Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N′-(Diphenylmethylene)-3-(3-nitrophenyl)-1′,3′-dioxospiro[cyclopropane-2′-indan]-2-carbohydrazide

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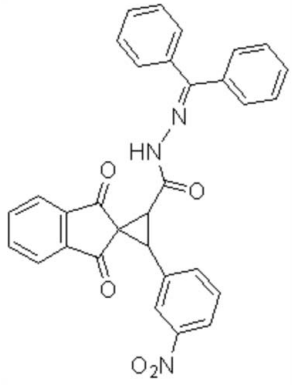
Received 26 September 2007; accepted 5 October 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.122; data-to-parameter ratio = 13.0.

In the title compound, $C_{31}H_{21}N_3O_5$, the indan ring system makes dihedral angles of 53.26 (6) with the nitrobenzene ring, and 66.50 (6) and 58.39 (7)° with the two phenyl rings. The crystal packing is stabilized by weak intermolecular N—H···O and C—H···O hydrogen bonds.

Related literature

For related crystal structures, see: Satis Kumar *et al.* (2006); Chakkaravarthi *et al.* (2007). For standard bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{31}H_{21}N_3O_5$
M_r = 515.51
Triclinic, $P\overline{1}$
a = 9.4617 (4) Å
b = 12.8806 (5) Å
c = 12.9114 (8) Å
α = 108.212 (2)°
β = 108.535 (3)°
γ = 107.424 (2)°
V = 1270.69 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 (2) K
0.22 × 0.16 × 0.16 mm

Data collection

Bruker Kappa-APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.897, T_{max} = 0.985
23251 measured reflections
4593 independent reflections
3628 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.122
S = 1.02
4593 reflections
352 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O5^{i}	0.93	2.39	3.227 (2)	149
C29—H29···O1^{ii}	0.93	2.57	3.406 (2)	149
N2—H2*A*···O3^{iii}	0.86	2.59	3.324 (3)	144

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2310).

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  doi:10.1107/S160053680704891X

supplementary materials

Acta Cryst. (2007). E**63**, o4290 [**doi:10.1107/S160053680704891X**]

N'-(Diphenylmethylene)-3-(3-nitrophenyl)-1',3'-dioxospiro[cyclopropane-2'-indan]-2-carbohydrazide

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Comment

In the title compound, (I) (Fig. 1), all bond lengths and angles are normal (Allen *et al.*, 1987) and correspond to those observed in similar structures (Chakkaravarthi *et al.*, 2007; Satis Kumar *et al.*, 2006).

The benzene ring C1—C6 forms the dihedral angle of 53.26 (6)° with the indan ring system. The phenyl rings C20—C25 and C26—C31 form the dihedral angles of 66.50 (6)° and 58.39 (7)°, respectively, with the indan ring system. The five-(C8/C9/C10/C15/C16) and six-membered (C10—C15) rings in the indane group make a dihedral angle of 4.04 (9)°. The nitro group N1/O3/O4 is twisted out the attached benzene ring at 13.19 (16)°.

The crystal packing of (I) (Fig. 2) is stabilized by intermolecular C—H···O and N—H···O hydrogen bonds (Table 1).

Experimental

A mixture of 1-(diphenylmethylene)-3-oxo-1,2-aziditinumylide (0.23 g, 1 mmol) and 2-(*m*-nitro) benzylidine-1,3-indane dione (0.27 g, 1 mmol) was refluxed in dry toluene. The reaction was monitered by TLC. After its completion, the solvent was removed at reduced pressure. The crude product was subjected to column chromatography (silica gel 100–200 mesh) using hexane:ethyl acetate (7:3) as eluant. The compound was recrystallized from hexane:chloroform (1:1) solution.

Refinement

All H atoms were positioned geometrically (C—H 0.93–0.98 Å, N—H 0.86 Å) and refined using riding model, with U_{iso}(H) = 1.2Ueq(C,*N*).

