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(*Z*)-2-(4-Nitrobenzylidene)-1-benzofuran-3(2*H*)-one

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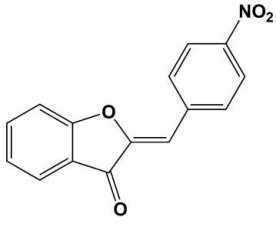
Key indicators: single-crystal X-ray study; T = 303 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.105; data-to-parameter ratio = 11.7.

In the crystal structure of the title compound, $C_{15}H_9NO_4$, weak C—H···O interactions generate rings with $R_2^2(8)$ motifs. The supramolecular aggregation is completed by the presence of C—H···O and van der Waals interactions.

Related literature

For the synthesis and biological activity of substituted aurones, see: Varma & Varma (1992); Beney *et al.* (2001); Sim *et al.* (2008). For the assignment of conformations and the orientation of the substituents, see: Nardelli (1983, 1995); Klyne & Prelog (1960). For hydrogen bonds, see: Desiraju & Steiner (1999). For graph-set analysis of hydrogen bonds, see: Etter *et al.* (1990); Bernstein *et al.* (1995). For the diverse theraputic properties of aurones, see: Villemin *et al.* (1998). Several multifunctionalized aurones have been reported to exhibit anti-malarial (Souard *et al.* 2010) and anti-histamine (Wang *et al.* 2007) properties.



Experimental

Crystal data

$C_{15}H_9NO_4$
M_r = 267.23
Triclinic, $P\overline{1}$
a = 6.6916 (2) Å
b = 7.4708 (2) Å
c = 12.6414 (3) Å
α = 100.459 (1)°
β = 93.019 (2)°
γ = 102.043 (1)°
V = 605.09 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 303 K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.932, T_{max} = 0.955
12519 measured reflections
2116 independent reflections
1869 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.105
S = 1.03
2116 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15···O1	0.93	2.32	2.9547 (16)	125
C9—H9···O2^{i}	0.93	2.50	3.2951 (14)	143

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZJ2025).

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(*Z*)-2-(4-Nitrobenzylidene)-1-benzofuran-3(2*H*)-one

J. Satyanarayana Reddy, N. Ravikumar, J. Venkata Prasad, G. Gopi Krishna and K. Anand Solomon

S1. Comment

Aurones belong flavonoids family, which are structurally isomers of flavones. They form essential structural scaffolds in many natural and synthetic molecules possessing diverse therapeutic properties (Villemin *et al.* 1998) Several multifunctionalized aurones were reported to exhibit anti-malarial (Souard *et al.* 2010) and anti-histamine (Wang *et al.* 2007) properties.

The title compound (Fig.1),$C_{15}H_9NO_4$,crystallized in triclinic space group P-1 with two molecules in the assymetric unit (Fig.2).The crystal structure of (I) is stabilized by C—H···O interactions.The range of H···O distances (Table 1) found in (I) agrees with those found for C—H···O hydrogen bonds (Desiraju & Steiner,1999). The coumaranone moiety at C10 is in co-planar conformation [C7—C8—C9—C10=179.55 (13)°].The translational related molecules interact with each other *via* weak C—H···O [C9—H9···O2: H9···O2 = 2.50 Å, θ = 143°] hydrogen bonds along the *c* axis, and form a one dimensional chain (Fig. 3).

S2. Experimental

3-coumaranone was allowed to react with 4-nitrobenzaldehyde in ethanolic solution of potassium hydroxide for 30 minutes to yield the title compound (Fig.4). The pure product was obtained by recrystallization in methanol.

S3. 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.

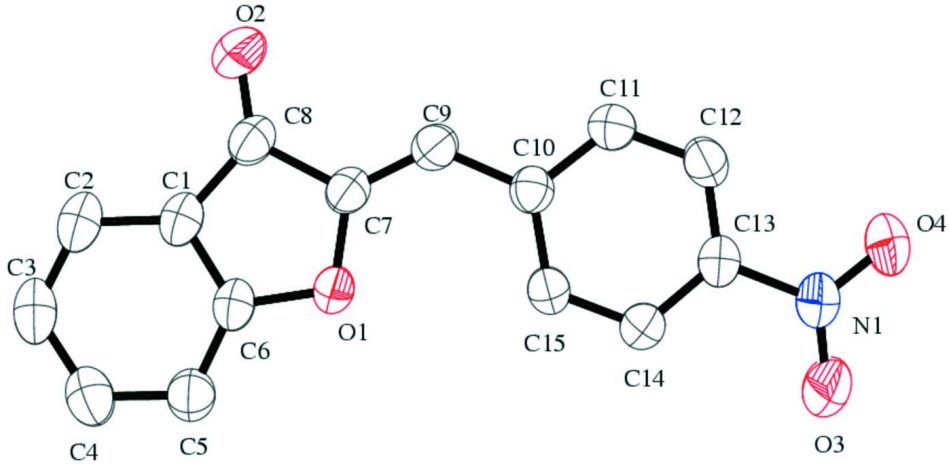

Figure 1

ORTEP diagram of (*Z*)-2-(4-nitrobenzylidene)benzofuran-3(2*H*)-one. (Thermal ellipsoids are at 50% probability level).

