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# Crystal structure and Hirshfeld surface analysis of (2*E*)-1-phenyl-3-(1*H*-pyrrol-2-yl)propen-1-one

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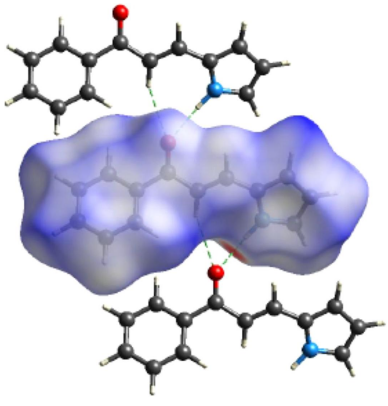
The title compound, $C_{13}H_{11}NO$, adopts an *E* configuration about the C=C double bond. The pyrrole ring is inclined to the phenyl ring at an angle of 44.94 (8)°. In the crystal, molecules are linked by N—H···O hydrogen bonds, forming ribbons parallel to (020) in zigzag *C*(7) chains along the *a* axis. These ribbons are connected *via* C—H···$\pi$ interactions, forming a three-dimensional network. No significant $\pi$–$\pi$ interactions are observed.

## 1. Chemical context

The chemistry of carbo- and heterocyclic aromatic compounds is the most important branch of organic chemistry (Khalilov *et al.*, 2022; Akkurt *et al.*, 2023). Synthetic organic chemistry is growing tremendously, with recently developed aromatic systems that are designed for various research and commercial purposes (Maharramov *et al.*, 2021, 2022; Erenler *et al.*, 2022). Nowadays, five- and six-membered heterocyclic systems find broad applications in different branches of chemistry, as well as coordination chemistry (Gurbanov *et al.*, 2021; Mahmoudi *et al.*, 2021), drug design and development (Donmez & Turkyılmaz, 2022; Askerova, 2022), and materials science (Velásquez *et al.*, 2019; Afkhami *et al.*, 2019). The pyrrole motif is the most widespread five-membered heteroaromatic ring system in nitrogen heterocycles (Mahmoudi *et al.*, 2017). It is an essential structural motif present in many natural tetrapyrrole scaffolds of heme and related cofactors (chlorophyll a, heme b, vitamin B12 and factor 430), and other bioactive molecules, like porphobilinogen, nargenicin, prodigiosin, *etc.* (Walsh *et al.*, 2006; Sobhi & Faisal, 2023). Chalcones incorporating N-heterocyclic, especially pyrrole, scaffolds with various biological and pharmacological activities, such as antioxidant, antibacterial, antifungal, antileishmanial, anticancer, antitubercular, antimalarial and other properties, have been reviewed recently (Mezgebe *et al.*, 2023). In addition, the incorporation of diverse pharmacophore groups in a pyrrole scaffold has led to the development of more desired compounds, such as elopiprazole, lorpiprazole, isamoltane, obatoclax, *etc.* (Bhardwaj *et al.*, 2015; Atalay *et al.*, 2022). Thus, in the framework of our studies in heterocyclic chemistry (Naghiyev *et al.*, 2020, 2021, 2022), we report herein the crystal structure and Hirshfeld surface analysis of the title compound, (2*E*)-1-phenyl-3-(1*H*-pyrrol-2-yl)propen-1-one.



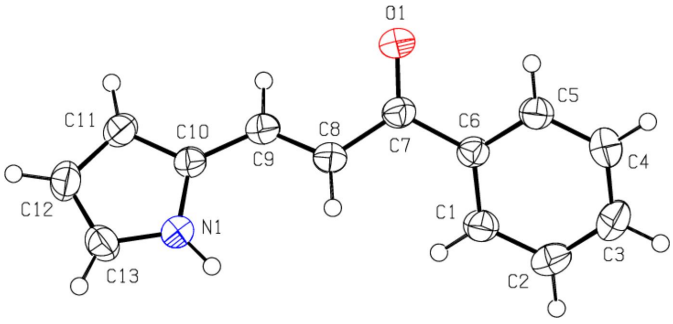
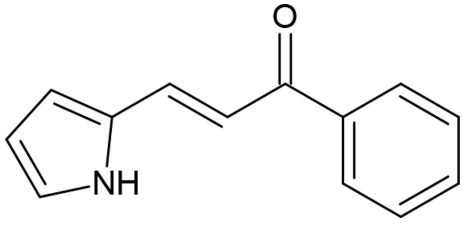



**Figure 1**
The molecular structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.




## 2. Structural commentary

The title compound (Fig. 1) shows an *E* configuration about the C=C double bond. The pyrrole ring (atoms N1/C10–C13) is inclined to the phenyl ring (C1–C6) by 44.94 (8)°, the torsion angles being C5—C6—C7—C8 = −156.04 (13)°, C5—C6—C7—O1 = 22.6 (2)°, C6—C7—C8—C9 = −163.76 (13)°, C7—C8—C9—C10 = −172.34 (13)°, O1—C7—C8—C9 = 17.6 (2)° and C8—C9—C10—C11 = 173.37 (14)°. The geometrical parameters of the the title compound are in agreement with those reported for similar compounds; see the *Database survey* section.