Figures

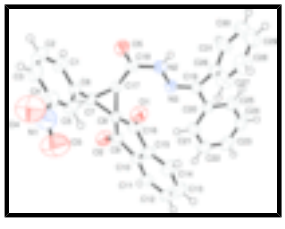

Fig. 1. The molecular structure of (I), showing the atomic labels and 50% probability displacement ellipsoids.

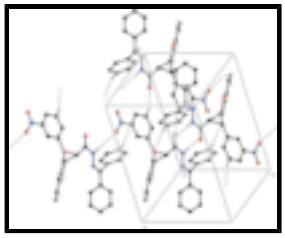

Fig. 2. The packing of (I), viewed down the *c* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

N'-(Diphenylmethylene)-3-(3-nitrophenyl)-1',3'-dioxospiro[cyclopropane-2'- indan]-2-carbohydrazide

Crystal data

$C_{31}H_{21}N_3O_5$	$Z = 2$
$M_r = 515.51$	$F_{000} = 536$
Triclinic, $P\bar{1}$	$D_x = 1.347$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.4617$ (4) Å	Cell parameters from 7426 reflections
$b = 12.8806$ (5) Å	$\theta = 2.4$–25.0º
$c = 12.9114$ (8) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 108.212$ (2)º	$T = 295$ (2) K
$\beta = 108.535$ (3)º	Prism, colourless
$\gamma = 107.424$ (2)º	0.22 × 0.16 × 0.16 mm
$V = 1270.69$ (11) Å^3	

Data collection

Bruker Kappa-APEXII diffractometer	4593 independent reflections
Radiation source: fine-focus sealed tube	3628 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.029$
$T = 295$(2) K	$\theta_{max} = 25.3$º
ω and φ scans	$\theta_{min} = 2.4$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -11 \rightarrow 11$
$T_{min} = 0.897$, $T_{max} = 0.985$	$k = -15 \rightarrow 15$
23251 measured reflections	$l = -13 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.044$	H-atom parameters constrained
$wR(F^2) = 0.122$	$w = 1/[\sigma^2(F_o^2) + (0.0544P)^2 + 0.4755P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$