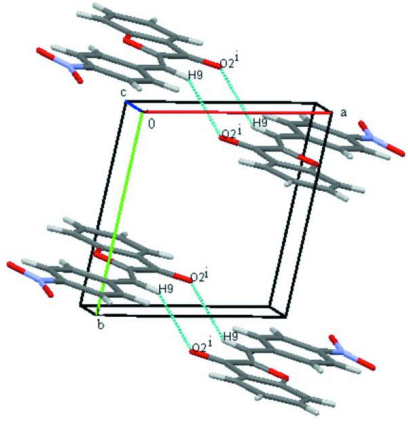

Figure 2

Crystal packing diagram of the title compound.

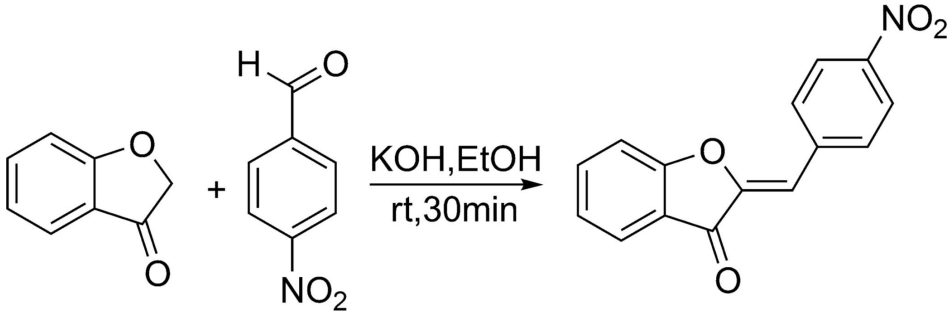

Figure 3

The synthetic scheme of the title compound.

(*Z*)-2-(4-Nitrobenzylidene)-1-benzofuran-3(2*H*)-one

Crystal data

$C_{15}H_9NO_4$
$M_r = 267.23$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.6916$ (2) Å
$b = 7.4708$ (2) Å
$c = 12.6414$ (3) Å
$\alpha = 100.459$ (1)°
$\beta = 93.019$ (2)°
$\gamma = 102.043$ (1)°
$V = 605.09$ (3) Å^3
$Z = 2$
$F(000) = 276$
$D_x = 1.467$ Mg m^{-3}
Melting point: 460 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7266 reflections
$\theta = 2.8$–30.5°
$\mu = 0.11$ mm^{-1}
$T = 303$ K
Block, yellow
0.30 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min} = 0.932$, $T_{max} = 0.955$
12519 measured reflections
2116 independent reflections
1869 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.8°$
$h = -7 \rightarrow 7$
$k = -8 \rightarrow 8$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.105$
$S = 1.03$
2116 reflections
181 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0599P)^2 + 0.1178P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.8384 (2)	0.28398 (18)	−0.19093 (11)	0.0456 (3)
C2	0.7837 (2)	0.3025 (2)	−0.29555 (11)	0.0548 (4)
H2	0.6469	0.2729	−0.3234	0.066*

