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3,3-Dimethyl-5-phenyl-3,4-dihydro-1*H*-benzo[*b*]carbazole-1,6,11(2*H*,5*H*)-trione

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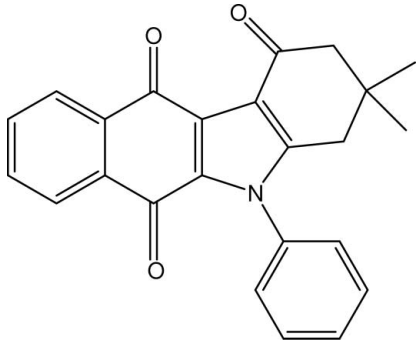
Key indicators: single-crystal X-ray study; T = 105 K; mean σ(C–C) = 0.002 Å; R factor = 0.052; wR factor = 0.131; data-to-parameter ratio = 20.5.

In the title compound, $C_{24}H_{19}NO_3$, the six-membered ring with the methyl substituents is in an envelope conformation. The crystal structure is stabilized by C—H···O, C—H···π and π–π interactions; the latter involve centroid–centroid distances of 3.680 (1) and 3.802 (1) Å.

Related literature

For bond-length data, see: Allen *et al.* (1987). For related literature, see: Cone *et al.* (1989); Cremer & Pople (1975); Hu *et al.* (2006); Fun *et al.* (2007).



Experimental

Crystal data

$C_{24}H_{19}NO_3$
M_r = 369.40
Monoclinic, $P2_1/c$
a = 10.0097 (4) Å
b = 10.3559 (3) Å
c = 18.8030 (6) Å
β = 113.032 (2)°
V = 1793.74 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 105.0 (1) K
0.44 × 0.44 × 0.21 mm

Data collection

Bruker SMART APEX II CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.923, T_{max} = 0.981
20016 measured reflections
5227 independent reflections
3937 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.131
S = 1.04
5227 reflections
255 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 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
C4—H4A···O1^{i}	0.93	2.59	3.360 (2)	140
C7—H7A···O2^{ii}	0.93	2.37	3.272 (2)	163
C18—H18A···O2^{iii}	0.93	2.40	3.262 (2)	155
C15—H15B···$Cg1^{iii}$	0.97	2.82	3.742 (2)	158

Symmetry codes: (i) $-x+2, -y+1, -z$; (ii) $-x+1, -y+2, -z$; (iii) $-x+1, -y+1, -z$. Note: $Cg1$ is the centroid of the C3–C8 ring.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2149).

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supplementary materials

Acta Cryst. (2007). E**63**, o3146 [**doi:10.1107/S1600536807027213**]

3,3-Dimethyl-5-phenyl-3,4-dihydro-1*H*-benzo[*b*]carbazole-1,6,11(2*H*,5*H*)-trione

H.-K. Fun, J. B.-J. Teh, Y. Liu and J.-H. Xu

Comment

Benzo[*b*]carbazole-6,11-diones, as bisannulated indoloquinones, are important synthetic targets (Cone *et al.*, 1989). However, a majority of the present synthetic methods for them are based on rather long reaction sequences. We have recently reported a direct one-pot synthesis of benzo[*b*]carbazole-6,11-diones (Hu *et al.*, 2006). The title compound, a derivative of benzo[*b*]carbazole-6,11-dione, was isolated from the *C*,*N*-dialkylation of the cyclic β-enaminone of 5,5-dimethyl-3-(phenylamino)cyclohex-2-en-1-one by 2,3-dichloro-1,4-naphthalenedione.

Bond lengths and angles in the title compound have normal values (Allen *et al.*, 1987), comparable to a related structure (Fun *et al.*, 2007). The C11—C16 ring adopts an envelope conformation, with C14 deviating from the plane of the other five atoms by 0.621 (1) Å. The puckering parameters are Q = 0.453 (2) Å, θ = 50.1 (3)° and φ = 170.7 (3)° (Cremer & Pople, 1975). The C17—C22 ring is almost perpendicular to the pyrrole ring; the dihedral angle between the N1/C1/C10/C11/C16 and C17—C22 rings is 77.92 (8)°.