4593 reflections	$\Delta\rho_{max} = 0.41$ e Å^{-3}
352 parameters	$\Delta\rho_{min} = -0.33$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	−0.04259 (18)	0.28990 (11)	0.30518 (12)	0.0562 (4)
O2	−0.38449 (18)	−0.09220 (12)	−0.04041 (12)	0.0600 (4)
O3	−0.4375 (4)	0.4332 (2)	0.2466 (3)	0.1238 (9)
O4	−0.3681 (3)	0.59338 (18)	0.2206 (3)	0.1264 (9)
O5	0.13052 (18)	0.34678 (13)	0.11804 (15)	0.0704 (5)
N1	−0.3744 (3)	0.49416 (19)	0.2027 (2)	0.0828 (6)
N2	0.20415 (18)	0.23100 (13)	0.19914 (14)	0.0457 (4)
H2A	0.3038	0.2883	0.2454	0.055*
N3	0.16360 (17)	0.12174 (13)	0.20421 (13)	0.0406 (3)
C1	−0.1963 (3)	0.34378 (19)	−0.0334 (2)	0.0558 (5)
H1	−0.1547	0.3114	−0.0851	0.067*
C2	−0.2192 (3)	0.4456 (2)	−0.0283 (2)	0.0688 (6)
H2	−0.1950	0.4805	−0.0774	0.083*
C3	−0.2776 (3)	0.49552 (19)	0.0488 (2)	0.0651 (6)
H3	−0.2938	0.5642	0.0529	0.078*
C4	−0.3116 (2)	0.44166 (17)	0.1199 (2)	0.0554 (5)
C5	−0.2928 (2)	0.33816 (16)	0.11500 (18)	0.0474 (5)
H5	−0.3192	0.3028	0.1632	0.057*
C6	−0.2340 (2)	0.28869 (15)	0.03732 (16)	0.0408 (4)
C7	−0.2306 (2)	0.16839 (15)	0.01203 (15)	0.0384 (4)
H7	−0.3194	0.1049	−0.0687	0.046*
C8	−0.1958 (2)	0.11749 (14)	0.10371 (15)	0.0366 (4)
C9	−0.3020 (2)	−0.01311 (15)	0.06427 (16)	0.0399 (4)
C10	−0.2864 (2)	−0.02621 (15)	0.17684 (16)	0.0383 (4)
C11	−0.3501 (2)	−0.13041 (17)	0.18977 (19)	0.0473 (5)
H11	−0.4181	−0.2061	0.1219	0.057*
C12	−0.3093 (3)	−0.1183 (2)	0.3065 (2)	0.0568 (5)
H12	−0.3509	−0.1870	0.3176	0.068*
C13	−0.2078 (3)	−0.0061 (2)	0.4074 (2)	0.0605 (6)
H13	−0.1817	−0.0006	0.4853	0.073*
C14	−0.1441 (3)	0.09819 (19)	0.39477 (18)	0.0547 (5)
H14	−0.0760	0.1738	0.4629	0.066*
C15	−0.1851 (2)	0.08654 (16)	0.27771 (16)	0.0408 (4)
C16	−0.1291 (2)	0.18194 (16)	0.23871 (16)	0.0402 (4)
C17	−0.0803 (2)	0.14712 (15)	0.04513 (15)	0.0370 (4)
H17	−0.0884	0.0759	−0.0178	0.044*
C18	0.0907 (2)	0.25044 (16)	0.12286 (17)	0.0428 (4)
C19	0.2746 (2)	0.11628 (15)	0.28863 (15)	0.0376 (4)
C20	0.2312 (2)	−0.00189 (15)	0.29322 (15)	0.0379 (4)
C21	0.0669 (2)	−0.08342 (17)	0.24699 (18)	0.0490 (5)