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

*Cg*1 and *Cg*2 are the centroids of the phenyl (C1–C6) and 1*H*-pyrrole (N1/C10–C13) rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*N*···O1$^{i}$ | 0.872 (17) | 2.119 (17) | 2.9561 (18) | 160.7 (14) |
| C2—H2···*Cg*1$^{ii}$ | 0.93 | 2.82 | 3.450 (2) | 126 |
| C5—H5···*Cg*1$^{iii}$ | 0.93 | 2.91 | 3.5233 (19) | 124 |
| C9—H9···*Cg*2$^{iv}$ | 0.93 | 3.00 | 3.6207 (18) | 126 |
| C13—H13···*Cg*2$^{v}$ | 0.93 | 2.95 | 3.593 (2) | 127 |

Symmetry codes: (i) $x-1, y, z$; (ii) $-x, -y, -z+1$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x+1, -y, -z+1$; (v) $-x, -y+1, -z+1$.

## 3. Supramolecular features and Hirshfeld surface analysis

In the crystal, molecules are linked by N—H···O hydrogen bonds, forming ribbons parallel to (020) in zigzag *C*(7) chains along the *a* axis (Bernstein *et al.*, 1995; Table 1 and Fig. 2). These ribbons are connected *via* C—H···$\pi$ interactions, forming a three-dimensional network (Table 1 and Fig. 3). No significant $\pi$–$\pi$ interactions are observed.

The Hirshfeld surfaces of the title molecule and the two-dimensional fingerprints were computed with *CrystalExplorer17.5* (Spackman *et al.*, 2021). The $d_{\rm norm}$ mappings for the title compound were performed in the range from −0.4746 (red) to +1.2616 (blue) a.u. On the $d_{\rm norm}$ surfaces, bright-red spots indicate the locations of the N—H···O interactions [Table 1 and Figs. 4(*a*) and 4(*b*)].