The crystal structure is stabilized by intermolecular C—H···O interactions (Fig. 2 and Table 1) and also C—H···π interactions involving the C3—C8 ring (centroid *Cg*1) (Table 1). π-π interactions provide additional stability; the centroid-centroid distance between the N1/C1/C10/C11/C16 rings at (*x*, *y*, *z*) and (1 − *x*, 1 − *y*, −*z*) is 3.802 (1) Å, and that between the N1/C1/C10/C11/C16 rings at (*x*, *y*, *z*) and the C1—C3/C8—C10 ring at (1 − *x*, 1 − *y*, −*z*) is 3.680 (1) Å.

Experimental

A mixture of 2,3-dichloro-1,4-naphthalenedione (1.1 mmol), 5,5-dimethyl-3-(phenylamino)cyclohex-2-en-1-one (1 mmol) and Na_2CO_3 (2.5 mmol) in DMF (15 ml) was heated under reflux for 6 h with magnetic stirring and TLC monitoring of the reaction. The solvent was removed under reduced pressure, and the residual solid was separated by flash chromatography on a silica gel column, with petroleum ether-ethyl acetate as eluents, to give the title compound. Single crystals were obtained by slow evaporation of a petroleum ether-ethyl acetate (3:1) solvent system (yield 75%); m.p 532–533 K.

Refinement

H atoms were positioned geometrically and treated as riding, with C—H = 0.93–0.97Å and the U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

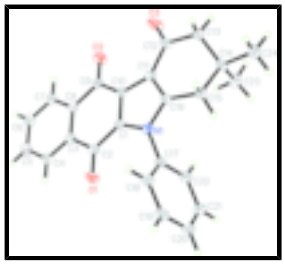

Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atomic numbering.

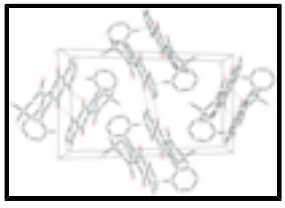

Fig. 2. The crystal packing of the title compound, viewed down the *a* axis. H atoms not involved in intermolecular hydrogen bonding (dashed lines) have been omitted.

3,3-Dimethyl-5-phenyl-3,4-dihydro-1*H*-benzo[*b*]carbazole-1,6,11(2*H*,5H)-trione

Crystal data

$C_{24}H_{19}NO_3$	F_{000} = 776
M_r = 369.40	D_x = 1.368 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 4781 reflections
a = 10.0097 (4) Å	θ = 2.2–30.0º
b = 10.3559 (3) Å	μ = 0.09 mm^{-1}
c = 18.8030 (6) Å	T = 105.0 (1) K
β = 113.032 (2)º	Block, yellow
V = 1793.74 (11) Å^3	0.44 × 0.44 × 0.21 mm
Z = 4	

Data collection

Bruker SMART APEX II CCD diffractometer	5227 independent reflections
Radiation source: fine-focus sealed tube	3937 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.045
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 30.0º
T = 105.0(1) K	θ_{min} = 2.2º
ω scans	h = −14→10
Absorption correction: multi-scan (SADABS; Bruker, 2005)	k = −14→14
T_{min} = 0.923, T_{max} = 0.981	l = −23→26
20016 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.052$	H-atom parameters constrained
$wR(F^2) = 0.131$	$w = 1/[\sigma^2(F_o^2) + (0.058P)^2 + 0.6108P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
5227 reflections	$\Delta\rho_{max} = 0.40$ e Å^{-3}
255 parameters	$\Delta\rho_{min} = -0.25$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. The data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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 $F^2 > 2$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	0.88629 (12)	0.46854 (10)	0.06989 (7)	0.0276 (3)
O2	0.48911 (12)	0.84168 (10)	0.04046 (7)	0.0294 (3)
O3	0.29406 (13)	0.73100 (11)	0.10322 (8)	0.0364 (3)
N1	0.65186 (13)	0.43131 (11)	0.12615 (7)	0.0167 (2)
C1	0.67700 (15)	0.53791 (13)	0.08874 (8)	0.0165 (3)
C2	0.79625 (15)	0.55284 (13)	0.06292 (8)	0.0188 (3)
C3	0.80114 (15)	0.68082 (13)	0.02733 (8)	0.0177 (3)
C4	0.91277 (16)	0.70517 (14)	0.00263 (8)	0.0216 (3)
H4A	0.9824	0.6422	0.0082	0.026*
C5	0.92026 (17)	0.82360 (15)	−0.03028 (9)	0.0257 (3)
H5A	0.9950	0.8398	−0.0467	0.031*
C6	0.81637 (17)	0.91787 (15)	−0.03875 (9)	0.0256 (3)
H6A	0.8215	0.9968	−0.0612	0.031*
C7	0.70500 (17)	0.89488 (14)	−0.01394 (8)	0.0213 (3)
H7A	0.6361	0.9585	−0.0194	0.026*
C8	0.69637 (15)	0.77623 (13)	0.01928 (8)	0.0179 (3)
C9	0.57515 (15)	0.75543 (13)	0.04574 (8)	0.0181 (3)