H21	−0.0173	−0.0647	0.2100	0.059*
C22	0.0260 (3)	−0.19161 (18)	0.2548 (2)	0.0573 (5)
H22	−0.0850	−0.2443	0.2249	0.069*
C23	0.1482 (3)	−0.22227 (18)	0.30635 (19)	0.0577 (5)
H23	0.1204	−0.2958	0.3108	0.069*
C24	0.3110 (3)	−0.14361 (19)	0.35109 (19)	0.0591 (5)
H24	0.3942	−0.1644	0.3853	0.071*
C25	0.3536 (2)	−0.03331 (18)	0.34610 (18)	0.0501 (5)
H25	0.4650	0.0201	0.3784	0.060*
C26	0.4357 (2)	0.22278 (15)	0.38371 (16)	0.0399 (4)
C27	0.4430 (3)	0.29707 (19)	0.49105 (19)	0.0573 (5)
H27	0.3483	0.2794	0.5029	0.069*
C28	0.5895 (3)	0.3971 (2)	0.5805 (2)	0.0691 (6)
H28	0.5936	0.4462	0.6527	0.083*
C29	0.7288 (3)	0.42418 (19)	0.5633 (2)	0.0664 (6)
H29	0.8272	0.4924	0.6232	0.080*
C30	0.7234 (3)	0.3510 (2)	0.4581 (2)	0.0684 (6)
H30	0.8186	0.3689	0.4470	0.082*
C31	0.5770 (2)	0.25060 (19)	0.36821 (19)	0.0559 (5)
H31	0.5741	0.2014	0.2966	0.067*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0672 (9)	0.0370 (7)	0.0434 (8)	0.0101 (7)	0.0201 (7)	0.0111 (6)
O2	0.0658 (9)	0.0413 (8)	0.0422 (8)	0.0044 (7)	0.0148 (7)	0.0117 (7)
O3	0.172 (2)	0.1117 (17)	0.180 (2)	0.0977 (17)	0.134 (2)	0.0836 (18)
O4	0.165 (2)	0.0690 (12)	0.190 (2)	0.0774 (14)	0.111 (2)	0.0548 (14)
O5	0.0535 (9)	0.0567 (9)	0.0936 (12)	0.0135 (7)	0.0150 (8)	0.0547 (9)
N1	0.0938 (16)	0.0619 (13)	0.1136 (19)	0.0499 (12)	0.0576 (15)	0.0383 (13)
N2	0.0356 (8)	0.0403 (8)	0.0557 (10)	0.0118 (7)	0.0133 (7)	0.0277 (8)
N3	0.0398 (8)	0.0393 (8)	0.0456 (9)	0.0180 (7)	0.0179 (7)	0.0234 (7)
C1	0.0592 (13)	0.0612 (12)	0.0597 (13)	0.0285 (10)	0.0282 (11)	0.0392 (11)
C2	0.0696 (15)	0.0650 (14)	0.0885 (17)	0.0294 (12)	0.0341 (14)	0.0559 (14)
C3	0.0604 (13)	0.0428 (11)	0.0872 (17)	0.0232 (10)	0.0213 (12)	0.0357 (12)
C4	0.0493 (11)	0.0402 (10)	0.0689 (14)	0.0207 (9)	0.0211 (10)	0.0205 (10)
C5	0.0454 (11)	0.0407 (10)	0.0558 (12)	0.0184 (8)	0.0211 (9)	0.0243 (9)
C6	0.0355 (9)	0.0388 (9)	0.0429 (10)	0.0144 (8)	0.0117 (8)	0.0206 (8)
C7	0.0398 (9)	0.0374 (9)	0.0332 (9)	0.0152 (7)	0.0123 (8)	0.0167 (8)
C8	0.0371 (9)	0.0335 (9)	0.0350 (9)	0.0123 (7)	0.0146 (8)	0.0154 (7)
C9	0.0361 (9)	0.0362 (9)	0.0420 (10)	0.0134 (8)	0.0159 (8)	0.0157 (8)
C10	0.0345 (9)	0.0413 (9)	0.0455 (10)	0.0182 (8)	0.0208 (8)	0.0229 (8)
C11	0.0416 (10)	0.0445 (10)	0.0616 (12)	0.0189 (8)	0.0252 (9)	0.0290 (9)
C12	0.0654 (13)	0.0616 (13)	0.0750 (15)	0.0351 (11)	0.0448 (12)	0.0474 (12)
C13	0.0814 (16)	0.0750 (15)	0.0582 (13)	0.0449 (13)	0.0452 (12)	0.0446 (13)
C14	0.0707 (14)	0.0575 (12)	0.0437 (11)	0.0312 (11)	0.0312 (10)	0.0239 (10)
C15	0.0465 (10)	0.0430 (10)	0.0418 (10)	0.0227 (8)	0.0252 (9)	0.0215 (8)
C16	0.0419 (10)	0.0375 (10)	0.0392 (10)	0.0162 (8)	0.0185 (8)	0.0161 (8)