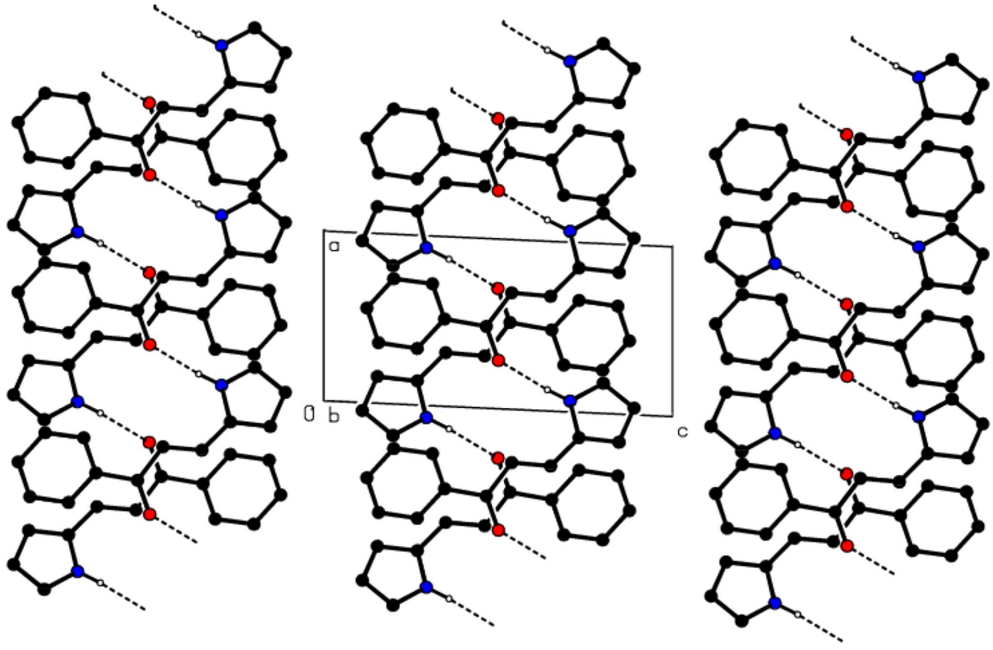



**Figure 2**
View of the N—H···O hydrogen bonds of the title compound down the *b* axis.

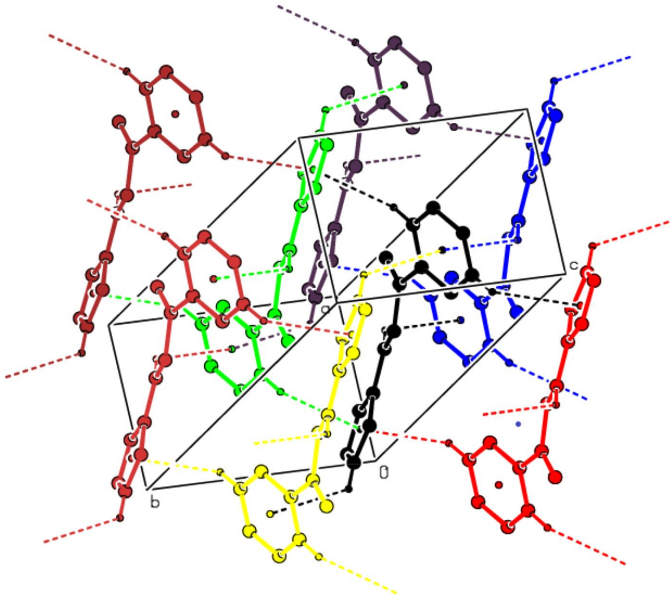



**Figure 3**
View of the C—H···$\pi$ interactions of the title compound in the unit cell.

The fingerprint plots (Fig. 5) reveal that while H···H interactions [Fig. 5(*b*); 48.4%] make the largest contributions to the surface contacts (Table 1), C···H/H···C [Fig. 5(*c*); 31.7%] and O···H/H···O [Fig. 5(*d*); 11.3%] contacts are also important. Other less notable interactions are C···C (3.7%), N···H/H···N (3.1%) and O···C/C···O (1.8%).

## 4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.43, last update November 2022; Groom *et al.*, 2016) for the '(2*E*)-1-phenyl-3-(1*H*-pyrrol-2-yl)prop-2-en-1-one' skeleton of the title compound yielded two hits, namely, 1-(3-chlorophenyl)-3-(3-furyl)prop-2-en-1-one (CSD refcode NUQFOW; Zingales *et al.*, 2015) and (*E*)-3-(2-furyl)-1-phenylprop-2-en-1-one (NOTCUW01; Vázquez-Vuelvas *et al.*,

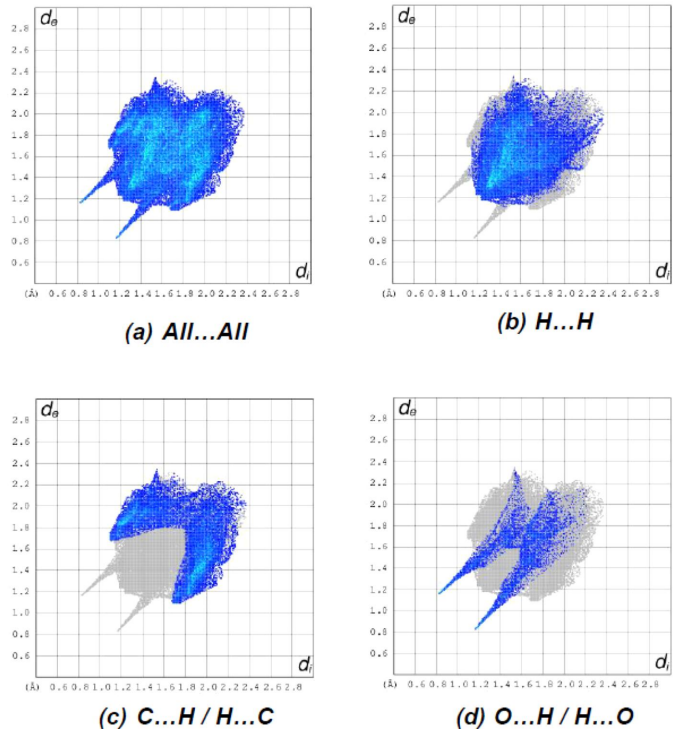



**Figure 5**
The two-dimensional fingerprint plots of the title compound, showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) C···H/H···C and (*d*) O···H/H···O interactions.