C10	0.56930 (15)	0.62804 (13)	0.07879 (8)	0.0164 (3)
C11	0.47292 (15)	0.57373 (13)	0.11076 (8)	0.0172 (3)
C12	0.34326 (16)	0.62263 (14)	0.12104 (9)	0.0211 (3)
C13	0.27163 (16)	0.52641 (14)	0.15548 (9)	0.0221 (3)
H13A	0.2027	0.4760	0.1137	0.027*
H13B	0.2170	0.5739	0.1796	0.027*
C14	0.37449 (16)	0.43246 (13)	0.21565 (8)	0.0197 (3)
C15	0.46719 (15)	0.36058 (13)	0.17948 (8)	0.0185 (3)
H15A	0.5454	0.3151	0.2195	0.022*
H15B	0.4077	0.2974	0.1426	0.022*
C16	0.52900 (15)	0.45310 (13)	0.13976 (8)	0.0168 (3)
C17	0.75680 (15)	0.33105 (13)	0.16409 (8)	0.0179 (3)
C18	0.77517 (17)	0.22589 (14)	0.12389 (9)	0.0233 (3)
H18A	0.7206	0.2173	0.0712	0.028*
C19	0.87714 (18)	0.13282 (15)	0.16385 (10)	0.0285 (4)
H19A	0.8896	0.0603	0.1379	0.034*
C20	0.95985 (18)	0.14733 (16)	0.24163 (10)	0.0313 (4)
H20A	1.0289	0.0853	0.2677	0.038*
C21	0.94077 (18)	0.25331 (16)	0.28107 (10)	0.0299 (4)
H21A	0.9970	0.2628	0.3335	0.036*
C22	0.83737 (16)	0.34590 (14)	0.24236 (9)	0.0227 (3)
H22A	0.8226	0.4168	0.2687	0.027*
C23	0.47307 (18)	0.50570 (15)	0.28774 (9)	0.0262 (3)
H23A	0.5320	0.4453	0.3258	0.039*
H23D	0.4146	0.5542	0.3083	0.039*
H23B	0.5344	0.5635	0.2743	0.039*
C24	0.28358 (18)	0.33466 (15)	0.23837 (10)	0.0267 (3)
H24D	0.3466	0.2730	0.2738	0.040*
H24A	0.2189	0.2907	0.1930	0.040*
H24B	0.2281	0.3789	0.2625	0.040*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0270 (6)	0.0222 (5)	0.0408 (6)	0.0090 (4)	0.0211 (5)	0.0088 (5)
O2	0.0330 (6)	0.0195 (5)	0.0423 (7)	0.0108 (5)	0.0219 (5)	0.0095 (5)
O3	0.0316 (7)	0.0221 (5)	0.0662 (9)	0.0117 (5)	0.0309 (6)	0.0124 (6)
N1	0.0182 (6)	0.0132 (5)	0.0197 (6)	0.0024 (4)	0.0085 (5)	0.0021 (4)
C1	0.0164 (7)	0.0144 (6)	0.0181 (6)	0.0015 (5)	0.0061 (5)	0.0005 (5)
C2	0.0182 (7)	0.0177 (6)	0.0200 (7)	0.0016 (5)	0.0070 (6)	0.0002 (5)
C3	0.0179 (7)	0.0172 (6)	0.0168 (6)	−0.0006 (5)	0.0055 (5)	−0.0006 (5)
C4	0.0199 (7)	0.0224 (7)	0.0233 (7)	0.0000 (6)	0.0094 (6)	−0.0001 (6)
C5	0.0256 (8)	0.0258 (7)	0.0287 (8)	−0.0055 (6)	0.0139 (7)	0.0001 (6)
C6	0.0292 (8)	0.0196 (7)	0.0285 (8)	−0.0049 (6)	0.0119 (7)	0.0028 (6)
C7	0.0254 (8)	0.0157 (6)	0.0224 (7)	0.0001 (5)	0.0089 (6)	0.0001 (5)
C8	0.0201 (7)	0.0150 (6)	0.0169 (6)	−0.0004 (5)	0.0054 (5)	−0.0009 (5)
C9	0.0198 (7)	0.0158 (6)	0.0184 (6)	0.0020 (5)	0.0070 (5)	0.0002 (5)
C10	0.0174 (7)	0.0146 (6)	0.0171 (6)	0.0015 (5)	0.0065 (5)	−0.0005 (5)

