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8-*tert*-Butyl-7,10-diphenyl-6,10-dihydro-5*H*-benzo[*h*]pyrazolo[3,4-*b*]quinoline

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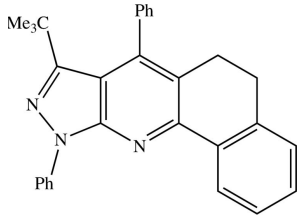
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.004 Å; R factor = 0.071; wR factor = 0.238; data-to-parameter ratio = 17.4.

In the title compound, $C_{30}H_{27}N_3$, the non-aromatic carbocyclic ring adopts an almost perfect screw-boat conformation; the molecules are linked into cyclic centrosymmetric dimers by pairs of C—H···π(pyridyl) hydrogen bonds.

Related literature

In the 8-methyl analogue (II) (Portilla *et al.*, 2005) the molecules are linked into sheets by a combination of C—H···π(arene) and C—H···π(pyridyl) hydrogen bonds, while in 3-*tert*-butyl-4-(4-nitrophenyl)-1-phenyl-1*H*-pyrazolo[3,4-*b*]-pyridine (Abonia *et al.*, 2005), the molecules are linked into chains of rings by a combination of C—H···O and C—H···π(arene) hydrogen bonds.

For related literature, see: Cremer & Pople (1975); Evans & Boeyens (1989); Quiroga *et al.* (2001).



Experimental

Crystal data

$C_{30}H_{27}N_3$
M_r = 429.55
Triclinic, $P\overline{1}$
a = 9.516 (2) Å
b = 10.406 (3) Å
c = 11.868 (5) Å
α = 99.52 (4)°
β = 100.42 (2)°
γ = 91.55 (4)°
V = 1137.9 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 120 (2) K
0.41 × 0.23 × 0.11 mm

Data collection

Bruker-Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.977, T_{max} = 0.992
28777 measured reflections
5226 independent reflections
2735 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.238
S = 1.03
5226 reflections
301 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected bond lengths (Å).

C6*A*—C7	1.399 (3)	N10—C10*A*	1.376 (3)
C7—C7*A*	1.415 (3)	C10*A*—N11	1.332 (3)
C7*A*—C8	1.446 (3)	N11—C11*A*	1.352 (3)
C8—N9	1.322 (3)	C11*A*—C6*A*	1.414 (3)
N9—N10	1.373 (3)	C7*A*—C10*A*	1.410 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C72—H72···*Cg*^{i}	0.95	2.70	3.607 (3)	159

Symmetry code: (i) $-x+1, -y+1, -z+1$. *Cg* is the centroid of the pyridyl ring

Data collection: *COLLECT* (Hooft, 1999); cell refinement: *DIRAX/LSQ* (Duisenberg *et al.*, 2000); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005) and *WinGX* (Farrugia, 1999); program(s) used to refine structure: *OSCAIL* (McArdle, 2003) and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2364).

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supplementary materials

Acta Cryst. (2007). E**63**, o2690-o2691 [**doi:10.1107/S1600536807017631**]

8-*tert*-Butyl-7,10-diphenyl-6,10-dihydro-5*H*-benzo[*h*]pyrazolo[3,4-*b*]quinoline

J. N. Low, J. Cobo, J. Portilla, J. Quiroga and C. Glidewell

Comment

Pyrazolo[3,4-b]quinolines are of interest as possible antiviral and antimalarial agents, and because of their other biological properties, such as parasiticidic, bactericidal, vasodilator, and enzyme-inhibitory activity (Quiroga *et al.*, 2001). Here we report the structure of the title compound (I) (Fig. 2) as a new example of this class of compound.

Within the molecule of (I), the bond distances show strong bond fixation within the pyrazolo ring, and electronic delocalisation in the aryl and pyridyl rings (Table 1). For the C4A/C5/C6/C6A/C11A/C11B the ring-puckering parameters (Cremer & Pople, 1975) are θ = 116.6 (5)° and φ = 269.7 (5)°, very close to the ideal values, θ = 112.5° and φ = (60k + 30)° (k = integer) for an idealised screw-boat conformation (Evans & Boeyens, 1989).

In the crystal structure, molecules of (I) are linked by paired C—H..π(pyridyl) hydrogen bonds (Table 2) to form cyclic centrosymmetric dimers, but there are no direction-specific interactions between adjacent dimers.