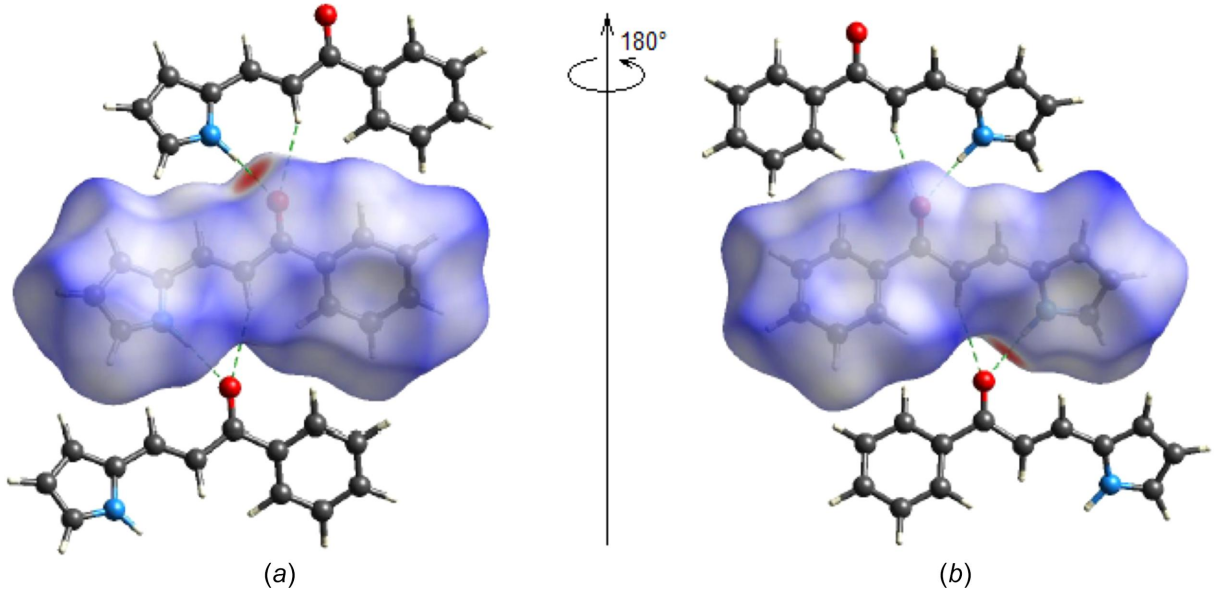



**Figure 4**
(*a*) Front and (*b*) back sides of the three-dimensional Hirshfeld surface of the title compound mapped over $d_{norm}$, with a fixed colour scale of −0.4746 to +1.2616 a.u.

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{13}H_{11}NO$ |
| $M_r$ | 197.23 |
| Crystal system, space group | Triclinic, $P\overline{1}$ |
| Temperature (K) | 293 |
| $a, b, c$ (Å) | 5.7855 (16), 7.3347 (19), 12.424 (3) |
| $\alpha, \beta, \gamma$ (°) | 106.519 (8), 91.912 (9), 92.326 (9) |
| $V$ (Å$^3$) | 504.5 (2) |
| $Z$ | 2 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.08 |
| Crystal size (mm) | 0.12 × 0.11 × 0.10 |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| Absorption correction | Multi-scan (*SADABS*; Krause *et al.*, 2015) |
| $T_{min}$, $T_{max}$ | 0.688, 0.746 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 18072, 2535, 1908 |
| $R_{int}$ | 0.042 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.673 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.049, 0.108, 1.06 |
| No. of reflections | 2535 |
| No. of parameters | 139 |
| H-atom treatment | H atoms treated by a mixture of independent and constrained refinement |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.18, −0.16 |

Computer programs: *APEX2* and *SAINT* (Bruker, 2007), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

2015). When the positions of the pyrrole and phenyl rings are switched, additional hits are found, namely, 1-(2,4-dimethylfuran-3-yl)-3-phenylprop-2-en-1-one (MISXUL; Khalilov *et al.*, 2023), 1-(3-furyl)-3-[3-(trifluoromethyl)phenyl]prop-2-en-1-one (KUDNAA; Bákowicz *et al.*, 2015) and (2*E*)-3-(4-chlorophenyl)-1-(1*H*-pyrrol-2-yl)prop-2-en-1-one (XIYYOU; Bukhari *et al.*, 2008).

In the crystal of NUQFOW, molecules stack along the *a* axis; however, there are no significant intermolecular interactions present. In the crystal of NOTCUW01, molecules are connected by weak C—H···O hydrogen bonds and C—H···$\pi$ interactions, forming ribbons extending along the *c* axis. In the crystal of MISXUL, pairs of molecules are linked by C—H···O hydrogen bonds, forming dimers with $R_2^2(14)$ ring motifs. The molecules are connected *via* C—H···$\pi$ interactions, forming a three-dimensional network. No $\pi$–$\pi$ interactions are observed. In KUDNAA, molecules are linked by intermolecular C—H···O interactions, forming zigzag chains with $C(5)$ motifs along the *b* axis. In addition, molecules are connected by face-to-face $\pi$–$\pi$ stacking interactions [centroid–centroid distances = 3.926 (3) and 3.925 (2) Å] between the opposing benzene and furan rings of the molecules along the *c* axis. In XIYYOU, intermolecular N—H···O hydrogen bonds link the molecules into centrosymmetric $R_2^2(10)$ dimers. There are C—H···$\pi$ interactions between the benzene and pyrrole rings and a benzene C—H group. A weak $\pi$–$\pi$ interaction between the pyrrole rings [centroid–centroid distance = 3.8515 (11) Å] further stabilizes the structure. There is also a $\pi$-interaction between the pyrrole ring and the carbonyl group, with an O···$\pi$ distance of 3.4825 (18) Å.

