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3-Phenyl-1-(pyrrol-2-yl)prop-2-en-1-one

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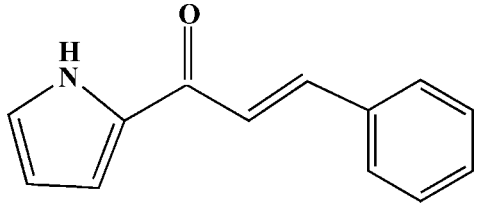
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.054; wR factor = 0.137; data-to-parameter ratio = 15.2.

The title molecule, $C_{13}H_{11}NO$, is almost flat, the angle between the pyrrole and the phenyl rings being 10.9 (1)°. The atoms of the central C_3O unit are coplanar, with a mean deviation from the plane of 0.001 (1) Å. The angles between this plane and the pyrrole and phenyl rings are 3.3 (1) and 8.0 (1)°, respectively. The molecules form centrosymmetric dimers through a pair of N—H···O hydrogen bonds with an $R_2^2(10)$ motif.

Related literature

For details of the biological and the pharmaceutical properties of chalcones, see: Chen *et al.* (1999); Dimmock *et al.* (1999); Go *et al.* (2005); Lin *et al.* (2002); Lunardi *et al.* (2003); Opletalova (2000). For other related literature, see: Gong & Shen (2007); Kumaran *et al.* (1996); Shanmuga Sundara Raj *et al.* (1997, 1998). For a description of hydrogen-bond motifs, see: Etter *et al.* (1990).



Experimental

Crystal data

$C_{13}H_{11}NO$
M_r = 197.23
Monoclinic, $C2/c$
a = 19.848 (4) Å
b = 5.6435 (12) Å
c = 19.325 (4) Å
β = 101.535 (4)°
V = 2120.9 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.34 × 0.13 × 0.11 mm

Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.974, T_{max} = 0.991
5274 measured reflections
2069 independent reflections
1164 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.137
S = 1.00
2069 reflections
136 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
N1—H1···O1^{i}	0.86	2.02	2.817 (2)	155
C7—H7···O1	0.93	2.51	2.835 (3)	101

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FB2072).

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supporting information

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3-Phenyl-1-(pyrrol-2-yl)prop-2-en-1-one

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S1. Comment

Chalcone derivatives possess wide variety of pharmaceutical properties, such as anticancer, antibacterial, antiviral, antiprotozoal, insecticidal and enzyme-inhibitory ones (Dimmock *et al.*, 1999; Go *et al.*, 2005; Opletalova, 2000). Some of the substituted chalcones are also reported to possess antileishmanial (Chen *et al.*, 1999), antitubercular (Lin *et al.*, 2002), trypanocidal (Lunardi *et al.*, 2003) activities. As a part of our ongoing efforts in the chalcone compounds (Gong & Shen, 2007), the title compound is reported here for the first time.

In the title compound, $C_{13}H_{11}NO$, the bond lengths and angles are usual. The –NH groups are involved as donors to form centrosymmetric dimers with a motif $R^2_2(10)$ through N—H···O hydrogen bonds (Etter *et al.*, 1990) - (Fig. 2). There is a pyrrole-H···π-phenyl-ring interaction as indicate the geometric parameters C2—H2···Centroid(phenyl) (1 - *x*, *y*, 3/2 - *z*) where the distance H···centroid and C2···centroid equal to 2.90 and 3.666 (3) Å, respectively, and the angle C2—H2···Centroid(phenyl) equals to 141° (Spek, 2003).

S2. Experimental

2-Acetylpyrrole (2.18 g, 20.0 mmol) was added to a solution of benzaldehyde (1.06 g, 10.0 mmol) in methanol (65 ml). Then potassium hydroxide (1.12 g, 20 mmol) and ammonia (25%, 50 ml) were added to the solution and refluxed for 12 h. The resulting solution was cooled and the solvent was evaporated under vacuum to give an orange precipitate which was separated by filtration, washed with iced ethanol (95%) and water to pH = 7. Recrystallization from dichloromethane gave light yellow prism-like crystals with average size of about 1.50x0.35x0.25 mm. Yield: 0.89 g (45%).

