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# 2-(4-Nitrophenyl)-5-phenylfuran

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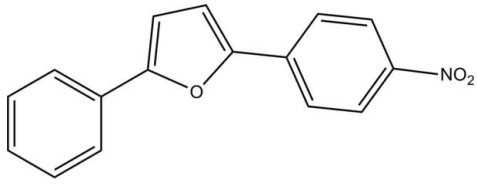
Key indicators: single-crystal X-ray study; $T$ = 113 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.063; $wR$ factor = 0.174; data-to-parameter ratio = 16.1.

The molecular skeleton of the title molecule, $C_{16}H_{11}NO_3$, is nearly planar with the two aromatic rings forming a dihedral angle of 2.73 (7)°. In the crystal, weak intermolecular C—H···O hydrogen bonds link molecules into ribbons extended along [101]. The crystal packing exhibits also $\pi$–$\pi$ interactions, as indicated by the short centroid–centroid distances between the aromatic rings [3.681 (3) Å] and between the aromatic and furan rings [3.811 (3) Å] of neighbouring molecules.

## Related literature

For details of the synthesis, see: Wang *et al.* (2009).




## Experimental

*Crystal data*

$C_{16}H_{11}NO_3$
$M_r$ = 265.26
Monoclinic, $P2_1/n$
$a$ = 7.3213 (15) Å
$b$ = 16.290 (3) Å
$c$ = 10.904 (2) Å
$\beta$ = 100.81 (3)°
$V$ = 1277.3 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 113 K
0.24 × 0.22 × 0.19 mm

*Data collection*

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min}$ = 0.977, $T_{max}$ = 0.982
10136 measured reflections
2924 independent reflections
1168 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.070

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.174
$S$ = 1.00
2924 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.19 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C3—H3···O3$^{i}$ | 0.95 | 2.51 | 3.373 (3) | 152 |
| C12—H12···O2$^{ii}$ | 0.95 | 2.61 | 3.435 (3) | 146 |

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $x+1, y, z+1$.

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

This work was funded in 2007 as a selected project in scientific and technological activities for returned scholars by the State Personnel Ministry.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2666).

## References

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Rigaku/MSC (2005). *CrystalClear* and *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wang, G., Guan, Z., Tang, R. & He, Y. (2009). *J. Heterocycl. Chem.* **46**, 540–543.

# supplementary materials

*Acta Cryst.* (2010). E**66**, o128 [ **doi:10.1107/S160053680905288X** ]

# 2-(4-Nitrophenyl)-5-phenylfuran

**Z. Guan, Y. He and G. Wang**

## Comment

The title compound, (I), has been obtained as a by-product in our ongoing research of highly substituted furan derivatives (Wang *et al.*, 2009).

In (I) (Fig. 1), two aromatic rings form a dihedral angle of 2.73 (7) °. Weak intermolecular C—H···O hydrogen bonds (Table 1) and π-π stacking interactions with centroid-centroid separations of 3.681 (3) and 3.811 (3) Å consolidate the crystal packing.

## Experimental

A solution of ethyl 2-benzoyl-4-(4-nitrophenyl)-4-oxobutanoate (0.353 g, 0.7 mmol) in ionic liquid [bmim]$HSO_4$ (1.6 g, 6.7 mmol) was stirred at 150 °C for 4 h in oil bath. After cooling to r.t., the reaction mixture was extracted with diethyl ether thoroughly. The combined extracts were washed with water, brine,dried ($Na_2SO_4$),and filtered. The solvents were removed and the residue was purified by flash chromatography (petroleum ether / dichloromethane 2:1) to get Ethyl 5-(4-nitrophenyl)-2-phenylfuran-3-carboxylate (240 mg, 71%) and the title compound (50 mg,14%) as yellow crystals.

## Refinement

All H-atoms were positioned geometrically and refined using a riding model, with d(C—H) = 0.95 Å, $U_{iso}$=1.2$U_{eq}$(C).

## Figures

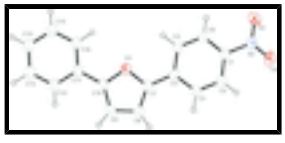


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

## 2-(4-Nitrophenyl)-5-phenylfuran

*Crystal data*

| | |
|---|---|
| $C_{16}H_{11}NO_3$ | $F$(000) = 552 |
| $M_r$ = 265.26 | $D_x$ = 1.379 Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation, λ = 0.71073 Å |
| $a$ = 7.3213 (15) Å | Cell parameters from 3226 reflections |
| $b$ = 16.290 (3) Å | θ = 2.3–27.7° |
| $c$ = 10.904 (2) Å | μ = 0.10 mm$^{-1}$ |
| β = 100.81 (3)° | $T$ = 113 K |

| | |
|---|---|
| $V$ = 1277.3 (4) Å$^3$ | Block, orange |
| $Z$ = 4 | 0.24 × 0.22 × 0.19 mm |