## 5. Synthesis and crystallization

The title compound was synthesized according to a recently reported procedure (Li *et al.*, 2022), and colourless crystals were obtained upon recrystallization from an ethanol/water (3:1 *v*/*v*) solution.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The C-bound H atoms were placed in calculated positions (0.93 Å) and refined as riding atoms with $U_{iso}(H) = 1.2U_{eq}(C)$. The N-bound H atom was located in a difference map and refined with $U_{iso}(H) = 1.2U_{eq}(N)$. Three reflections (001, 010 and 020) were omitted in the final cycles of refinement.

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The contributions of the authors are as follows: conceptualization, IGM, ANK and AMM; methodology, IB and MA; investigation, ASA and FNN; writing (original draft), MA, AB and ANK; writing (review and editing of the manuscript), MA and ANK; visualization, MA, IGM and FNN; funding acquisition, ASA, AB and FNN; resources, AB, ASA and MA; supervision, MA and ANK.

## References

Afkhami, F. A., Mahmoudi, G., Khandar, A. A., Franconetti, A., Zangrando, E., Qureshi, N., Lipkowski, J., Gurbanov, A. V. & Frontera, A. (2019). *Eur. J. Inorg. Chem.* **2019**, 262–270.
Akkurt, M., Maharramov, A. M., Shikhaliyev, N. G., Qajar, A. M., Atakishiyeva, G., Shikhaliyeva, I. M., Niyazova, A. A. & Bhattarai, A. (2023). *UNEC J. Eng. Appl. Sci.* **3**, 33–39.
Askerova, U. F. (2022). *UNEC J. Eng. Appl. Sci.* **2**, 58–64.
Atalay, V. E., Atish, I. S., Shahin, K. F., Kashikchi, E. S. & Karahan, M. (2022). *UNEC J. Eng. Appl. Sci.* **2**, 33–40.
Bąkowicz, J., Galica, T. & Turowska-Tyrk, I. (2015). *Z. Kristallogr. Cryst. Mater.* **230**, 131–137.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bhardwaj, V., Gumber, D., Abbot, V., Dhiman, S. & Sharma, P. (2015). *RSC Adv.* **5**, 15233–15266.
Bruker (2007). *APEX2* 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.
Donmez, M. & Turkyılmaz, M. (2022). *UNEC J. Eng. Appl. Sci.* **2**, 43–48.
Erenler, R., Dag, B. & Ozbek, B. B. (2022). *UNEC J. Eng. Appl. Sci.* **2**, 26–32.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Gurbanov, A. V., Mertsalov, D. F., Zubkov, F. I., Nadirova, M. A., Nikitina, E. V., Truong, H. H., Grigoriev, M. S., Zaytsev, V. P., Mahmudov, K. T. & Pombeiro, A. J. L. (2021). *Crystals*, **11**, 112.

Khalilov, A. N., Khrustalev, V. N., Samigullina, A. I., Akkurt, M., Rzayev, R. M., Bhattarai, A. & Mamedov, İ. G. (2023). *Acta Cryst.* E**79**, 736–740.

Khalilov, A. N., Khrustalev, V. N., Tereshina, T. A., Akkurt, M., Rzayev, R. M., Akobirshoeva, A. A. & Mamedov, İ. G. (2022). *Acta Cryst.* E**78**, 525–529.

Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.

Li, J., Zheng, H., Lu, H., Li, J., Yao, L., Wang, Y., Zhou, X., Nie, J., Zhu, X. & Fu, Z. (2022). *Eur. Polym. J.* **176**, 111393.

Maharramov, A. M., Shikhaliyev, N. G., Zeynalli, N. R., Niyazova, A. A., Garazade, Kh. A. & Shikhaliyeva, I. M. (2021). *UNEC J. Eng. Appl. Sci.* **1**, 5–11.

Maharramov, A. M., Suleymanova, G. T., Qajar, A. M., Niyazova, A. A., Ahmadova, N. E., Shikhaliyeva, I. M., Garazade, Kh. A., Nenajdenko, V. G. & Shikaliyev, N. G. (2022). *UNEC J. Eng. Appl. Sci.* **2**, 64–73.

Mahmoudi, G., Zangrando, E., Bauzá, A., Maniukiewicz, W., Carballo, R., Gurbanov, A. V. & Frontera, A. (2017). *CrystEngComm*, **19**, 3322–3330.

Mahmoudi, G., Zangrando, E., Miroslaw, B., Gurbanov, A. V., Babashkina, M. G., Frontera, A. & Safin, D. A. (2021). *Inorg. Chim. Acta*, **519**, 120279.