S3. Refinement

All the H atoms could be distinguished in the difference Fourier map. Nevertheless, the H atoms were set into idealized positions and constrained by the riding motion formalism: The C—H and N—H distances were set to 0.93 and 0.86 Å, respectively, while U_{iso}=1.2U_{eq} of the pertinent carrier atom.

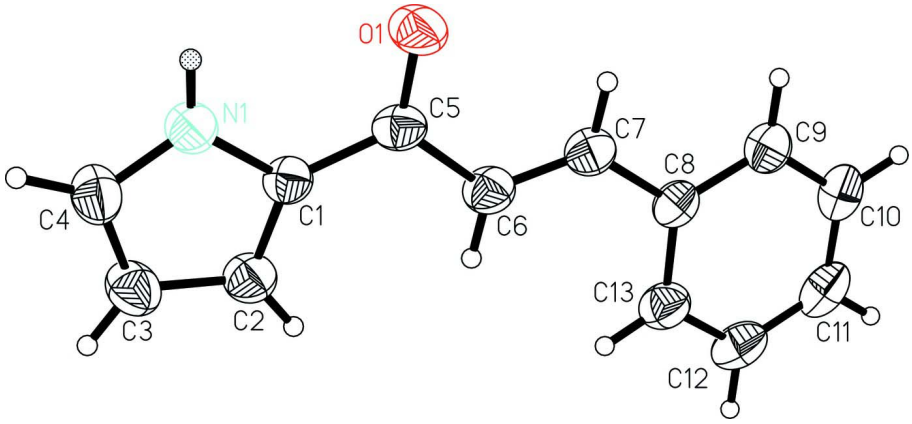

Figure 1

The title molecule with the displacement ellipsoids shown at the 30% probability level, and with the H atoms shown as spheres of arbitrary radii.

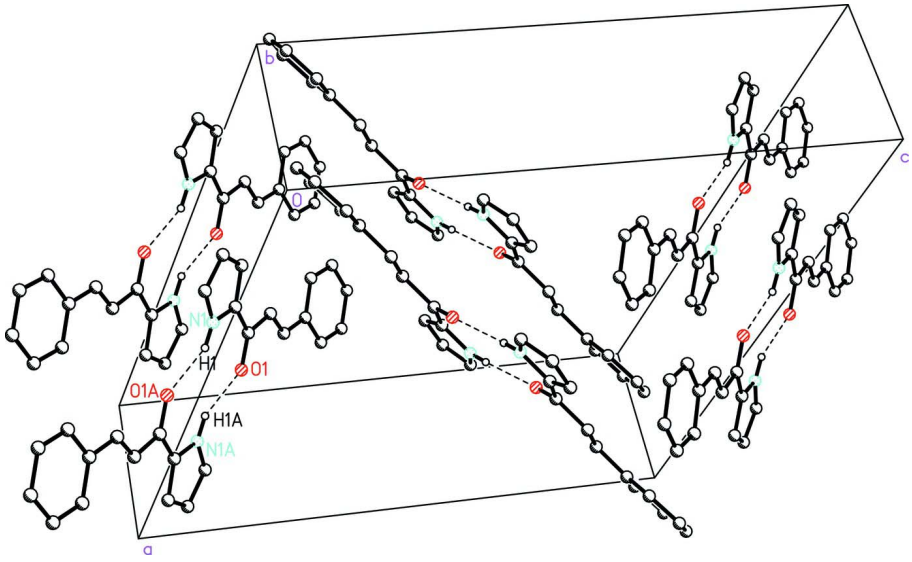

Figure 2

A motif showing the N—H···.O hydrogen bonds. The H atoms not involved in hydrogen bonding have been omitted for clarity.