C17	0.0431 (10)	0.0364 (9)	0.0354 (9)	0.0178 (8)	0.0191 (8)	0.0190 (8)
C18	0.0414 (10)	0.0437 (10)	0.0479 (11)	0.0180 (8)	0.0198 (9)	0.0272 (9)
C19	0.0375 (9)	0.0412 (9)	0.0373 (9)	0.0200 (8)	0.0173 (8)	0.0185 (8)
C20	0.0416 (10)	0.0401 (9)	0.0332 (9)	0.0201 (8)	0.0162 (8)	0.0166 (8)
C21	0.0426 (10)	0.0478 (11)	0.0590 (12)	0.0222 (9)	0.0204 (9)	0.0273 (10)
C22	0.0537 (12)	0.0433 (11)	0.0708 (14)	0.0163 (9)	0.0279 (11)	0.0263 (10)
C23	0.0791 (15)	0.0439 (11)	0.0579 (13)	0.0296 (11)	0.0321 (12)	0.0285 (10)
C24	0.0673 (14)	0.0555 (12)	0.0573 (13)	0.0368 (11)	0.0178 (11)	0.0301 (11)
C25	0.0458 (11)	0.0504 (11)	0.0509 (11)	0.0231 (9)	0.0145 (9)	0.0250 (9)
C26	0.0400 (9)	0.0382 (9)	0.0412 (10)	0.0180 (8)	0.0160 (8)	0.0193 (8)
C27	0.0552 (12)	0.0532 (12)	0.0556 (13)	0.0228 (10)	0.0266 (11)	0.0148 (10)
C28	0.0760 (16)	0.0503 (12)	0.0553 (14)	0.0252 (12)	0.0218 (12)	0.0049 (11)
C29	0.0562 (14)	0.0425 (11)	0.0641 (15)	0.0085 (10)	0.0078 (11)	0.0148 (11)
C30	0.0456 (12)	0.0648 (14)	0.0737 (16)	0.0091 (11)	0.0232 (11)	0.0255 (13)
C31	0.0478 (12)	0.0581 (12)	0.0500 (12)	0.0159 (10)	0.0236 (10)	0.0167 (10)

Geometric parameters (Å, °)

O1—C16	1.211 (2)	C12—H12	0.9300
O2—C9	1.211 (2)	C13—C14	1.381 (3)
O3—N1	1.228 (3)	C13—H13	0.9300
O4—N1	1.205 (3)	C14—C15	1.381 (3)
O5—C18	1.212 (2)	C14—H14	0.9300
N1—C4	1.465 (3)	C15—C16	1.487 (2)
N2—C18	1.352 (2)	C17—C18	1.497 (2)
N2—N3	1.3719 (19)	C17—H17	0.9800
N2—H2A	0.8600	C19—C20	1.479 (2)
N3—C19	1.288 (2)	C19—C26	1.489 (2)
C1—C2	1.377 (3)	C20—C21	1.384 (3)
C1—C6	1.387 (3)	C20—C25	1.386 (2)
C1—H1	0.9300	C21—C22	1.375 (3)
C2—C3	1.368 (3)	C21—H21	0.9300
C2—H2	0.9300	C22—C23	1.372 (3)
C3—C4	1.371 (3)	C22—H22	0.9300
C3—H3	0.9300	C23—C24	1.367 (3)
C4—C5	1.382 (3)	C23—H23	0.9300
C5—C6	1.374 (3)	C24—C25	1.384 (3)
C5—H5	0.9300	C24—H24	0.9300
C6—C7	1.493 (2)	C25—H25	0.9300
C7—C17	1.483 (2)	C26—C31	1.373 (3)
C7—C8	1.519 (2)	C26—C27	1.382 (3)
C7—H7	0.9800	C27—C28	1.377 (3)
C8—C16	1.486 (2)	C27—H27	0.9300
C8—C9	1.492 (2)	C28—C29	1.367 (3)
C8—C17	1.538 (2)	C28—H28	0.9300
C9—C10	1.481 (2)	C29—C30	1.364 (3)
C10—C11	1.383 (2)	C29—H29	0.9300
C10—C15	1.384 (2)	C30—C31	1.380 (3)
C11—C12	1.375 (3)	C30—H30	0.9300