C11	0.0172 (7)	0.0146 (6)	0.0194 (6)	0.0013 (5)	0.0069 (5)	−0.0009 (5)
C12	0.0199 (7)	0.0182 (6)	0.0268 (7)	0.0024 (5)	0.0110 (6)	−0.0001 (6)
C13	0.0200 (7)	0.0201 (7)	0.0297 (8)	0.0014 (5)	0.0135 (6)	0.0018 (6)
C14	0.0211 (7)	0.0169 (6)	0.0248 (7)	−0.0002 (5)	0.0130 (6)	−0.0015 (5)
C15	0.0180 (7)	0.0158 (6)	0.0236 (7)	−0.0006 (5)	0.0102 (6)	0.0000 (5)
C16	0.0165 (7)	0.0152 (6)	0.0192 (6)	0.0006 (5)	0.0075 (5)	−0.0013 (5)
C17	0.0159 (7)	0.0143 (6)	0.0247 (7)	0.0022 (5)	0.0093 (6)	0.0050 (5)
C18	0.0231 (8)	0.0204 (7)	0.0277 (8)	0.0038 (6)	0.0112 (6)	0.0011 (6)
C19	0.0318 (9)	0.0191 (7)	0.0425 (9)	0.0096 (6)	0.0232 (8)	0.0074 (7)
C20	0.0254 (8)	0.0310 (8)	0.0430 (10)	0.0135 (7)	0.0195 (8)	0.0204 (7)
C21	0.0227 (8)	0.0362 (9)	0.0279 (8)	0.0055 (7)	0.0067 (7)	0.0120 (7)
C22	0.0205 (7)	0.0225 (7)	0.0254 (7)	0.0009 (6)	0.0093 (6)	0.0030 (6)
C23	0.0347 (9)	0.0212 (7)	0.0248 (7)	−0.0019 (6)	0.0139 (7)	−0.0028 (6)
C24	0.0306 (8)	0.0218 (7)	0.0340 (8)	−0.0012 (6)	0.0192 (7)	0.0012 (6)

Geometric parameters (Å, °)

