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2-[(3,5-Dimethyl-1-phenyl-1*H*-pyrazol-4-yl)methylidene]indan-1,3-dione

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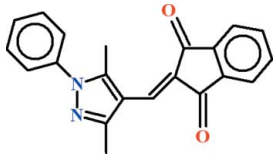
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.112; data-to-parameter ratio = 13.0.

In the title compound, $C_{21}H_{16}N_2O_2$, the five-membered heterocyclic ring makes a dihedral angle of 47.06 (6)° with the attached benzene ring, whereas the indan-1,3-dione ring system and the benzene ring are oriented at a dihedral angle of 21.92 (7)°. In the crystal, inversion dimers linked by pairs of C—H···O hydrogen bonds generate $R_2^2(22)$ loops. Aromatic π–π stacking interactions [centroid–centroid distances = 3.8325 (12)–3.8600 (12) Å] also occur.

Related literature

For background to donor–acceptor chromophores, see: Asiri *et al.* (2006); Asiri & Khan (2009); Koyuncu *et al.* (2010); Kulhanek *et al.* (2011); Wang *et al.* (2011). For related structures, see: Belyakov *et al.* (2008); Fun *et al.* (2010). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{21}H_{16}N_2O_2$
M_r = 328.36
Monoclinic, $C2/c$
a = 14.6655 (3) Å
b = 7.8902 (2) Å
c = 28.6651 (7) Å
β = 98.251 (1)°
V = 3282.61 (13) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.26 × 0.23 × 0.21 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.975, T_{max} = 0.985
12302 measured reflections
2970 independent reflections
2106 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.112
S = 1.01
2970 reflections
228 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C18—H18···O1^{i}	0.93	2.58	3.377 (3)	145

Symmetry code: (i) $-x, y, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6509).

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supplementary materials

Acta Cryst. (2011). E**67**, o3419 [**doi:10.1107/S1600536811049488**]

2-[(3,5-Dimethyl-1-phenyl-1*H*-pyrazol-4-yl)methylidene]indan-1,3-dione

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Comment

Formation of the donor acceptor chromophores by the nucleophilic addition of an active hydrogen compound to a carbonyl group followed by a dehydration reaction is known as knoevenagel condensation (Asiri & Khan, 2009). Donor acceptor chromophores are applicable in the field of materials science such as third order non-linear optical (NLO) (Asiri *et al.* 2006), photonic materials and devices, optical limiting (Kulhanek *et al.* 2011), electrochemical sensing (Koyuncu *et al.* 2010) and langmuir film (Wang *et al.* 2011). Due to wide application of donor acceptor chromophores, we are reporting here the synthesiz and crystal structure of the title compound (I), (Fig. 1).

The crystal structures of (II) *i.e.*, 2-(4,5,6,7,8,9-hexahydro-6a-azaphenylen-2-ylmethylene)indan-1,3-dione (Belyakov *et al.*, 2008) and (III) *i.e.*, 4-((*E*)((3,5-dimethyl- 1-phenyl-1*H*-pyrazol-4-yl)methylene)amino)-1,5-dimethyl-2-phenyl -1,2-dihydro-3*H*-pyrazol-3-one have been published which contain the moities present in (I).

In (I), the group A (C1—C9/O1/O2) of indan-1, 3-dione, the heterocyclic five membered ring B (C11/C12/C14/N1/N2) and the benzene ring C (C16—C21) of the aldehyde moiety are planar with r. m. s. deviation of 0.0345, 0.0099 and 0.0035 Å, respectively. The dihedral angle between A/B, A/C and B/C is 39.77 (4), 21.92 (7) and 47.06 (6)°, respectively. The title compound consists of dimers due to intermolecular H-bonds of C—H···O type, where O-atom is of carbonyl and H-atom is of benzene ring. This H-bondings form a $R_2^2(22)$ (Fig. 2) ring motif (Bernstein *et al.*, 1995). There exists π–π interactions between the centroids of the rings of indan-1, 3-dione moieties at the separation of 3.8325 (12)–3.8600 (12) A°.