Mezgebe, K., Melaku, Y. & Mulugeta, E. (2023). *ACS Omega*, **8**, 19194–19211.

Naghiyev, F. N., Akkurt, M., Askerov, R. K., Mamedov, I. G., Rzayev, R. M., Chyrka, T. & Maharramov, A. M. (2020). *Acta Cryst.* E**76**, 720–723.

Naghiyev, F. N., Khrustalev, V. N., Novikov, A. P., Akkurt, M., Rzayev, R. M., Akobirshoeva, A. A. & Mamedov, I. G. (2022). *Acta Cryst.* E**78**, 554–558.

Naghiyev, F. N., Tereshina, T. A., Khrustalev, V. N., Akkurt, M., Rzayev, R. M., Akobirshoeva, A. A. & Mamedov, İ. G. (2021). *Acta Cryst.* E**77**, 516–521.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Sobhi, R. M. & Faisal, R. M. (2023). *UNEC J. Eng. Appl. Sci.* **3**, 21–32.

Spackman, P. R., Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Jayatilaka, D. & Spackman, M. A. (2021). *J. Appl. Cryst.* **54**, 1006–1011.

Spek, A. L. (2020). *Acta Cryst.* E**76**, 1–11.

Vázquez-Vuelvas, O. F., Enríquez-Figueroa, R. A., García-Ortega, H., Flores-Alamo, M. & Pineda-Contreras, A. (2015). *Acta Cryst.* E**71**, 161–164.

Velásquez, J. D., Mahmoudi, G., Zangrando, E., Gurbanov, A. V., Zubkov, F. I., Zorlu, Y., Masoudiasl, A. & Echeverría, J. (2019). *CrystEngComm*, **21**, 6018–6025.

Walsh, C. T., Garneau-Tsodikova, S. & Howard-Jones, A. R. (2006). *Nat. Prod. Rep.* **23**, 517–531.

Zingales, S. K., Wallace, M. Z. & Padgett, C. W. (2015). *Acta Cryst.* E**71**, o707.

# supporting information

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## Crystal structure and Hirshfeld surface analysis of (2*E*)-1-phenyl-3-(1*H*-pyrrol-2-yl)propen-1-one

**Ayten S. Safarova, Ali N. Khalilov, Mehmet Akkurt, Abel M. Maharramov, Ajaya Bhattarai, Farid N. Naghiyev and İbrahim G. Mamedov**

### Computing details

**(2*E*)-1-Phenyl-3-(1*H*-pyrrol-2-yl)propen-1-one**

*Crystal data*

$C_{13}H_{11}NO$
$M_r$ = 197.23
Triclinic, $P\overline{1}$
$a$ = 5.7855 (16) Å
$b$ = 7.3347 (19) Å
$c$ = 12.424 (3) Å
$\alpha$ = 106.519 (8)°
$\beta$ = 91.912 (9)°
$\gamma$ = 92.326 (9)°
$V$ = 504.5 (2) Å$^3$
$Z$ = 2
$F(000)$ = 208
$D_x$ = 1.298 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 5813 reflections
$\theta$ = 2.9–27.4°
$\mu$ = 0.08 mm$^{-1}$
$T$ = 293 K
Block, colorless
0.12 × 0.11 × 0.10 mm

*Data collection*

Bruker APEXII CCD diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
$T_{min}$ = 0.688, $T_{max}$ = 0.746
18072 measured reflections
2535 independent reflections
1908 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.042
$\theta_{max}$ = 28.6°, $\theta_{min}$ = 2.9°
$h$ = −7→7
$k$ = −9→9
$l$ = −16→16

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.108
$S$ = 1.06
2535 reflections
139 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0348P)^2 + 0.1277P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.15 e Å$^{-3}$