3-Phenyl-1-(pyrrol-2-yl)prop-2-en-1-one

Crystal data

$C_{13}H_{11}NO$
$M_r = 197.23$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 19.848\ (4)$ Å
$b = 5.6435\ (12)$ Å
$c = 19.325\ (4)$ Å
$\beta = 101.535\ (4)°$
$V = 2120.9\ (8)$ Å^3
$Z = 8$

$F(000) = 832$
$D_x = 1.235$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 642 reflections
$\theta = 2.7–24.7°$
$\mu = 0.08$ mm^{-1}
$T = 293$ K
Prism, light yellow
0.34 × 0.13 × 0.11 mm

Data collection

Bruker APEX area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.974, T_{max} = 0.991
5274 measured reflections
2069 independent reflections
1164 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 26.0°, θ_{min} = 2.1°
h = −24→23
k = −6→6
l = −14→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.137
S = 1.00
2069 reflections
136 parameters
0 restraints
44 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 0.0616P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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	0.54821 (8)	0.1673 (3)	0.58099 (8)	0.0776 (5)
N1	0.41400 (9)	0.2050 (3)	0.50060 (9)	0.0635 (5)
H1	0.4349	0.0847	0.4874	0.076*
C1	0.44232 (11)	0.3625 (4)	0.55205 (10)	0.0547 (6)
C2	0.39177 (12)	0.5253 (4)	0.55675 (12)	0.0673 (7)
H2	0.3961	0.6536	0.5875	0.081*
C3	0.33346 (12)	0.4656 (4)	0.50787 (13)	0.0762 (7)
H3	0.2916	0.5456	0.4997	0.091*
C4	0.34890 (12)	0.2665 (4)	0.47383 (12)	0.0724 (7)
H4	0.3191	0.1871	0.4380	0.087*
C5	0.51165 (12)	0.3362 (4)	0.59096 (11)	0.0586 (6)
C6	0.53729 (12)	0.5178 (4)	0.64459 (11)	0.0640 (6)
H6	0.5083	0.6427	0.6503	0.077*
C7	0.59949 (12)	0.5118 (4)	0.68497 (11)	0.0609 (6)
H7	0.6274	0.3860	0.6775	0.073*
C8	0.62940 (11)	0.6813 (4)	0.74025 (10)	0.0564 (6)

C9	0.69227 (11)	0.6324 (4)	0.78395 (11)	0.0645 (6)
H9	0.7159	0.4953	0.7767	0.077*
C10	0.72018 (13)	0.7842 (5)	0.83802 (13)	0.0733 (7)
H10	0.7622	0.7486	0.8671	0.088*
C11	0.68593 (15)	0.9879 (5)	0.84886 (13)	0.0780 (8)
H11	0.7046	1.0898	0.8855	0.094*
C12	0.62420 (14)	1.0411 (4)	0.80554 (13)	0.0782 (7)
H12	0.6011	1.1794	0.8128	0.094*
C13	0.59620 (13)	0.8898 (4)	0.75115 (12)	0.0699 (7)
H13	0.5547	0.9283	0.7216	0.084*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0839 (12)	0.0726 (11)	0.0687 (11)	0.0236 (9)	−0.0030 (8)	−0.0209 (8)
N1	0.0670 (12)	0.0654 (12)	0.0563 (11)	0.0096 (10)	0.0076 (9)	−0.0115 (10)
C1	0.0643 (14)	0.0543 (14)	0.0453 (12)	0.0030 (11)	0.0102 (11)	−0.0051 (11)
C2	0.0730 (15)	0.0639 (16)	0.0651 (15)	0.0084 (13)	0.0138 (13)	−0.0107 (12)
C3	0.0672 (15)	0.0833 (18)	0.0767 (17)	0.0166 (14)	0.0114 (14)	−0.0072 (14)
C4	0.0619 (15)	0.0858 (18)	0.0661 (15)	0.0029 (14)	0.0051 (12)	−0.0102 (14)
C5	0.0749 (16)	0.0527 (14)	0.0486 (13)	0.0075 (12)	0.0134 (11)	−0.0024 (11)
C6	0.0732 (15)	0.0575 (15)	0.0609 (14)	0.0051 (12)	0.0123 (12)	−0.0109 (11)
C7	0.0684 (14)	0.0583 (15)	0.0579 (14)	0.0009 (12)	0.0174 (12)	−0.0049 (11)
C8	0.0646 (14)	0.0539 (14)	0.0521 (13)	−0.0081 (12)	0.0154 (11)	−0.0037 (11)
C9	0.0660 (15)	0.0655 (15)	0.0631 (15)	−0.0076 (12)	0.0157 (12)	−0.0018 (12)
C10	0.0717 (16)	0.0802 (18)	0.0669 (16)	−0.0221 (15)	0.0110 (12)	−0.0012 (14)
C11	0.104 (2)	0.0711 (19)	0.0591 (15)	−0.0342 (16)	0.0157 (15)	−0.0060 (13)
C12	0.108 (2)	0.0550 (15)	0.0728 (18)	−0.0107 (15)	0.0210 (16)	−0.0106 (13)
C13	0.0828 (16)	0.0579 (14)	0.0672 (16)	−0.0021 (13)	0.0105 (13)	−0.0049 (12)