Experimental

A mixture of 3,5-dimethyl-1-phenylpyrazole-4-carbaldehyde (1.0 g, 5.0 mmol), indan-1, 3-dione (0.73 g, 5.0 mmol) and a few drops of pyridine in ethanol (15 ml) was heated for 3 h. The progress of the reaction was monitored by TLC. The solid that separated from the cooled mixture was collected and recrystallized from a methanol-chloroform mixture to give the yellow prisms of (I).

Yellow: 85%, m.p. 469–470 K.

IR (KBr) ν_{max} cm^{-1}: 3035 (Ar—H), 2859 (C—H), 1663 (C═O), 1578 (C═C).

Refinement

The H-atoms were positioned geometrically (C–H = 0.93–0.96 Å) and refined as riding with $U_{iso}(H) = xU_{eq}(C)$, where x = 1.5 for methyl and x = 1.2 for aryl H-atoms.

Figures

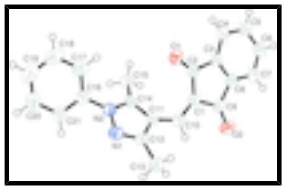

Fig. 1. View of the title compound with displacement ellipsoids drawn at the 50% probability level. H-atoms are shown as small spheres of arbitrary radii.

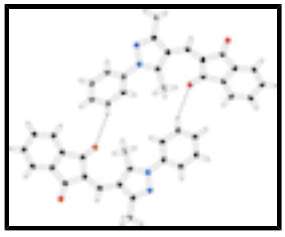

Fig. 2. The partial packing (*PLATON*; Spek, 2009) which shows that molecules form dimers with $R_2^2(22)$ ring motif.

2-[(3,5-Dimethyl-1-phenyl-1*H*-pyrazol-4-yl)methylidene]indan-1,3-dione

Crystal data

$C_{21}H_{16}N_2O_2$	$F(000) = 1376$
$M_r = 328.36$	$D_x = 1.329$ Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 2106 reflections
a = 14.6655 (3) Å	θ = 1.4–25.3°
b = 7.8902 (2) Å	μ = 0.09 mm^{-1}
c = 28.6651 (7) Å	*T* = 296 K
β = 98.251 (1)°	Prism, yellow
V = 3282.61 (13) Å^3	0.26 × 0.23 × 0.21 mm
Z = 8	

Data collection

Bruker Kappa APEXII CCD diffractometer	2970 independent reflections
Radiation source: fine-focus sealed tube	2106 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.034$
Detector resolution: 8.00 pixels mm^{-1}	$\theta_{max} = 25.3°$, $\theta_{min} = 1.4°$
ω scans	$h = -17\rightarrow17$
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	$k = -6\rightarrow9$
$T_{min} = 0.975$, $T_{max} = 0.985$	$l = -34\rightarrow34$
12302 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods

Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.042$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.112$	H-atom parameters constrained
$S = 1.01$	$w = 1/[\sigma^2(F_o^2) + (0.0522P)^2 + 0.9126P]$ where $P = (F_o^2 + 2F_c^2)/3$
2970 reflections	$(\Delta/\sigma)_{max} < 0.001$
228 parameters	$\Delta\rho_{max} = 0.12$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.23$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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	0.07106 (8)	0.30881 (19)	0.11877 (4)	0.0564 (5)
O2	0.23637 (9)	0.04176 (19)	0.00898 (4)	0.0608 (5)
N1	0.34865 (9)	0.1867 (2)	0.23313 (5)	0.0473 (5)
N2	0.25797 (9)	0.1475 (2)	0.23590 (5)	0.0439 (5)
C1	0.17883 (11)	0.1490 (2)	0.07845 (6)	0.0419 (6)
C2	0.09301 (11)	0.2414 (3)	0.08361 (6)	0.0423 (6)
C3	0.03786 (11)	0.2486 (2)	0.03591 (6)	0.0403 (6)
C4	−0.04905 (12)	0.3164 (3)	0.02282 (6)	0.0475 (6)
C5	−0.08681 (13)	0.3072 (3)	−0.02408 (7)	0.0537 (7)
C6	−0.03758 (14)	0.2345 (3)	−0.05695 (7)	0.0557 (7)
C7	0.04935 (13)	0.1681 (3)	−0.04398 (6)	0.0519 (7)
C8	0.08677 (11)	0.1748 (2)	0.00319 (6)	0.0414 (6)
C9	0.17632 (12)	0.1113 (3)	0.02737 (6)	0.0450 (6)
C10	0.25407 (11)	0.1176 (2)	0.11037 (6)	0.0441 (6)
C11	0.26939 (11)	0.1368 (2)	0.16062 (6)	0.0418 (6)
C12	0.35529 (11)	0.1768 (2)	0.18786 (6)	0.0441 (6)
C13	0.44513 (12)	0.2131 (3)	0.17115 (7)	0.0616 (8)
C14	0.20881 (11)	0.1150 (2)	0.19334 (6)	0.0418 (6)
C15	0.11558 (11)	0.0380 (3)	0.18802 (6)	0.0559 (7)
C16	0.22738 (12)	0.1517 (2)	0.28101 (6)	0.0440 (6)
C17	0.14828 (13)	0.2378 (3)	0.28667 (7)	0.0577 (8)
C18	0.12018 (16)	0.2438 (3)	0.33060 (9)	0.0709 (9)
C19	0.17138 (19)	0.1645 (3)	0.36842 (8)	0.0743 (10)
C20	0.25092 (17)	0.0804 (3)	0.36263 (7)	0.0682 (9)