O1—C2	1.2244 (17)	C13—H13A	0.9700
O2—C9	1.2176 (17)	C13—H13B	0.9700
O3—C12	1.2187 (17)	C14—C23	1.530 (2)
N1—C16	1.3693 (18)	C14—C24	1.530 (2)
N1—C1	1.3839 (17)	C14—C15	1.5398 (19)
N1—C17	1.4505 (17)	C15—C16	1.4901 (19)
C1—C10	1.3822 (18)	C15—H15A	0.9700
C1—C2	1.4622 (19)	C15—H15B	0.9700
C2—C3	1.4942 (19)	C17—C18	1.378 (2)
C3—C4	1.391 (2)	C17—C22	1.382 (2)
C3—C8	1.4052 (19)	C18—C19	1.391 (2)
C4—C5	1.389 (2)	C18—H18A	0.9300
C4—H4A	0.9300	C19—C20	1.378 (2)
C5—C6	1.389 (2)	C19—H19A	0.9300
C5—H5A	0.9300	C20—C21	1.379 (2)
C6—C7	1.387 (2)	C20—H20A	0.9300
C6—H6A	0.9300	C21—C22	1.390 (2)
C7—C8	1.3963 (19)	C21—H21A	0.9300
C7—H7A	0.9300	C22—H22A	0.9300
C8—C9	1.496 (2)	C23—H23A	0.9600
C9—C10	1.4691 (18)	C23—H23D	0.9600
C10—C11	1.4362 (19)	C23—H23B	0.9600
C11—C16	1.3905 (18)	C24—H24D	0.9600
C11—C12	1.4745 (19)	C24—H24A	0.9600
C12—C13	1.513 (2)	C24—H24B	0.9600
C13—C14	1.541 (2)		
C16—N1—C1	108.59 (11)	C23—C14—C24	109.19 (12)
C16—N1—C17	123.82 (11)	C23—C14—C15	109.86 (12)
C1—N1—C17	125.47 (11)	C24—C14—C15	109.29 (12)
C10—C1—N1	108.68 (12)	C23—C14—C13	110.58 (12)
C10—C1—C2	125.34 (12)	C24—C14—C13	108.87 (12)
N1—C1—C2	125.98 (12)	C15—C14—C13	109.02 (12)

O1—C2—C1	123.46 (13)	C16—C15—C14	110.52 (11)
O1—C2—C3	121.92 (13)	C16—C15—H15A	109.5
C1—C2—C3	114.62 (12)	C14—C15—H15A	109.5
C4—C3—C8	119.99 (13)	C16—C15—H15B	109.5
C4—C3—C2	118.80 (13)	C14—C15—H15B	109.5
C8—C3—C2	121.21 (12)	H15A—C15—H15B	108.1
C5—C4—C3	119.96 (14)	N1—C16—C11	109.22 (12)
C5—C4—H4A	120.0	N1—C16—C15	124.55 (12)
C3—C4—H4A	120.0	C11—C16—C15	126.24 (12)
C4—C5—C6	120.21 (14)	C18—C17—C22	121.62 (13)
C4—C5—H5A	119.9	C18—C17—N1	121.47 (13)
C6—C5—H5A	119.9	C22—C17—N1	116.91 (12)
C7—C6—C5	120.32 (14)	C17—C18—C19	118.57 (14)
C7—C6—H6A	119.8	C17—C18—H18A	120.7
C5—C6—H6A	119.8	C19—C18—H18A	120.7
C6—C7—C8	120.00 (14)	C20—C19—C18	120.46 (15)
C6—C7—H7A	120.0	C20—C19—H19A	119.8
C8—C7—H7A	120.0	C18—C19—H19A	119.8
C7—C8—C3	119.52 (13)	C19—C20—C21	120.35 (14)
C7—C8—C9	118.40 (13)	C19—C20—H20A	119.8
C3—C8—C9	122.08 (12)	C21—C20—H20A	119.8
O2—C9—C10	123.31 (13)	C20—C21—C22	119.93 (15)
O2—C9—C8	120.47 (13)	C20—C21—H21A	120.0
C10—C9—C8	116.21 (12)	C22—C21—H21A	120.0
C1—C10—C11	107.15 (12)	C17—C22—C21	119.05 (14)
C1—C10—C9	120.38 (12)	C17—C22—H22A	120.5
C11—C10—C9	132.31 (12)	C21—C22—H22A	120.5
C16—C11—C10	106.36 (12)	C14—C23—H23A	109.5
C16—C11—C12	119.88 (13)	C14—C23—H23D	109.5
C10—C11—C12	133.65 (12)	H23A—C23—H23D	109.5
O3—C12—C11	124.19 (14)	C14—C23—H23B	109.5
O3—C12—C13	121.06 (13)	H23A—C23—H23B	109.5
C11—C12—C13	114.75 (12)	H23D—C23—H23B	109.5
C12—C13—C14	115.95 (12)	C14—C24—H24D	109.5
C12—C13—H13A	108.3	C14—C24—H24A	109.5
C14—C13—H13A	108.3	H24D—C24—H24A	109.5
C12—C13—H13B	108.3	C14—C24—H24B	109.5
C14—C13—H13B	108.3	H24D—C24—H24B	109.5
H13A—C13—H13B	107.4	H24A—C24—H24B	109.5
C16—N1—C1—C10	0.16 (15)	C1—C10—C11—C12	176.89 (15)
C17—N1—C1—C10	−163.70 (12)	C9—C10—C11—C12	1.6 (3)
C16—N1—C1—C2	−179.09 (13)	C16—C11—C12—O3	173.72 (15)
C17—N1—C1—C2	17.0 (2)	C10—C11—C12—O3	−1.9 (3)
C10—C1—C2—O1	−176.81 (14)	C16—C11—C12—C13	−6.89 (19)
N1—C1—C2—O1	2.3 (2)	C10—C11—C12—C13	177.52 (14)
C10—C1—C2—C3	3.6 (2)	O3—C12—C13—C14	−146.12 (15)
N1—C1—C2—C3	−177.25 (12)	C11—C12—C13—C14	34.47 (18)
O1—C2—C3—C4	−1.0 (2)	C12—C13—C14—C23	65.39 (16)
C1—C2—C3—C4	178.52 (13)	C12—C13—C14—C24	−174.65 (12)