C11—H11	0.9300	C31—H31	0.9300
C12—C13	1.380 (3)		
O4—N1—O3	122.9 (2)	C14—C15—C10	120.78 (17)
O4—N1—C4	118.4 (2)	C14—C15—C16	128.81 (17)
O3—N1—C4	118.68 (19)	C10—C15—C16	110.37 (15)
C18—N2—N3	121.34 (14)	O1—C16—C8	127.48 (16)
C18—N2—H2A	119.3	O1—C16—C15	126.23 (16)
N3—N2—H2A	119.3	C8—C16—C15	106.26 (14)
C19—N3—N2	116.68 (14)	C7—C17—C18	121.70 (15)
C2—C1—C6	121.1 (2)	C7—C17—C8	60.32 (11)
C2—C1—H1	119.4	C18—C17—C8	119.45 (14)
C6—C1—H1	119.4	C7—C17—H17	114.9
C3—C2—C1	120.2 (2)	C18—C17—H17	114.9
C3—C2—H2	119.9	C8—C17—H17	114.9
C1—C2—H2	119.9	O5—C18—N2	120.11 (17)
C2—C3—C4	118.20 (19)	O5—C18—C17	123.29 (16)
C2—C3—H3	120.9	N2—C18—C17	116.58 (15)
C4—C3—H3	120.9	N3—C19—C20	116.59 (15)
C3—C4—C5	122.9 (2)	N3—C19—C26	123.70 (15)
C3—C4—N1	118.74 (19)	C20—C19—C26	119.60 (14)
C5—C4—N1	118.3 (2)	C21—C20—C25	118.00 (16)
C6—C5—C4	118.45 (18)	C21—C20—C19	120.89 (15)
C6—C5—H5	120.8	C25—C20—C19	121.10 (16)
C4—C5—H5	120.8	C22—C21—C20	121.12 (18)
C5—C6—C1	119.13 (17)	C22—C21—H21	119.4
C5—C6—C7	122.89 (16)	C20—C21—H21	119.4
C1—C6—C7	117.43 (17)	C23—C22—C21	120.37 (19)
C17—C7—C6	126.45 (15)	C23—C22—H22	119.8
C17—C7—C8	61.64 (11)	C21—C22—H22	119.8
C6—C7—C8	125.85 (15)	C24—C23—C22	119.34 (18)
C17—C7—H7	111.4	C24—C23—H23	120.3
C6—C7—H7	111.4	C22—C23—H23	120.3
C8—C7—H7	111.4	C23—C24—C25	120.73 (19)
C16—C8—C9	106.86 (14)	C23—C24—H24	119.6
C16—C8—C7	128.31 (14)	C25—C24—H24	119.6
C9—C8—C7	118.67 (14)	C24—C25—C20	120.42 (19)
C16—C8—C17	119.38 (14)	C24—C25—H25	119.8
C9—C8—C17	118.39 (14)	C20—C25—H25	119.8
C7—C8—C17	58.04 (11)	C31—C26—C27	118.73 (18)
O2—C9—C10	127.28 (16)	C31—C26—C19	122.37 (17)
O2—C9—C8	125.76 (16)	C27—C26—C19	118.90 (16)
C10—C9—C8	106.96 (14)	C28—C27—C26	120.5 (2)
C11—C10—C15	121.26 (17)	C28—C27—H27	119.7
C11—C10—C9	129.33 (17)	C26—C27—H27	119.7
C15—C10—C9	109.33 (14)	C29—C28—C27	120.1 (2)
C12—C11—C10	117.74 (19)	C29—C28—H28	120.0
C12—C11—H11	121.1	C27—C28—H28	120.0
C10—C11—H11	121.1	C30—C29—C28	119.9 (2)
C11—C12—C13	121.18 (18)	C30—C29—H29	120.0