C21	0.27950 (13)	0.0733 (3)	0.31885 (6)	0.0536 (7)
H4	−0.08104	0.36672	0.04493	0.0570*
H5	−0.14557	0.34996	−0.03377	0.0644*
H6	−0.06392	0.23049	−0.08844	0.0668*
H7	0.08189	0.12017	−0.06624	0.0623*
H10	0.30449	0.07647	0.09756	0.0529*
H13A	0.49379	0.20906	0.19738	0.0924*
H13B	0.44309	0.32379	0.15712	0.0924*
H13C	0.45628	0.12989	0.14820	0.0924*
H15A	0.07018	0.12581	0.18772	0.0838*
H15B	0.11146	−0.03737	0.21392	0.0838*
H15C	0.10477	−0.02420	0.15897	0.0838*
H17	0.11393	0.29166	0.26111	0.0693*
H18	0.06657	0.30145	0.33466	0.0850*
H19	0.15205	0.16794	0.39792	0.0891*
H20	0.28568	0.02796	0.38831	0.0818*
H21	0.33335	0.01622	0.31488	0.0643*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0561 (8)	0.0723 (10)	0.0421 (7)	0.0083 (7)	0.0117 (6)	−0.0049 (7)
O2	0.0533 (8)	0.0730 (11)	0.0585 (8)	0.0118 (7)	0.0158 (6)	−0.0066 (7)
N1	0.0349 (8)	0.0581 (11)	0.0483 (9)	−0.0067 (7)	0.0035 (6)	−0.0007 (8)
N2	0.0348 (8)	0.0530 (10)	0.0433 (8)	−0.0046 (7)	0.0032 (6)	0.0014 (7)
C1	0.0384 (9)	0.0464 (11)	0.0407 (9)	−0.0030 (8)	0.0053 (7)	0.0007 (9)
C2	0.0416 (10)	0.0472 (12)	0.0390 (10)	−0.0033 (8)	0.0087 (8)	0.0025 (9)
C3	0.0412 (10)	0.0400 (11)	0.0402 (10)	−0.0041 (8)	0.0076 (7)	0.0044 (8)
C4	0.0455 (10)	0.0516 (13)	0.0465 (10)	0.0007 (9)	0.0106 (8)	0.0068 (9)
C5	0.0453 (11)	0.0605 (14)	0.0532 (12)	0.0008 (10)	−0.0001 (9)	0.0100 (10)
C6	0.0595 (12)	0.0637 (15)	0.0407 (10)	−0.0042 (11)	−0.0038 (9)	0.0023 (10)
C7	0.0575 (12)	0.0560 (14)	0.0424 (10)	−0.0013 (10)	0.0076 (9)	−0.0030 (9)
C8	0.0417 (10)	0.0424 (12)	0.0402 (10)	−0.0053 (8)	0.0062 (7)	0.0013 (8)
C9	0.0428 (10)	0.0458 (12)	0.0476 (10)	−0.0032 (9)	0.0103 (8)	−0.0001 (9)
C10	0.0392 (10)	0.0460 (12)	0.0474 (10)	−0.0028 (8)	0.0073 (8)	−0.0007 (9)
C11	0.0359 (9)	0.0448 (12)	0.0436 (10)	−0.0005 (8)	0.0020 (7)	0.0018 (8)
C12	0.0369 (9)	0.0488 (12)	0.0463 (10)	−0.0027 (8)	0.0045 (7)	0.0022 (9)
C13	0.0403 (10)	0.0857 (17)	0.0585 (12)	−0.0126 (11)	0.0060 (9)	0.0028 (11)
C14	0.0341 (9)	0.0442 (12)	0.0456 (10)	−0.0015 (8)	0.0006 (7)	0.0042 (9)
C15	0.0423 (10)	0.0678 (15)	0.0557 (11)	−0.0129 (10)	0.0009 (8)	0.0091 (11)
C16	0.0419 (10)	0.0437 (12)	0.0471 (10)	−0.0080 (9)	0.0089 (8)	−0.0040 (9)
C17	0.0499 (12)	0.0578 (14)	0.0670 (13)	−0.0009 (10)	0.0136 (10)	0.0003 (11)
C18	0.0641 (14)	0.0630 (16)	0.0935 (18)	−0.0102 (12)	0.0383 (13)	−0.0158 (14)
C19	0.1054 (19)	0.0613 (16)	0.0645 (15)	−0.0224 (14)	0.0406 (14)	−0.0123 (13)
C20	0.0982 (18)	0.0600 (16)	0.0470 (12)	−0.0066 (13)	0.0127 (11)	−0.0033 (11)
C21	0.0598 (12)	0.0527 (13)	0.0483 (11)	0.0012 (10)	0.0073 (9)	−0.0045 (10)

Geometric parameters (Å, °)