O1—C2—C3—C8	179.56 (14)	C12—C13—C14—C15	−55.50 (16)
C1—C2—C3—C8	−0.87 (19)	C23—C14—C15—C16	−73.91 (15)
C8—C3—C4—C5	−0.3 (2)	C24—C14—C15—C16	166.31 (12)
C2—C3—C4—C5	−179.67 (13)	C13—C14—C15—C16	47.42 (15)
C3—C4—C5—C6	−0.1 (2)	C1—N1—C16—C11	0.41 (15)
C4—C5—C6—C7	0.5 (2)	C17—N1—C16—C11	164.60 (12)
C5—C6—C7—C8	−0.4 (2)	C1—N1—C16—C15	−179.61 (13)
C6—C7—C8—C3	0.0 (2)	C17—N1—C16—C15	−15.4 (2)
C6—C7—C8—C9	179.64 (13)	C10—C11—C16—N1	−0.79 (15)
C4—C3—C8—C7	0.3 (2)	C12—C11—C16—N1	−177.47 (12)
C2—C3—C8—C7	179.69 (12)	C10—C11—C16—C15	179.23 (13)
C4—C3—C8—C9	−179.28 (13)	C12—C11—C16—C15	2.6 (2)
C2—C3—C8—C9	0.1 (2)	C14—C15—C16—N1	155.83 (13)
C7—C8—C9—O2	−2.2 (2)	C14—C15—C16—C11	−24.20 (19)
C3—C8—C9—O2	177.36 (14)	C16—N1—C17—C18	111.91 (16)
C7—C8—C9—C10	178.78 (12)	C1—N1—C17—C18	−86.59 (17)
C3—C8—C9—C10	−1.62 (19)	C16—N1—C17—C22	−68.08 (17)
N1—C1—C10—C11	−0.64 (15)	C1—N1—C17—C22	93.42 (16)
C2—C1—C10—C11	178.62 (13)	C22—C17—C18—C19	0.3 (2)
N1—C1—C10—C9	175.32 (12)	N1—C17—C18—C19	−179.65 (13)
C2—C1—C10—C9	−5.4 (2)	C17—C18—C19—C20	−1.3 (2)
O2—C9—C10—C1	−174.82 (14)	C18—C19—C20—C21	1.1 (2)
C8—C9—C10—C1	4.13 (19)	C19—C20—C21—C22	0.2 (2)
O2—C9—C10—C11	0.0 (2)	C18—C17—C22—C21	0.9 (2)
C8—C9—C10—C11	178.92 (14)	N1—C17—C22—C21	−179.09 (13)
C1—C10—C11—C16	0.88 (15)	C20—C21—C22—C17	−1.2 (2)
C9—C10—C11—C16	−174.42 (14)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4A···O1^{i}	0.93	2.59	3.360 (2)	140
C7—H7A···O2^{ii}	0.93	2.37	3.272 (2)	163
C18—H18A···O2^{iii}	0.93	2.40	3.262 (2)	155
C15—H15B···Cg1^{iii}	0.97	2.82	3.742 (2)	158