C11—C12—H12	119.4	C28—C29—H29	120.0
C13—C12—H12	119.4	C29—C30—C31	120.2 (2)
C12—C13—C14	121.23 (19)	C29—C30—H30	119.9
C12—C13—H13	119.4	C31—C30—H30	119.9
C14—C13—H13	119.4	C26—C31—C30	120.5 (2)
C13—C14—C15	117.80 (19)	C26—C31—H31	119.7
C13—C14—H14	121.1	C30—C31—H31	119.7
C15—C14—H14	121.1		
C18—N2—N3—C19	−172.85 (17)	C9—C8—C16—C15	4.82 (18)
C6—C1—C2—C3	1.1 (3)	C7—C8—C16—C15	156.24 (16)
C1—C2—C3—C4	0.1 (3)	C17—C8—C16—C15	−132.99 (15)
C2—C3—C4—C5	−1.4 (3)	C14—C15—C16—O1	−4.2 (3)
C2—C3—C4—N1	−179.9 (2)	C10—C15—C16—O1	178.21 (18)
O4—N1—C4—C3	−12.1 (4)	C14—C15—C16—C8	173.92 (19)
O3—N1—C4—C3	164.8 (3)	C10—C15—C16—C8	−3.63 (19)
O4—N1—C4—C5	169.4 (2)	C6—C7—C17—C18	7.1 (3)
O3—N1—C4—C5	−13.8 (4)	C8—C7—C17—C18	−108.25 (17)
C3—C4—C5—C6	1.4 (3)	C6—C7—C17—C8	115.38 (19)
N1—C4—C5—C6	179.94 (18)	C16—C8—C17—C7	−119.16 (17)
C4—C5—C6—C1	−0.2 (3)	C9—C8—C17—C7	107.79 (17)
C4—C5—C6—C7	−171.44 (17)	C16—C8—C17—C18	−7.3 (2)
C2—C1—C6—C5	−1.1 (3)	C9—C8—C17—C18	−140.32 (16)
C2—C1—C6—C7	170.69 (19)	C7—C8—C17—C18	111.88 (17)
C5—C6—C7—C17	−114.6 (2)	N3—N2—C18—O5	−178.34 (18)
C1—C6—C7—C17	74.0 (2)	N3—N2—C18—C17	0.2 (3)
C5—C6—C7—C8	−35.8 (3)	C7—C17—C18—O5	−35.5 (3)
C1—C6—C7—C8	152.77 (17)	C8—C17—C18—O5	−106.8 (2)
C17—C7—C8—C16	104.13 (19)	C7—C17—C18—N2	146.06 (17)
C6—C7—C8—C16	−12.2 (3)	C8—C17—C18—N2	74.7 (2)
C17—C7—C8—C9	−107.32 (17)	N2—N3—C19—C20	−179.47 (14)
C6—C7—C8—C9	136.39 (17)	N2—N3—C19—C26	4.4 (2)
C6—C7—C8—C17	−116.29 (19)	N3—C19—C20—C21	−25.2 (2)
C16—C8—C9—O2	175.67 (18)	C26—C19—C20—C21	151.17 (17)
C7—C8—C9—O2	21.0 (3)	N3—C19—C20—C25	156.18 (17)
C17—C8—C9—O2	−46.0 (2)	C26—C19—C20—C25	−27.5 (2)
C16—C8—C9—C10	−4.34 (18)	C25—C20—C21—C22	0.9 (3)
C7—C8—C9—C10	−159.01 (15)	C19—C20—C21—C22	−177.76 (18)
C17—C8—C9—C10	133.95 (15)	C20—C21—C22—C23	−1.5 (3)
O2—C9—C10—C11	5.5 (3)	C21—C22—C23—C24	0.7 (3)
C8—C9—C10—C11	−174.53 (17)	C22—C23—C24—C25	0.7 (3)
O2—C9—C10—C15	−177.83 (18)	C23—C24—C25—C20	−1.3 (3)
C8—C9—C10—C15	2.17 (19)	C21—C20—C25—C24	0.5 (3)
C15—C10—C11—C12	0.0 (3)	C19—C20—C25—C24	179.18 (18)
C9—C10—C11—C12	176.39 (17)	N3—C19—C26—C31	−91.3 (2)
C10—C11—C12—C13	−0.3 (3)	C20—C19—C26—C31	92.6 (2)
C11—C12—C13—C14	0.4 (3)	N3—C19—C26—C27	88.1 (2)
C12—C13—C14—C15	−0.2 (3)	C20—C19—C26—C27	−88.0 (2)
C13—C14—C15—C10	−0.1 (3)	C31—C26—C27—C28	0.1 (3)
C13—C14—C15—C16	−177.40 (18)	C19—C26—C27—C28	−179.36 (19)