C3	0.9366 (3)	0.3652 (2)	−0.35600 (12)	0.0595 (4)
H3	0.9037	0.3790	−0.4260	0.071*
C4	1.1407 (3)	0.4087 (2)	−0.31413 (12)	0.0586 (4)
H4	1.2417	0.4519	−0.3569	0.070*
C5	1.1987 (2)	0.3898 (2)	−0.21071 (12)	0.0526 (4)
H5	1.3355	0.4179	−0.1830	0.063*
C6	1.0423 (2)	0.32720 (17)	−0.15171 (10)	0.0431 (3)
C7	0.88073 (19)	0.22680 (18)	−0.01762 (11)	0.0429 (3)
C8	0.7214 (2)	0.21929 (19)	−0.10621 (12)	0.0485 (3)
C9	0.8470 (2)	0.17046 (18)	0.07516 (11)	0.0452 (3)
H9	0.7102	0.1217	0.0832	0.054*
C10	0.9913 (2)	0.17343 (17)	0.16591 (10)	0.0411 (3)
C11	0.9136 (2)	0.11596 (19)	0.25736 (11)	0.0470 (3)
H11	0.7727	0.0733	0.2574	0.056*
C12	1.0401 (2)	0.12085 (19)	0.34749 (11)	0.0477 (3)
H12	0.9866	0.0829	0.4083	0.057*
C13	1.2473 (2)	0.18320 (18)	0.34544 (10)	0.0444 (3)
C14	1.3322 (2)	0.23746 (19)	0.25581 (11)	0.0475 (3)
H14	1.4736	0.2769	0.2562	0.057*
C15	1.2041 (2)	0.23210 (18)	0.16603 (11)	0.0452 (3)
H15	1.2592	0.2677	0.1050	0.054*
N1	1.3855 (2)	0.19263 (19)	0.44088 (10)	0.0575 (3)
O1	1.07162 (13)	0.29789 (13)	−0.04757 (7)	0.0459 (3)
O2	0.53638 (16)	0.16865 (18)	−0.10414 (10)	0.0732 (4)
O3	1.5647 (2)	0.2687 (3)	0.44252 (12)	0.1051 (6)
O4	1.31586 (19)	0.12304 (19)	0.51458 (9)	0.0760 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0521 (8)	0.0404 (7)	0.0431 (7)	0.0118 (6)	−0.0073 (6)	0.0070 (5)
C2	0.0648 (9)	0.0512 (8)	0.0466 (8)	0.0140 (7)	−0.0133 (7)	0.0092 (6)
C3	0.0845 (11)	0.0537 (8)	0.0392 (7)	0.0150 (8)	−0.0068 (7)	0.0108 (6)
C4	0.0747 (10)	0.0542 (8)	0.0465 (8)	0.0093 (7)	0.0062 (7)	0.0142 (6)
C5	0.0543 (8)	0.0539 (8)	0.0483 (8)	0.0072 (6)	0.0001 (6)	0.0135 (6)
C6	0.0513 (8)	0.0395 (7)	0.0382 (7)	0.0108 (5)	−0.0043 (5)	0.0084 (5)
C7	0.0404 (7)	0.0435 (7)	0.0439 (7)	0.0085 (5)	−0.0025 (5)	0.0090 (5)
C8	0.0443 (8)	0.0499 (8)	0.0513 (8)	0.0110 (6)	−0.0058 (6)	0.0121 (6)
C9	0.0406 (7)	0.0476 (7)	0.0468 (8)	0.0085 (5)	0.0004 (6)	0.0102 (6)
C10	0.0443 (7)	0.0385 (6)	0.0405 (7)	0.0092 (5)	0.0016 (5)	0.0084 (5)
C11	0.0424 (7)	0.0525 (8)	0.0481 (8)	0.0108 (6)	0.0064 (6)	0.0143 (6)
C12	0.0537 (8)	0.0522 (8)	0.0414 (7)	0.0143 (6)	0.0092 (6)	0.0159 (6)
C13	0.0511 (8)	0.0451 (7)	0.0378 (7)	0.0124 (6)	−0.0011 (6)	0.0098 (5)
C14	0.0418 (7)	0.0547 (8)	0.0450 (8)	0.0055 (6)	−0.0003 (6)	0.0145 (6)
C15	0.0463 (7)	0.0510 (7)	0.0385 (7)	0.0067 (6)	0.0023 (5)	0.0145 (6)
N1	0.0585 (8)	0.0713 (8)	0.0436 (7)	0.0123 (6)	−0.0027 (6)	0.0187 (6)
O1	0.0426 (5)	0.0546 (5)	0.0400 (5)	0.0067 (4)	−0.0041 (4)	0.0154 (4)
O2	0.0437 (6)	0.1012 (9)	0.0775 (8)	0.0093 (6)	−0.0083 (5)	0.0363 (7)

O3	0.0651 (8)	0.1611 (15)	0.0821 (9)	−0.0170 (9)	−0.0255 (7)	0.0637 (10)
O4	0.0768 (8)	0.1133 (10)	0.0450 (6)	0.0215 (7)	0.0047 (5)	0.0342 (6)

Geometric parameters (Å, º)