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.2761 (2) | 0.1954 (2) | 0.68844 (12) | 0.0384 (3) |
| H1 | 0.152580 | 0.148144 | 0.636826 | 0.046* |
| C2 | 0.2561 (3) | 0.1996 (2) | 0.79934 (13) | 0.0454 (4) |
| H2 | 0.120202 | 0.152611 | 0.822105 | 0.055* |
| C3 | 0.4365 (3) | 0.2729 (2) | 0.87637 (13) | 0.0482 (4) |
| H3 | 0.421898 | 0.276227 | 0.951211 | 0.058* |
| C4 | 0.6386 (3) | 0.3416 (2) | 0.84307 (13) | 0.0455 (4) |
| H4 | 0.759276 | 0.393419 | 0.895615 | 0.055* |
| C5 | 0.6619 (2) | 0.3335 (2) | 0.73212 (12) | 0.0378 (3) |
| H5 | 0.800320 | 0.376468 | 0.709453 | 0.045* |
| C6 | 0.4805 (2) | 0.26175 (18) | 0.65370 (11) | 0.0324 (3) |
| C7 | 0.5128 (2) | 0.25283 (19) | 0.53401 (11) | 0.0354 (3) |
| C8 | 0.3085 (2) | 0.2513 (2) | 0.46122 (12) | 0.0383 (3) |
| H8 | 0.168759 | 0.287979 | 0.493566 | 0.046* |
| C9 | 0.3176 (2) | 0.19850 (19) | 0.34947 (11) | 0.0357 (3) |
| H9 | 0.455504 | 0.148284 | 0.321134 | 0.043* |
| C10 | 0.1436 (2) | 0.20911 (19) | 0.26803 (11) | 0.0335 (3) |
| C11 | 0.1590 (3) | 0.1715 (2) | 0.15357 (12) | 0.0407 (4) |
| H11 | 0.283975 | 0.120383 | 0.112231 | 0.049* |
| C12 | −0.0454 (3) | 0.2235 (2) | 0.11041 (13) | 0.0457 (4) |
| H12 | −0.081206 | 0.214416 | 0.035462 | 0.055* |
| C13 | −0.1829 (3) | 0.2901 (2) | 0.19837 (13) | 0.0436 (4) |
| H13 | −0.330437 | 0.334068 | 0.193755 | 0.052* |
| N1 | −0.0693 (2) | 0.28171 (17) | 0.29363 (10) | 0.0386 (3) |
| H1N | −0.130 (3) | 0.302 (2) | 0.3590 (14) | 0.046* |
| O1 | 0.70997 (17) | 0.25046 (16) | 0.49928 (8) | 0.0496 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0329 (7) | 0.0410 (8) | 0.0402 (8) | −0.0001 (6) | 0.0026 (6) | 0.0099 (6) |
| C2 | 0.0437 (9) | 0.0482 (9) | 0.0484 (9) | 0.0010 (7) | 0.0145 (7) | 0.0190 (7) |
| C3 | 0.0613 (10) | 0.0526 (9) | 0.0349 (8) | 0.0068 (8) | 0.0081 (7) | 0.0181 (7) |
| C4 | 0.0467 (9) | 0.0493 (9) | 0.0391 (9) | 0.0005 (7) | −0.0068 (7) | 0.0115 (7) |
| C5 | 0.0338 (7) | 0.0404 (8) | 0.0402 (8) | 0.0016 (6) | 0.0029 (6) | 0.0128 (6) |
| C6 | 0.0320 (7) | 0.0324 (7) | 0.0331 (7) | 0.0059 (5) | 0.0044 (6) | 0.0089 (5) |
| C7 | 0.0335 (7) | 0.0379 (7) | 0.0349 (7) | 0.0053 (6) | 0.0059 (6) | 0.0096 (6) |
| C8 | 0.0315 (7) | 0.0474 (8) | 0.0371 (8) | 0.0078 (6) | 0.0052 (6) | 0.0127 (6) |
| C9 | 0.0328 (7) | 0.0373 (7) | 0.0380 (8) | 0.0013 (6) | 0.0052 (6) | 0.0120 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C10 | 0.0320 (7) | 0.0354 (7) | 0.0334 (7) | −0.0009 (5) | 0.0025 (6) | 0.0109 (6) |
| C11 | 0.0412 (8) | 0.0464 (8) | 0.0344 (8) | −0.0019 (6) | 0.0062 (6) | 0.0115 (6) |
| C12 | 0.0521 (10) | 0.0540 (9) | 0.0333 (8) | −0.0052 (7) | −0.0036 (7) | 0.0179 (7) |
| C13 | 0.0364 (8) | 0.0502 (9) | 0.0479 (9) | 0.0019 (7) | −0.0054 (7) | 0.0207 (7) |
| N1 | 0.0360 (7) | 0.0472 (7) | 0.0338 (7) | 0.0031 (5) | 0.0048 (5) | 0.0129 (5) |
| O1 | 0.0330 (6) | 0.0771 (8) | 0.0403 (6) | 0.0057 (5) | 0.0088 (5) | 0.0181 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.378 (2) | C8—C9 | 1.3346 (19) |
| C1—C6 | 1.3886 (19) | C8—H8 | 0.9300 |
| C1—H1 | 0.9300 | C9—C10 | 1.4237 (19) |
| C2—C3 | 1.375 (2) | C9—H9 | 0.9300 |
| C2—H2 | 0.9300 | C10—N1 | 1.3728 (18) |
| C3—C4 | 1.377 (2) | C10—C11 | 1.3761 (19) |
| C3—H3 | 0.9300 | C11—C12 | 1.394 (2) |
| C4—C5 | 1.374 (2) | C11—H11 | 0.9300 |
| C4—H4 | 0.9300 | C12—C13 | 1.361 (2) |
| C5—C6 | 1.3867 (19) | C12—H12 | 0.9300 |
| C5—H5 | 0.9300 | C13—N1 | 1.3526 (18) |
| C6—C7 | 1.4882 (19) | C13—H13 | 0.9300 |
| C7—O1 | 1.2318 (16) | N1—H1N | 0.871 (16) |
| C7—C8 | 1.462 (2) | | |
| | | | |
| C2—C1—C6 | 120.07 (14) | C9—C8—C7 | 121.56 (13) |
| C2—C1—H1 | 120.0 | C9—C8—H8 | 119.2 |
| C6—C1—H1 | 120.0 | C7—C8—H8 | 119.2 |
| C3—C2—C1 | 120.16 (14) | C8—C9—C10 | 128.38 (13) |
| C3—C2—H2 | 119.9 | C8—C9—H9 | 115.8 |
| C1—C2—H2 | 119.9 | C10—C9—H9 | 115.8 |
| C2—C3—C4 | 120.20 (14) | N1—C10—C11 | 106.72 (12) |
| C2—C3—H3 | 119.9 | N1—C10—C9 | 124.28 (12) |
| C4—C3—H3 | 119.9 | C11—C10—C9 | 128.65 (13) |
| C5—C4—C3 | 119.93 (14) | C10—C11—C12 | 108.08 (13) |
| C5—C4—H4 | 120.0 | C10—C11—H11 | 126.0 |
| C3—C4—H4 | 120.0 | C12—C11—H11 | 126.0 |
| C4—C5—C6 | 120.48 (13) | C13—C12—C11 | 107.23 (13) |
| C4—C5—H5 | 119.8 | C13—C12—H12 | 126.4 |
| C6—C5—H5 | 119.8 | C11—C12—H12 | 126.4 |
| C5—C6—C1 | 119.12 (13) | N1—C13—C12 | 108.61 (14) |
| C5—C6—C7 | 119.03 (12) | N1—C13—H13 | 125.7 |
| C1—C6—C7 | 121.83 (12) | C12—C13—H13 | 125.7 |
| O1—C7—C8 | 121.73 (13) | C13—N1—C10 | 109.35 (12) |
| O1—C7—C6 | 119.52 (13) | C13—N1—H1N | 125.1 (10) |
| C8—C7—C6 | 118.74 (12) | C10—N1—H1N | 124.9 (10) |
| | | | |
| C6—C1—C2—C3 | 1.3 (2) | O1—C7—C8—C9 | 17.6 (2) |
| C1—C2—C3—C4 | −0.4 (2) | C6—C7—C8—C9 | −163.76 (13) |