Geometric parameters (Å, º)

O1—C5	1.236 (2)	C7—C8	1.468 (3)
N1—C4	1.338 (3)	C7—H7	0.9300
N1—C1	1.368 (2)	C8—C13	1.385 (3)
N1—H1	0.8600	C8—C9	1.387 (3)
C1—C2	1.377 (3)	C9—C10	1.379 (3)
C1—C5	1.438 (3)	C9—H9	0.9300
C2—C3	1.381 (3)	C10—C11	1.373 (3)
C2—H2	0.9300	C10—H10	0.9300
C3—C4	1.367 (3)	C11—C12	1.372 (3)
C3—H3	0.9300	C11—H11	0.9300
C4—H4	0.9300	C12—C13	1.382 (3)
C5—C6	1.474 (3)	C12—H12	0.9300
C6—C7	1.322 (3)	C13—H13	0.9300
C6—H6	0.9300		
C4—N1—C1	109.70 (18)	C6—C7—C8	127.4 (2)

C4—N1—H1	125.2	C6—C7—H7	116.3
C1—N1—H1	125.2	C8—C7—H7	116.3
N1—C1—C2	106.42 (18)	C13—C8—C9	118.3 (2)
N1—C1—C5	121.59 (19)	C13—C8—C7	121.9 (2)
C2—C1—C5	132.0 (2)	C9—C8—C7	119.8 (2)
C1—C2—C3	108.3 (2)	C10—C9—C8	120.9 (2)
C1—C2—H2	125.8	C10—C9—H9	119.5
C3—C2—H2	125.8	C8—C9—H9	119.5
C4—C3—C2	107.0 (2)	C11—C10—C9	120.0 (2)
C4—C3—H3	126.5	C11—C10—H10	120.0
C2—C3—H3	126.5	C9—C10—H10	120.0
N1—C4—C3	108.6 (2)	C12—C11—C10	119.9 (2)
N1—C4—H4	125.7	C12—C11—H11	120.0
C3—C4—H4	125.7	C10—C11—H11	120.0
O1—C5—C1	121.92 (19)	C11—C12—C13	120.2 (3)
O1—C5—C6	121.0 (2)	C11—C12—H12	119.9
C1—C5—C6	117.1 (2)	C13—C12—H12	119.9
C7—C6—C5	123.2 (2)	C12—C13—C8	120.6 (2)
C7—C6—H6	118.4	C12—C13—H13	119.7
C5—C6—H6	118.4	C8—C13—H13	119.7

C4—N1—C1—C2	0.4 (2)	C1—C5—C6—C7	178.6 (2)
C4—N1—C1—C5	178.7 (2)	C5—C6—C7—C8	−179.1 (2)
N1—C1—C2—C3	−0.3 (3)	C6—C7—C8—C13	−7.4 (3)
C5—C1—C2—C3	−178.3 (2)	C6—C7—C8—C9	171.7 (2)
C1—C2—C3—C4	0.1 (3)	C13—C8—C9—C10	1.6 (3)
C1—N1—C4—C3	−0.3 (3)	C7—C8—C9—C10	−177.45 (19)
C2—C3—C4—N1	0.2 (3)	C8—C9—C10—C11	−0.5 (3)
N1—C1—C5—O1	−1.8 (3)	C9—C10—C11—C12	−0.5 (4)
C2—C1—C5—O1	175.9 (2)	C10—C11—C12—C13	0.2 (4)
N1—C1—C5—C6	179.22 (18)	C11—C12—C13—C8	1.0 (4)
C2—C1—C5—C6	−3.0 (4)	C9—C8—C13—C12	−1.9 (3)
O1—C5—C6—C7	−0.4 (3)	C7—C8—C13—C12	177.2 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86	2.02	2.817 (2)	155
C7—H7···O1	0.93	2.51	2.835 (3)	101

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