*Data collection*

| | |
|---|---|
| Rigaku Saturn CCD area-detector diffractometer | 2924 independent reflections |
| Radiation source: rotating anode | 1168 reflections with $I > 2\sigma(I)$ |
| confocal | $R_{int}$ = 0.070 |
| Detector resolution: 7.31 pixels mm$^{-1}$ | $\theta_{max}$ = 27.6°, $\theta_{min}$ = 3.1° |
| ω and φ scans | $h$ = −9→9 |
| Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005) | $k$ = −21→21 |
| $T_{min}$ = 0.977, $T_{max}$ = 0.982 | $l$ = −12→14 |
| 10136 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)]$ = 0.063 | $w = 1/[\sigma^2(F_o^2) + (0.0654P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2)$ = 0.174 | $(\Delta/\sigma)_{max} < 0.001$ |
| $S$ = 1.00 | $\Delta\rho_{max}$ = 0.22 e Å$^{-3}$ |
| 2924 reflections | $\Delta\rho_{min}$ = −0.19 e Å$^{-3}$ |
| 182 parameters | Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.086 (10) |
| Secondary atom site location: difference Fourier map | |

*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 | 0.83658 (18) | 0.47058 (7) | 0.09998 (13) | 0.0540 (5) |

| | | | | |
|---|---|---|---|---|
| O2 | 0.3323 (3) | 0.56325 (12) | −0.48419 (15) | 0.0968 (7) |
| O3 | 0.3467 (3) | 0.69148 (10) | −0.43913 (17) | 0.0971 (7) |
| N1 | 0.3792 (3) | 0.61960 (13) | −0.41169 (19) | 0.0685 (6) |
| C1 | 0.4782 (3) | 0.60055 (13) | −0.2862 (2) | 0.0528 (6) |
| C2 | 0.5230 (3) | 0.66262 (13) | −0.2022 (2) | 0.0632 (7) |
| H2 | 0.4856 | 0.7174 | −0.2240 | 0.076* |
| C3 | 0.6219 (3) | 0.64521 (13) | −0.0866 (2) | 0.0612 (7) |
| H3 | 0.6524 | 0.6882 | −0.0275 | 0.073* |
| C4 | 0.6791 (3) | 0.56563 (12) | −0.05378 (19) | 0.0504 (6) |
| C5 | 0.6301 (3) | 0.50391 (12) | −0.1400 (2) | 0.0569 (6) |
| H5 | 0.6657 | 0.4489 | −0.1185 | 0.068* |
| C6 | 0.5298 (3) | 0.52119 (12) | −0.2572 (2) | 0.0595 (6) |
| H6 | 0.4971 | 0.4787 | −0.3169 | 0.071* |
| C7 | 0.7901 (3) | 0.55033 (12) | 0.0684 (2) | 0.0554 (6) |
| C9 | 0.9599 (3) | 0.54956 (13) | 0.2595 (2) | 0.0696 (8) |
| H9 | 1.0268 | 0.5672 | 0.3382 | 0.084* |
| C8 | 0.8639 (3) | 0.59996 (14) | 0.1642 (2) | 0.0700 (8) |
| H8 | 0.8530 | 0.6580 | 0.1666 | 0.084* |
| C10 | 0.9392 (3) | 0.47133 (13) | 0.2184 (2) | 0.0547 (6) |
| C11 | 1.0059 (3) | 0.39286 (13) | 0.2725 (2) | 0.0552 (6) |
| C12 | 1.0985 (3) | 0.38948 (14) | 0.3963 (2) | 0.0673 (7) |
| H12 | 1.1158 | 0.4382 | 0.4450 | 0.081* |
| C13 | 1.1648 (3) | 0.31612 (15) | 0.4481 (2) | 0.0787 (8) |
| H13 | 1.2278 | 0.3145 | 0.5326 | 0.094* |
| C14 | 1.1415 (4) | 0.24587 (16) | 0.3802 (3) | 0.0848 (9) |
| H14 | 1.1872 | 0.1953 | 0.4173 | 0.102* |
| C15 | 1.0523 (4) | 0.24782 (14) | 0.2581 (3) | 0.0847 (9) |
| H15 | 1.0371 | 0.1986 | 0.2104 | 0.102* |
| C16 | 0.9841 (3) | 0.32104 (13) | 0.2038 (2) | 0.0683 (7) |
| H16 | 0.9221 | 0.3220 | 0.1191 | 0.082* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0608 (9) | 0.0479 (9) | 0.0501 (10) | 0.0013 (7) | 0.0021 (8) | 0.0039 (7) |
| O2 | 0.1211 (16) | 0.0947 (14) | 0.0616 (12) | 0.0146 (11) | −0.0160 (11) | −0.0143 (10) |
| O3 | 0.1200 (16) | 0.0727 (13) | 0.0855 (14) | 0.0136 (10) | −0.0141 (12) | 0.0234 (10) |
| N1 | 0.0684 (13) | 0.0728 (14) | 0.0594 (14) | 0.0080 (10) | −0.0007 (11) | 0.0052 (11) |
| C1 | 0.0501 (12) | 0.0567 (13) | 0.0489 (13) | 0.0029 (10) | 0.0023 (10) | 0.0059 (10) |
