C10	122.63 (17)
C3—C2—H2	119.2	C8—C9—H9	118.7
C1—C2—H2	119.2	C10—C9—H9	118.7
C2—C3—C4	121.01 (16)	O1—C10—C11	121.51 (15)

C2—C3—H3	119.5	O1—C10—C9	121.28 (15)
C4—C3—H3	119.5	C11—C10—C9	117.21 (15)
C5—C4—C3	117.21 (15)	N1—C11—C12	106.82 (14)
C5—C4—C8	119.73 (15)	N1—C11—C10	121.50 (15)
C3—C4—C8	123.05 (15)	C12—C11—C10	131.68 (15)
C6—C5—C4	121.33 (16)	C11—C12—C13	107.66 (16)
C6—C5—H5	119.3	C11—C12—H12	126.2
C4—C5—H5	119.3	C13—C12—H12	126.2
C5—C6—C1	121.27 (16)	C14—C13—C12	107.15 (17)
C5—C6—H6	119.4	C14—C13—H13	126.4
C1—C6—H6	119.4	C12—C13—H13	126.4
C1—C7—H7A	109.5	N1—C14—C13	108.70 (16)
C1—C7—H7B	109.5	N1—C14—H14	125.7
H7A—C7—H7B	109.5	C13—C14—H14	125.7
C6—C1—C2—C3	1.0 (3)	C8—C9—C10—O1	7.2 (3)
C7—C1—C2—C3	−177.82 (18)	C8—C9—C10—C11	−172.94 (16)
C1—C2—C3—C4	0.1 (3)	C14—N1—C11—C12	−0.66 (19)
C2—C3—C4—C5	−1.4 (3)	C14—N1—C11—C10	179.84 (15)
C2—C3—C4—C8	177.45 (18)	O1—C10—C11—N1	1.2 (3)
C3—C4—C5—C6	1.6 (3)	C9—C10—C11—N1	−178.62 (15)
C8—C4—C5—C6	−177.28 (16)	O1—C10—C11—C12	−178.12 (17)
C4—C5—C6—C1	−0.5 (3)	C9—C10—C11—C12	2.0 (3)
C2—C1—C6—C5	−0.8 (3)	N1—C11—C12—C13	0.1 (2)
C7—C1—C6—C5	178.01 (18)	C10—C11—C12—C13	179.52 (18)
C5—C4—C8—C9	171.77 (17)	C11—C12—C13—C14	0.5 (2)
C3—C4—C8—C9	−7.0 (3)	C11—N1—C14—C13	1.0 (2)
C4—C8—C9—C10	179.85 (16)	C12—C13—C14—N1	−0.9 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86	2.07	2.8525 (19)	151

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

Fig. 1

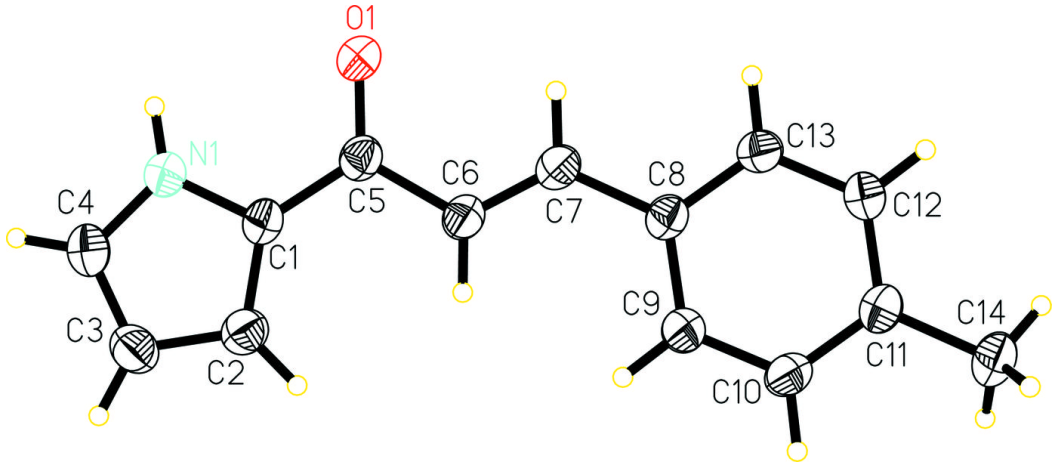

Fig. 2