In the 8-methyl analogue (II) (Portilla *et al.*, 2005) the molecules are linked into sheets by a combination of C—H···π(arene) and C—H···π(pyridyl) hydrogen bonds, while in (III) (Abonia *et al.*, 2005), the molecules are linked into chains of rings by a combination of C—H···O and C—H···π(arene) hydrogen bonds.

Experimental

A mixture of 5-amino-3-tert-butyl-1-phenylpyrazole (1 mmol) and 2-benzylidene-1-tetralone (1 mmol) was thoroughly mixed at room temperature. The mixture was heated in an oil-bath at 423 K for 3.5 min. It was then cooled to ambient temperature and permitted to solidify. The resulting solid was extracted with ethanol; the solvent was removed from the extract under reduced pressure and the product was recrystallised from ethanol/dimethylformamide (X:Y, v/v), to afford yellow crystals of the title compound (I) which were suitable for single-crystal X-ray diffraction. Yield 70%, m .p. 499-451 K;. MS (70 eV) m/z (%) 429 (56, M^+), 414 (100), 387 (16), 77 (20), 41 (18).

Refinement

All H atoms were located in difference maps and then treated as riding atoms in idealised positions with C—H distances 0.95 Å (aromatic), 0.98 Å (CH_3) or 0.99 Å (CH_2), and with $U_{iso}(H) = kU_{eq}(C)$, where k = 1.5 for the methyl groups and 1.2 for all other H atoms.

Figures

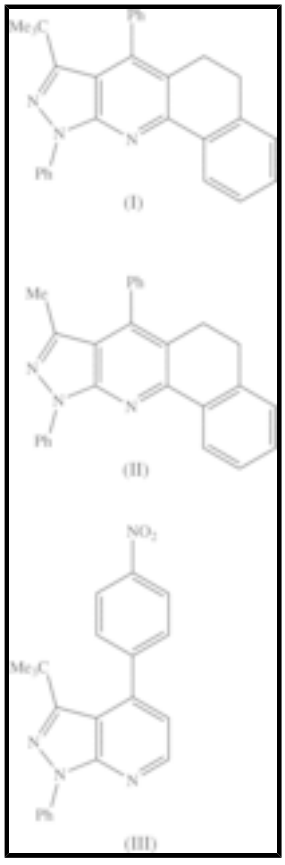


Fig. 1. Compounds (I), (II) and (III).

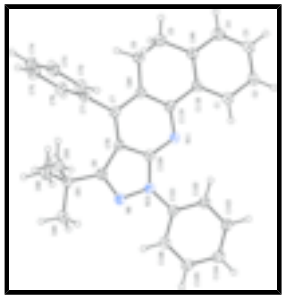


Fig. 2. The molecular structure of compound (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

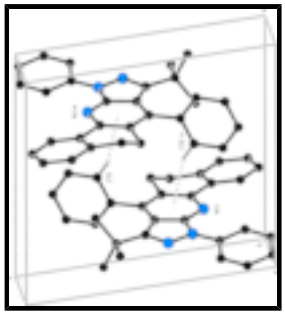


Fig. 3. Part of the crystal structure of compound (I) showing the formation of a centrosymmetric hydrogen-bonded dimer.. For the sake of clarity the H atoms not involved in the motif shown have been omitted. The atoms marked with an asterisk (*) are at the symmetry position (1 - x, 1 - y, 1 - z).

8-tert-Butyl-7,10-diphenyl-6,10-dihydro-5*H*-benzo[h]pyrazolo[3,4-b]quinoline

Crystal data

$C_{30}H_{27}N_3$	$Z = 2$
$M_r = 429.55$	$F_{000} = 456$
Triclinic, $P\overline{1}$	$D_x = 1.254$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.516$ (2) Å	Cell parameters from 5226 reflections
$b = 10.406$ (3) Å	$\theta = 3.1$–27.5º
$c = 11.868$ (5) Å	$\mu = 0.07$ mm^{-1}
$\alpha = 99.52$ (4)º	$T = 120$ (2) K
$\beta = 100.42$ (2)º	Plate, colourless
$\gamma = 91.55$ (4)º	0.41 × 0.23 × 0.11 mm
$V = 1137.9$ (7) Å^3	

