

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

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

Dong-Qing Li

Department of Chemistry and Biology, Yulin Normal University, Guangxi 537000, People's Republic of China

Correspondence e-mail: ldq00000@126.com

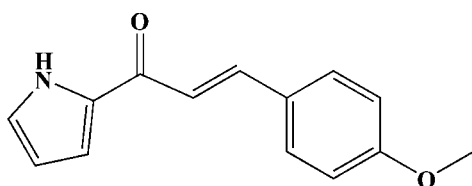
Received 18 July 2008; accepted 7 September 2008

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.048; wR factor = 0.125; data-to-parameter ratio = 15.3.

The title molecule, $\text{C}_{14}\text{H}_{13}\text{NO}_2$, is almost flat with a dihedral angle of 8.0 (1) $^\circ$ 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) $^\circ$. An intramolecular $\text{C}-\text{H}\cdots\text{O}$ 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 $\text{N}-\text{H}\cdots\text{O}$ 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

$\text{C}_{14}\text{H}_{13}\text{NO}_2$
 $M_r = 227.25$
 Monoclinic, $P2_1/c$
 $a = 5.0815$ (7) Å
 $b = 17.172$ (3) Å

$c = 13.973$ (2) Å
 $\beta = 97.878$ (3) $^\circ$
 $V = 1207.8$ (3) Å 3
 $Z = 4$
 Mo $K\alpha$ radiation

$\mu = 0.08$ 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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.019$

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
 $\Delta\rho_{\text{max}} = 0.13$ e Å $^{-3}$
 $\Delta\rho_{\text{min}} = -0.13$ e Å $^{-3}$

Table 1

Hydrogen-bond geometry (Å, $^\circ$).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|--|--------------|--------------------|-------------|----------------------|
| $\text{C7}-\text{H7}\cdots\text{O1}$ | 0.93 | 2.52 | 2.838 (2) | 100 |
| $\text{N1}-\text{H1}\cdots\text{O1}^i$ | 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.

The authors thank Yulin Normal University for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CS2091).

References

- Agrinskaya, N. V., Lukoshkin, V. A., Kudryavtsev, V. V., Nosova, G. I., Solovskaya, N. A. & Yakimanski, A. V. (1999). *Phys. Solid State*, **41**, 1914–1917.
- Bruker (2002). SMART and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bukhari, M. H., Siddiqui, H. L., Tahir, M. N., Chaudhary, M. A. & Iqbal, A. (2008). *Acta Cryst. E* **64**, o867–o868.
- Fun, H.-K., Chantrapromma, S., Patil, P. S., Karthikeyan, M. S. & Dharmaprakash, S. M. (2008). *Acta Cryst. E* **64**, o956–o957.
- Gong, Z.-Q., Liu, G.-S. & Xia, H.-Y. (2008). *Acta Cryst. E* **64**, o151.
- Indira, J., Prakash Karat, P. & Sarojini, B. K. (2002). *J. Cryst. Growth*, **242**, 209–214.
- Lin, Y. M., Zhou, Y., Flavin, M. T., Zhou, L. M., Nie, W. & Chen, F. C. (2002). *Bioorg. Med. Chem.* **10**, 2795–2802.
- Modzelewska, A., Catherine Petit, C., Achanta, G., Davidson, N. E., Huang, P. & Khan, S. R. (2006). *Bioorg. Med. Chem.* **14**, 3491–3495.
- Opletalova, V. (2000). *Ceska Slov. Farm.* **49**, 278–284.
- Opletalova, V. & Sedivy, D. (1999). *Ceska Slov. Farm.* **48**, 252–255.
- Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
- Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.
- Sogawa, S., Nihro, Y., Ueda, H., Miki, T., Matsumoto, H. & Satoh, T. (1994). *Biol. Pharm. Bull.* **17**, 251–256.

supplementary materials

Acta Cryst. (2008). E64, o1920 [doi:10.1107/S160053680802864X]

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

D.-Q. Li

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 $8.0(1)^\circ$ 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 $-0.6(3)^\circ$, meanwhile, O1 atom acts as an acceptor and is involved in an intramolecular C—H \cdots 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 \cdots 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 $d(\text{C—H}) = 0.93 \text{ \AA}$, $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$ for aromatic and ethylene; 0.96 \AA , $U_{\text{iso}} = 1.5U_{\text{eq}}(\text{C})$ for CH_3 atoms, and $d(\text{N—H}) = 0.86 \text{ \AA}$, $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{N})$ for pyrrole nitrogen atom.

Figures

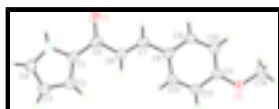


Fig. 1. The molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level and H atoms as spheres of arbitrary radius.

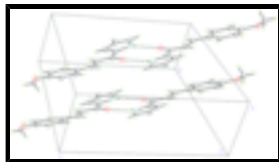


Fig. 2. Packing diagram of the title structure showing the N—H...O hydrogen bonding interactions.

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

Crystal data

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

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 | $R_{\text{int}} = 0.020$ |
| $T = 293(2) \text{ K}$ | $\theta_{\text{max}} = 26.0^\circ$ |
| φ and ω scans | $\theta_{\text{min}} = 1.9^\circ$ |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h = -6 \rightarrow 5$ |
| $T_{\text{min}} = 0.967$, $T_{\text{max}} = 0.988$ | $k = -20 \rightarrow 21$ |
| 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 |
| $wR(F^2) = 0.124$ | $w = 1/[\sigma^2(F_o^2) + (0.0557P)^2 + 0.1497P]$ |
| $S = 1.05$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 2369 reflections | $(\Delta/\sigma)_{\text{max}} < 0.001$ |
| 155 parameters | $\Delta\rho_{\text{max}} = 0.13 \text{ e \AA}^{-3}$ |
| | $\Delta\rho_{\text{min}} = -0.13 \text{ e \AA}^{-3}$ |

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

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

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|-------------|--------------|---------------|----------------------------------|
| 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 (\AA^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) |

supplementary materials

| | | | | | | |
|-----|-------------|-------------|-------------|-------------|-------------|--------------|
| 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 (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--------------------------------|-------|-------------|-------------|---------------|
| C7—H7 \cdots O1 | 0.93 | 2.52 | 2.838 (2) | 100 |
| N1—H1 \cdots O1 ⁱ | 0.86 | 2.03 | 2.8314 (17) | 155 |

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

Fig. 1

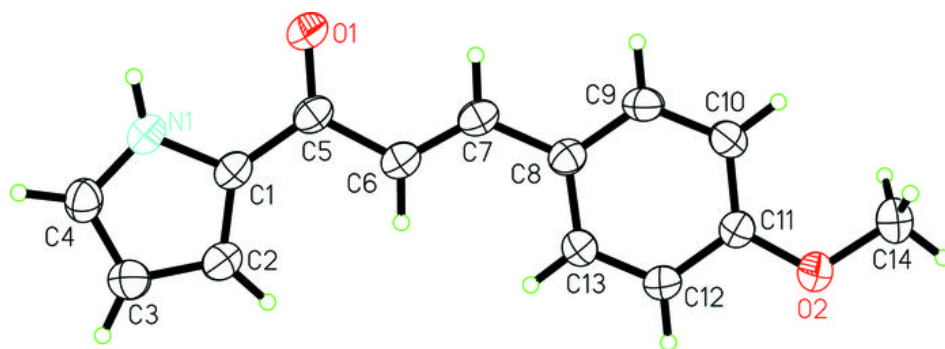


Fig. 2