C11—C10—C15—C14	0.2 (3)	C26—C27—C28—C29	0.5 (3)
C9—C10—C15—C14	−176.87 (17)	C27—C28—C29—C30	−1.0 (4)
C11—C10—C15—C16	177.93 (16)	C28—C29—C30—C31	0.9 (4)
C9—C10—C15—C16	0.9 (2)	C27—C26—C31—C30	−0.2 (3)
C9—C8—C16—O1	−177.06 (18)	C19—C26—C31—C30	179.25 (19)
C7—C8—C16—O1	−25.6 (3)	C29—C30—C31—C26	−0.3 (4)
C17—C8—C16—O1	45.1 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O5^{i}	0.93	2.39	3.227 (2)	149
C29—H29···O1^{ii}	0.93	2.57	3.406 (2)	149
N2—H2A···O3^{iii}	0.86	2.59	3.324 (3)	144

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

Fig. 1

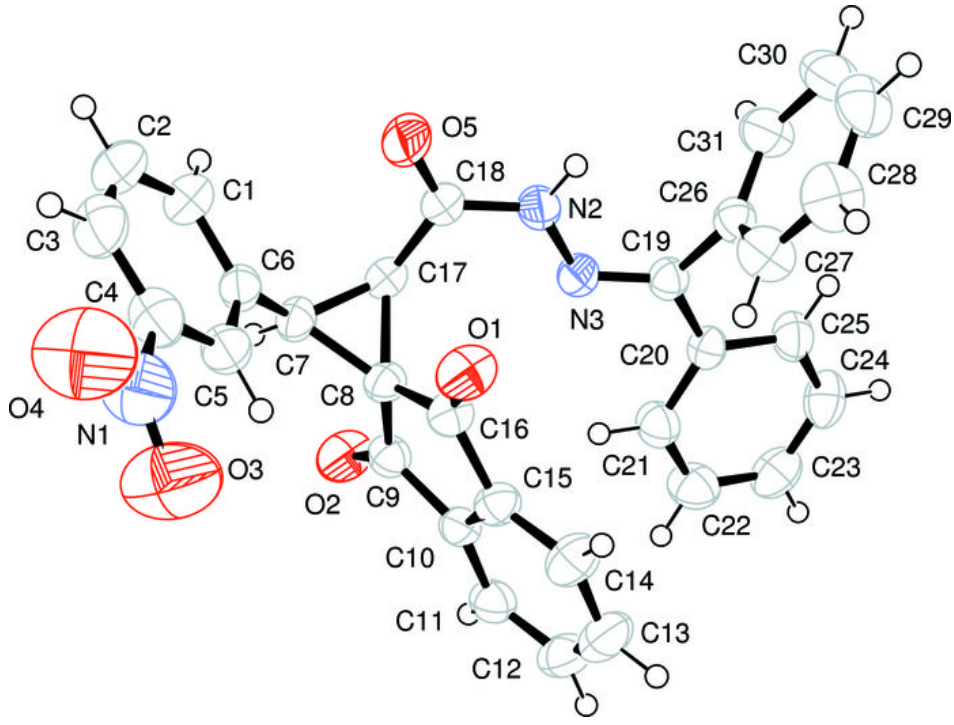
C30
C29
C31
C28
C26
C2
O5
C18
N2
C1
C3
C19
C27
C6
C17
C4
N3
C25
O1
C20
C24
C7
C5
C8
O4
C16
N1
C21
C23
O3
O2
C9
C15
C22
C10
C14
C11
C13
C12

Fig. 2