C1—C6	1.3780 (19)	C9—C10	1.4541 (18)
C1—C2	1.3922 (19)	C9—H9	0.9300
C1—C8	1.453 (2)	C10—C11	1.3935 (19)
C2—C3	1.365 (2)	C10—C15	1.3993 (19)
C2—H2	0.9300	C11—C12	1.3736 (19)
C3—C4	1.388 (2)	C11—H11	0.9300
C3—H3	0.9300	C12—C13	1.371 (2)
C4—C5	1.384 (2)	C12—H12	0.9300
C4—H4	0.9300	C13—C14	1.3816 (19)
C5—C6	1.369 (2)	C13—N1	1.4628 (18)
C5—H5	0.9300	C14—C15	1.3752 (19)
C6—O1	1.3837 (16)	C14—H14	0.9300
C7—C9	1.331 (2)	C15—H15	0.9300
C7—O1	1.3777 (16)	N1—O3	1.2127 (17)
C7—C8	1.4900 (18)	N1—O4	1.2150 (17)
C8—O2	1.2200 (17)		
C6—C1—C2	119.87 (14)	C7—C9—H9	115.1
C6—C1—C8	106.79 (12)	C10—C9—H9	115.1
C2—C1—C8	133.31 (13)	C11—C10—C15	118.52 (12)
C3—C2—C1	118.13 (14)	C11—C10—C9	118.28 (12)
C3—C2—H2	120.9	C15—C10—C9	123.20 (12)
C1—C2—H2	120.9	C12—C11—C10	121.54 (13)
C2—C3—C4	120.73 (14)	C12—C11—H11	119.2
C2—C3—H3	119.6	C10—C11—H11	119.2
C4—C3—H3	119.6	C13—C12—C11	118.23 (13)
C5—C4—C3	122.12 (15)	C13—C12—H12	120.9
C5—C4—H4	118.9	C11—C12—H12	120.9
C3—C4—H4	118.9	C12—C13—C14	122.37 (13)
C6—C5—C4	115.94 (14)	C12—C13—N1	119.42 (12)
C6—C5—H5	122.0	C14—C13—N1	118.21 (13)
C4—C5—H5	122.0	C15—C14—C13	118.91 (13)
C5—C6—C1	123.20 (13)	C15—C14—H14	120.5
C5—C6—O1	123.91 (12)	C13—C14—H14	120.5
C1—C6—O1	112.89 (12)	C14—C15—C10	120.40 (13)
C9—C7—O1	124.72 (12)	C14—C15—H15	119.8
C9—C7—C8	126.03 (13)	C10—C15—H15	119.8
O1—C7—C8	109.24 (11)	O3—N1—O4	122.99 (13)
O2—C8—C1	130.02 (13)	O3—N1—C13	118.44 (13)
O2—C8—C7	125.87 (14)	O4—N1—C13	118.57 (13)
C1—C8—C7	104.10 (11)	C7—O1—C6	106.90 (10)
C7—C9—C10	129.88 (13)		

C6—C1—C2—C3	−0.5 (2)	C7—C9—C10—C11	176.04 (13)
C8—C1—C2—C3	−178.41 (14)	C7—C9—C10—C15	−3.6 (2)
C1—C2—C3—C4	0.2 (2)	C15—C10—C11—C12	1.8 (2)
C2—C3—C4—C5	0.4 (2)	C9—C10—C11—C12	−177.82 (12)
C3—C4—C5—C6	−0.6 (2)	C10—C11—C12—C13	−0.4 (2)
C4—C5—C6—C1	0.2 (2)	C11—C12—C13—C14	−1.2 (2)
C4—C5—C6—O1	179.20 (12)	C11—C12—C13—N1	179.06 (12)
C2—C1—C6—C5	0.3 (2)	C12—C13—C14—C15	1.2 (2)
C8—C1—C6—C5	178.73 (12)	N1—C13—C14—C15	−179.02 (12)
C2—C1—C6—O1	−178.73 (11)	C13—C14—C15—C10	0.3 (2)
C8—C1—C6—O1	−0.35 (15)	C11—C10—C15—C14	−1.8 (2)
C6—C1—C8—O2	178.90 (15)	C9—C10—C15—C14	177.86 (12)
C2—C1—C8—O2	−3.0 (3)	C12—C13—N1—O3	−171.28 (15)
C6—C1—C8—C7	−1.28 (14)	C14—C13—N1—O3	9.0 (2)
C2—C1—C8—C7	176.79 (14)	C12—C13—N1—O4	9.1 (2)
C9—C7—C8—O2	3.7 (2)	C14—C13—N1—O4	−170.61 (13)
O1—C7—C8—O2	−177.66 (13)	C9—C7—O1—C6	175.88 (12)
C9—C7—C8—C1	−176.09 (13)	C8—C7—O1—C6	−2.75 (13)
O1—C7—C8—C1	2.52 (14)	C5—C6—O1—C7	−177.09 (12)
O1—C7—C9—C10	2.1 (2)	C1—C6—O1—C7	1.98 (14)
C8—C7—C9—C10	−179.55 (13)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···O1	0.93	2.32	2.9547 (16)	125
C9—H9···O2^{i}	0.93	2.50	3.2951 (14)	143

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