| C2 | 0.0694 (15) | 0.0474 (13) | 0.0655 (16) | 0.0056 (11) | −0.0063 (12) | 0.0013 (11) |
| C3 | 0.0701 (15) | 0.0471 (13) | 0.0605 (15) | 0.0021 (10) | −0.0031 (12) | −0.0038 (11) |
| C4 | 0.0537 (13) | 0.0457 (12) | 0.0507 (13) | −0.0042 (9) | 0.0072 (10) | 0.0037 (10) |
| C5 | 0.0726 (15) | 0.0420 (12) | 0.0540 (14) | 0.0031 (10) | 0.0063 (12) | 0.0040 (10) |
| C6 | 0.0739 (16) | 0.0502 (13) | 0.0516 (14) | −0.0001 (10) | 0.0048 (12) | −0.0039 (10) |
| C7 | 0.0614 (13) | 0.0468 (12) | 0.0547 (14) | 0.0027 (10) | 0.0029 (11) | 0.0032 (10) |
| C9 | 0.0815 (17) | 0.0579 (15) | 0.0600 (15) | −0.0001 (12) | −0.0111 (13) | −0.0044 (12) |
| C8 | 0.0825 (17) | 0.0520 (14) | 0.0660 (16) | 0.0046 (12) | −0.0102 (13) | −0.0033 (12) |
| C10 | 0.0535 (13) | 0.0579 (14) | 0.0484 (14) | −0.0008 (10) | −0.0015 (11) | 0.0047 (10) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C11 | 0.0484 (12) | 0.0554 (13) | 0.0588 (15) | −0.0014 (10) | 0.0023 (11) | 0.0082 (11) |
| C12 | 0.0727 (16) | 0.0644 (15) | 0.0594 (16) | 0.0006 (12) | −0.0015 (13) | 0.0066 (12) |
| C13 | 0.0857 (18) | 0.0737 (18) | 0.0680 (18) | 0.0021 (14) | −0.0076 (15) | 0.0174 (14) |
| C14 | 0.100 (2) | 0.0590 (16) | 0.087 (2) | 0.0009 (14) | −0.0049 (17) | 0.0195 (14) |
| C15 | 0.106 (2) | 0.0523 (15) | 0.087 (2) | −0.0018 (13) | −0.0051 (17) | 0.0046 (14) |
| C16 | 0.0772 (16) | 0.0555 (14) | 0.0641 (16) | −0.0037 (12) | −0.0074 (13) | 0.0029 (12) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C10 | 1.367 (2) | C9—C10 | 1.350 (3) |
| O1—C7 | 1.371 (2) | C9—C8 | 1.405 (3) |
| O2—N1 | 1.218 (2) | C9—H9 | 0.9500 |
| O3—N1 | 1.221 (2) | C8—H8 | 0.9500 |
| N1—C1 | 1.457 (3) | C10—C11 | 1.453 (3) |
| C1—C2 | 1.363 (3) | C11—C16 | 1.382 (3) |
| C1—C6 | 1.367 (3) | C11—C12 | 1.394 (3) |
| C2—C3 | 1.360 (3) | C12—C13 | 1.371 (3) |
| C2—H2 | 0.9500 | C12—H12 | 0.9500 |
| C3—C4 | 1.388 (3) | C13—C14 | 1.357 (3) |
| C3—H3 | 0.9500 | C13—H13 | 0.9500 |
| C4—C5 | 1.377 (3) | C14—C15 | 1.369 (3) |
| C4—C7 | 1.446 (3) | C14—H14 | 0.9500 |
| C5—C6 | 1.379 (3) | C15—C16 | 1.382 (3) |
| C5—H5 | 0.9500 | C15—H15 | 0.9500 |
| C6—H6 | 0.9500 | C16—H16 | 0.9500 |
| C7—C8 | 1.351 (3) | | |
| C10—O1—C7 | 107.20 (15) | C10—C9—H9 | 126.4 |
| O2—N1—O3 | 123.0 (2) | C8—C9—H9 | 126.4 |
| O2—N1—C1 | 118.64 (19) | C7—C8—C9 | 107.1 (2) |
| O3—N1—C1 | 118.31 (19) | C7—C8—H8 | 126.4 |
| C2—C1—C6 | 121.7 (2) | C9—C8—H8 | 126.4 |
| C2—C1—N1 | 119.23 (19) | C9—C10—O1 | 109.24 (17) |
| C6—C1—N1 | 119.06 (19) | C9—C10—C11 | 133.4 (2) |
| C3—C2—C1 | 119.2 (2) | O1—C10—C11 | 117.31 (18) |
| C3—C2—H2 | 120.4 | C16—C11—C12 | 118.48 (19) |
| C1—C2—H2 | 120.4 | C16—C11—C10 | 122.0 (2) |
| C2—C3—C4 | 121.1 (2) | C12—C11—C10 | 119.55 (19) |
| C2—C3—H3 | 119.5 | C13—C12—C11 | 120.3 (2) |
| C4—C3—H3 | 119.5 | C13—C12—H12 | 119.9 |
| C5—C4—C3 | 118.56 (19) | C11—C12—H12 | 119.9 |
| C5—C4—C7 | 122.16 (18) | C14—C13—C12 | 120.8 (2) |
| C3—C4—C7 | 119.27 (18) | C14—C13—H13 | 119.6 |
| C4—C5—C6 | 120.60 (19) | C12—C13—H13 | 119.6 |
| C4—C5—H5 | 119.7 | C13—C14—C15 | 120.0 (2) |
| C6—C5—H5 | 119.7 | C13—C14—H14 | 120.0 |
| C1—C6—C5 | 118.91 (19) | C15—C14—H14 | 120.0 |
| C1—C6—H6 | 120.5 | C14—C15—C16 | 120.3 (2) |
| C5—C6—H6 | 120.5 | C14—C15—H15 | 119.9 |
| C8—C7—O1 | 109.16 (18) | C16—C15—H15 | 119.9 |