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

Fig. 1

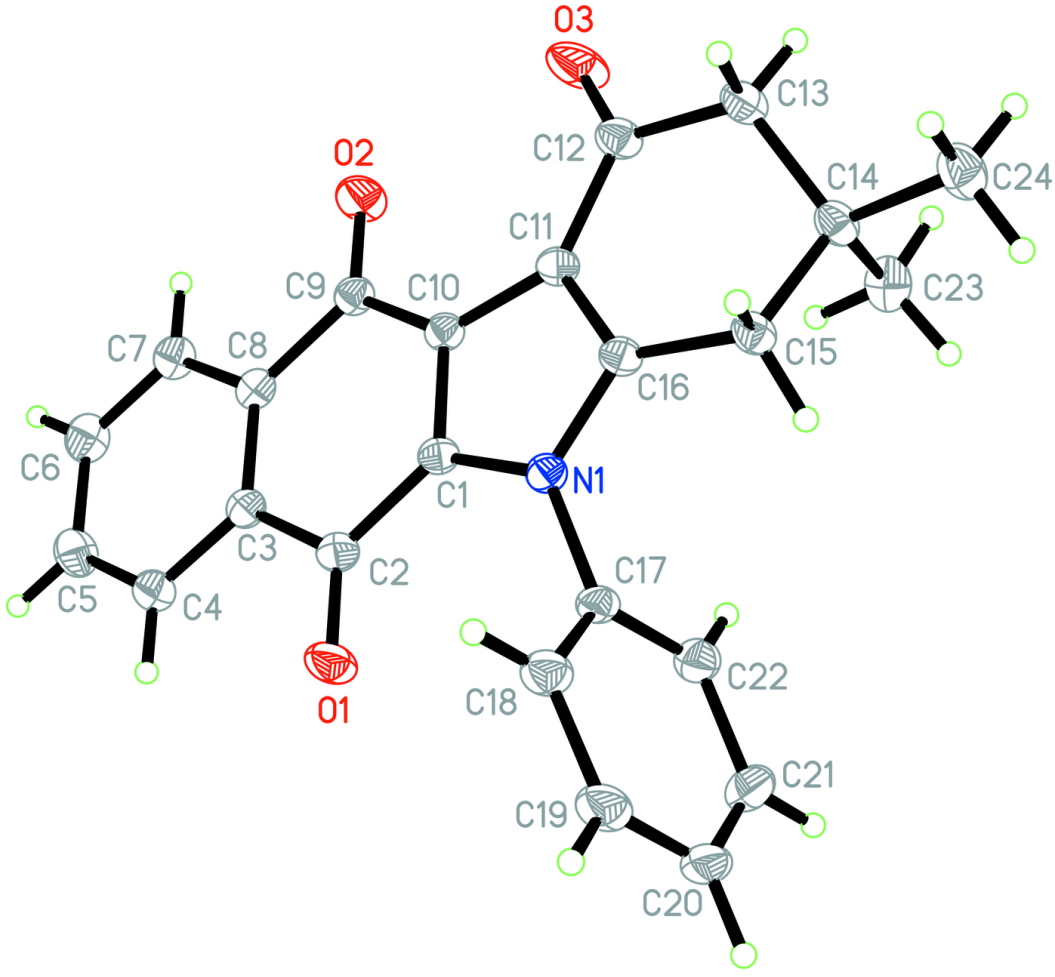
O3
C13
C12
O2
C14
C24
C11
C9
C10
C23
C7
C8
C15
C16
C6
N1
C1
C3
C2
C17
C5
C4
C22
O1
C18
C21
C19
C20

Fig. 2