O1—C2	1.223 (2)	C16—C17	1.374 (3)
O2—C9	1.220 (2)	C16—C21	1.380 (3)
N1—N2	1.3787 (19)	C17—C18	1.381 (3)
N1—C12	1.318 (2)	C18—C19	1.377 (3)
N2—C14	1.350 (2)	C19—C20	1.373 (4)
N2—C16	1.429 (2)	C20—C21	1.380 (3)
C1—C2	1.480 (2)	C4—H4	0.9300
C1—C9	1.489 (2)	C5—H5	0.9300
C1—C10	1.351 (2)	C6—H6	0.9300
C2—C3	1.487 (2)	C7—H7	0.9300
C3—C4	1.384 (2)	C10—H10	0.9300
C3—C8	1.388 (2)	C13—H13A	0.9600
C4—C5	1.381 (3)	C13—H13B	0.9600
C5—C6	1.390 (3)	C13—H13C	0.9600
C6—C7	1.379 (3)	C15—H15A	0.9600
C7—C8	1.385 (2)	C15—H15B	0.9600
C8—C9	1.482 (2)	C15—H15C	0.9600
C10—C11	1.434 (2)	C17—H17	0.9300
C11—C12	1.419 (2)	C18—H18	0.9300
C11—C14	1.392 (2)	C19—H19	0.9300
C12—C13	1.493 (2)	C20—H20	0.9300
C14—C15	1.484 (2)	C21—H21	0.9300
N2—N1—C12	104.58 (13)	C17—C18—C19	120.1 (2)
N1—N2—C14	112.65 (13)	C18—C19—C20	120.1 (2)
N1—N2—C16	118.54 (13)	C19—C20—C21	120.3 (2)
C14—N2—C16	128.77 (14)	C16—C21—C20	119.35 (19)
C2—C1—C9	107.17 (14)	C3—C4—H4	121.00
C2—C1—C10	130.24 (16)	C5—C4—H4	121.00
C9—C1—C10	122.11 (15)	C4—C5—H5	120.00
O1—C2—C1	128.67 (16)	C6—C5—H5	120.00
O1—C2—C3	124.66 (16)	C5—C6—H6	119.00
C1—C2—C3	106.57 (14)	C7—C6—H6	119.00
C2—C3—C4	128.51 (16)	C6—C7—H7	121.00
C2—C3—C8	109.87 (14)	C8—C7—H7	121.00
C4—C3—C8	121.62 (16)	C1—C10—H10	115.00
C3—C4—C5	117.97 (17)	C11—C10—H10	115.00
C4—C5—C6	120.46 (18)	C12—C13—H13A	109.00
C5—C6—C7	121.59 (18)	C12—C13—H13B	109.00
C6—C7—C8	118.03 (17)	C12—C13—H13C	109.00
C3—C8—C7	120.32 (16)	H13A—C13—H13B	109.00
C3—C8—C9	109.58 (15)	H13A—C13—H13C	109.00
C7—C8—C9	130.10 (16)	H13B—C13—H13C	109.00
O2—C9—C1	126.67 (16)	C14—C15—H15A	109.00
O2—C9—C8	126.62 (16)	C14—C15—H15B	109.00
C1—C9—C8	106.71 (15)	C14—C15—H15C	109.00
C1—C10—C11	130.99 (16)	H15A—C15—H15B	109.00

C10—C11—C12	125.10 (15)	H15A—C15—H15C	109.00
C10—C11—C14	129.85 (15)	H15B—C15—H15C	109.00
C12—C11—C14	105.00 (15)	C16—C17—H17	120.00
N1—C12—C11	111.71 (14)	C18—C17—H17	120.00
N1—C12—C13	119.87 (15)	C17—C18—H18	120.00
C11—C12—C13	128.37 (16)	C19—C18—H18	120.00
N2—C14—C11	106.01 (14)	C18—C19—H19	120.00
N2—C14—C15	122.38 (15)	C20—C19—H19	120.00
C11—C14—C15	130.47 (15)	C19—C20—H20	120.00
N2—C16—C17	119.90 (16)	C21—C20—H20	120.00
N2—C16—C21	119.37 (16)	C16—C21—H21	120.00
C17—C16—C21	120.70 (17)	C20—C21—H21	120.00
C16—C17—C18	119.49 (19)		
C12—N1—N2—C14	−0.43 (19)	C4—C3—C8—C7	0.4 (3)
C12—N1—N2—C16	−178.29 (15)	C4—C3—C8—C9	−179.10 (18)
N2—N1—C12—C11	1.86 (19)	C3—C4—C5—C6	−1.2 (3)
N2—N1—C12—C13	179.52 (16)	C4—C5—C6—C7	0.7 (4)
N1—N2—C14—C11	−1.14 (19)	C5—C6—C7—C8	0.3 (3)
N1—N2—C14—C15	167.82 (16)	C6—C7—C8—C3	−0.8 (3)
C16—N2—C14—C11	176.44 (16)	C6—C7—C8—C9	178.5 (2)
C16—N2—C14—C15	−14.6 (3)	C3—C8—C9—O2	−179.0 (2)
N1—N2—C16—C17	130.59 (19)	C3—C8—C9—C1	1.0 (2)
N1—N2—C16—C21	−47.4 (2)	C7—C8—C9—O2	1.7 (4)
C14—N2—C16—C17	−46.9 (3)	C7—C8—C9—C1	−178.41 (19)
C14—N2—C16—C21	135.2 (2)	C1—C10—C11—C12	−148.87 (18)
C9—C1—C2—O1	−173.0 (2)	C1—C10—C11—C14	34.2 (3)
C9—C1—C2—C3	3.3 (2)	C10—C11—C12—N1	179.86 (16)
C10—C1—C2—O1	−0.9 (4)	C10—C11—C12—C13	2.4 (3)
C10—C1—C2—C3	175.33 (17)	C14—C11—C12—N1	−2.57 (19)
C2—C1—C9—O2	177.3 (2)	C14—C11—C12—C13	−180.00 (19)
C2—C1—C9—C8	−2.7 (2)	C10—C11—C14—N2	179.55 (16)
C10—C1—C9—O2	4.5 (3)	C10—C11—C14—C15	11.8 (3)
C10—C1—C9—C8	−175.48 (16)	C12—C11—C14—N2	2.13 (18)
C2—C1—C10—C11	12.2 (3)	C12—C11—C14—C15	−165.60 (18)
C9—C1—C10—C11	−176.81 (18)	N2—C16—C17—C18	−178.80 (19)
O1—C2—C3—C4	−6.1 (3)	C21—C16—C17—C18	−0.9 (3)
O1—C2—C3—C8	173.65 (19)	N2—C16—C21—C20	178.66 (19)
C1—C2—C3—C4	177.46 (18)	C17—C16—C21—C20	0.7 (3)
C1—C2—C3—C8	−2.8 (2)	C16—C17—C18—C19	0.2 (3)
C2—C3—C4—C5	−179.6 (2)	C17—C18—C19—C20	0.5 (4)
C8—C3—C4—C5	0.7 (3)	C18—C19—C20—C21	−0.7 (4)
C2—C3—C8—C7	−179.42 (18)	C19—C20—C21—C16	0.1 (3)
C2—C3—C8—C9	1.1 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C18—H18···O1^{i}	0.93	2.58	3.377 (3)	145