| | | | |
|---|---|---|---|
| C8—C7—C4 | 133.11 (19) | C11—C16—C15 | 120.2 (2) |
| O1—C7—C4 | 117.73 (17) | C11—C16—H16 | 119.9 |
| C10—C9—C8 | 107.3 (2) | C15—C16—H16 | 119.9 |
| O2—N1—C1—C2 | −176.6 (2) | O1—C7—C8—C9 | −0.1 (3) |
| O3—N1—C1—C2 | 3.1 (3) | C4—C7—C8—C9 | −179.7 (2) |
| O2—N1—C1—C6 | 5.8 (3) | C10—C9—C8—C7 | −0.6 (3) |
| O3—N1—C1—C6 | −174.4 (2) | C8—C9—C10—O1 | 1.0 (3) |
| C6—C1—C2—C3 | 0.2 (4) | C8—C9—C10—C11 | 179.3 (2) |
| N1—C1—C2—C3 | −177.37 (19) | C7—O1—C10—C9 | −1.1 (2) |
| C1—C2—C3—C4 | 0.6 (4) | C7—O1—C10—C11 | −179.68 (19) |
| C2—C3—C4—C5 | −1.4 (3) | C9—C10—C11—C16 | −171.6 (2) |
| C2—C3—C4—C7 | 177.7 (2) | O1—C10—C11—C16 | 6.5 (3) |
| C3—C4—C5—C6 | 1.4 (3) | C9—C10—C11—C12 | 6.9 (4) |
| C7—C4—C5—C6 | −177.6 (2) | O1—C10—C11—C12 | −174.98 (19) |
| C2—C1—C6—C5 | −0.2 (4) | C16—C11—C12—C13 | −0.4 (4) |
| N1—C1—C6—C5 | 177.36 (19) | C10—C11—C12—C13 | −179.0 (2) |
| C4—C5—C6—C1 | −0.6 (4) | C11—C12—C13—C14 | 0.0 (4) |
| C10—O1—C7—C8 | 0.8 (2) | C12—C13—C14—C15 | 0.5 (4) |
| C10—O1—C7—C4 | −179.61 (18) | C13—C14—C15—C16 | −0.6 (4) |
| C5—C4—C7—C8 | 175.4 (2) | C12—C11—C16—C15 | 0.4 (4) |
| C3—C4—C7—C8 | −3.6 (4) | C10—C11—C16—C15 | 178.9 (2) |
| C5—C4—C7—O1 | −4.1 (3) | C14—C15—C16—C11 | 0.1 (4) |
| C3—C4—C7—O1 | 176.93 (19) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C3—H3···O3$^{i}$ | 0.95 | 2.51 | 3.373 (3) | 152. |
| C12—H12···O2$^{ii}$ | 0.95 | 2.61 | 3.435 (3) | 146. |

Symmetry codes: (i) *x*+1/2, −*y*+3/2, *z*+1/2; (ii) *x*+1, *y*, *z*+1.

**Fig. 1**