| | | | |
|---|---|---|---|
| C2—C3—C4—C5 | −1.2 (2) | C7—C8—C9—C10 | −172.34 (13) |
| C3—C4—C5—C6 | 1.9 (2) | C8—C9—C10—N1 | 1.1 (2) |
| C4—C5—C6—C1 | −1.0 (2) | C8—C9—C10—C11 | 173.37 (14) |
| C4—C5—C6—C7 | −179.23 (12) | N1—C10—C11—C12 | 0.50 (16) |
| C2—C1—C6—C5 | −0.7 (2) | C9—C10—C11—C12 | −172.82 (13) |
| C2—C1—C6—C7 | 177.54 (13) | C10—C11—C12—C13 | −0.54 (17) |
| C5—C6—C7—O1 | 22.6 (2) | C11—C12—C13—N1 | 0.37 (17) |
| C1—C6—C7—O1 | −155.56 (14) | C12—C13—N1—C10 | −0.06 (16) |
| C5—C6—C7—C8 | −156.04 (13) | C11—C10—N1—C13 | −0.27 (15) |
| C1—C6—C7—C8 | 25.76 (19) | C9—C10—N1—C13 | 173.41 (13) |

*Hydrogen-bond geometry (Å, º)*

Cg1 and Cg2 are the centroids of the (C1–C6) phenyl and (N1/C10–C13) 1H-pyrrole rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*N*···O1$^{i}$ | 0.872 (17) | 2.119 (17) | 2.9561 (18) | 160.7 (14) |
| C2—H2···*Cg*1$^{ii}$ | 0.93 | 2.82 | 3.450 (2) | 126 |
| C5—H5···*Cg*1$^{iii}$ | 0.93 | 2.91 | 3.5233 (19) | 124 |
| C9—H9···*Cg*2$^{iv}$ | 0.93 | 3.00 | 3.6207 (18) | 126 |
| C13—H13···*Cg*2$^{v}$ | 0.93 | 2.95 | 3.593 (2) | 127 |

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) −*x*, −*y*, −*z*+1; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) −*x*+1, −*y*, −*z*+1; (v) −*x*, −*y*+1, −*z*+1.