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

Fig. 1

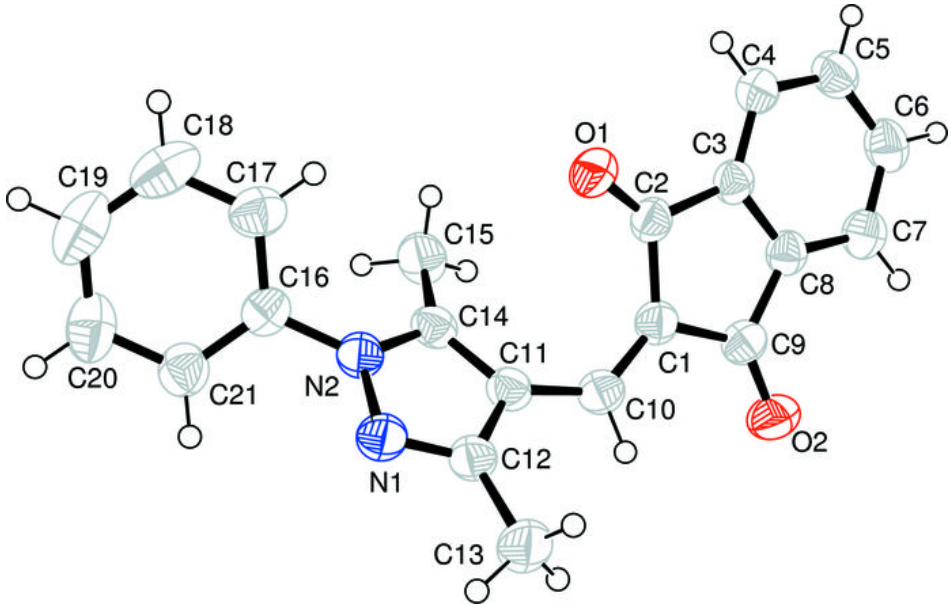
C4
C5
C6
C3
O1
C2
C7
C8
C18
C19
C17
C15
C16
C14
C11
C1
C9
C20
C21
N2
C10
O2
N1
C12
C13

Fig. 2