Data collection

Bruker-Nonius KappaCCD diffractometer	5226 independent reflections
Radiation source: Bruker–Nonius FR591 rotating anode	2735 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.061$
Detector resolution: 9.091 pixels mm^{-1}	$\theta_{max} = 27.5$º
$T = 120(2)$ K	$\theta_{min} = 3.1$º
φ and ω scans	$h = -12 \rightarrow 12$
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	$k = -13 \rightarrow 13$
$T_{min} = 0.977$, $T_{max} = 0.992$	$l = -15 \rightarrow 15$
28777 measured reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.1424P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.071$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.238$	$\Delta\rho_{max} = 0.37$ e Å^{-3}
$S = 1.03$	$\Delta\rho_{min} = -0.31$ e Å^{-3}
5226 reflections	Extinction correction: none
301 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	

Hydrogen site location: inferred from neighbouring sites

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.1837 (3)	0.3064 (3)	0.1069 (2)	0.0396 (6)
C2	0.0673 (3)	0.3333 (3)	0.0288 (2)	0.0444 (7)
C3	−0.0594 (3)	0.3643 (3)	0.0658 (2)	0.0425 (7)
C4	−0.0684 (3)	0.3690 (3)	0.1804 (2)	0.0423 (7)
C4A	0.0477 (3)	0.3419 (2)	0.2610 (2)	0.0362 (6)
C5	0.0376 (3)	0.3404 (3)	0.3840 (2)	0.0501 (7)
C6	0.1720 (3)	0.3745 (3)	0.4663 (2)	0.0466 (7)
C6A	0.2988 (3)	0.3109 (2)	0.42886 (19)	0.0328 (6)
C7	0.4173 (3)	0.2866 (2)	0.50956 (19)	0.0319 (6)
C71	0.4101 (3)	0.3216 (2)	0.6355 (2)	0.0336 (6)
C72	0.4450 (3)	0.4504 (2)	0.6922 (2)	0.0393 (6)
C73	0.4334 (3)	0.4871 (3)	0.8068 (2)	0.0426 (7)
C74	0.3865 (3)	0.3981 (3)	0.8668 (2)	0.0433 (7)
C75	0.3494 (3)	0.2704 (3)	0.8119 (2)	0.0464 (7)
C76	0.3612 (3)	0.2329 (3)	0.6964 (2)	0.0387 (6)
C7A	0.5359 (3)	0.2327 (2)	0.46623 (19)	0.0321 (6)
C8	0.6766 (3)	0.1911 (2)	0.5083 (2)	0.0336 (6)
C81	0.7608 (3)	0.1828 (3)	0.6284 (2)	0.0372 (6)
C82	0.6882 (3)	0.0770 (3)	0.6768 (2)	0.0585 (8)
C83	0.7713 (4)	0.3126 (3)	0.7121 (3)	0.0682 (10)
C84	0.9126 (3)	0.1438 (4)	0.6198 (2)	0.0644 (9)
N9	0.7386 (2)	0.1471 (2)	0.41949 (16)	0.0354 (5)
N10	0.6469 (2)	0.15871 (19)	0.31858 (16)	0.0326 (5)
C101	0.6912 (3)	0.1158 (2)	0.21105 (19)	0.0323 (6)
C102	0.6118 (3)	0.1379 (2)	0.1067 (2)	0.0377 (6)
C103	0.6587 (3)	0.0932 (3)	0.0044 (2)	0.0416 (7)
C104	0.7829 (3)	0.0277 (3)	0.0042 (2)	0.0411 (7)
C105	0.8610 (3)	0.0077 (3)	0.1081 (2)	0.0422 (7)
C106	0.8164 (3)	0.0519 (2)	0.2120 (2)	0.0379 (6)
C10A	0.5221 (3)	0.2093 (2)	0.34415 (19)	0.0307 (6)
N11	0.4113 (2)	0.23114 (18)	0.26481 (15)	0.0312 (5)
C11A	0.2992 (3)	0.2826 (2)	0.30822 (19)	0.0310 (6)
C11B	0.1760 (2)	0.3099 (2)	0.22402 (19)	0.0319 (6)
H1	0.2704	0.2851	0.0809	0.048*
H2	0.0739	0.3305	−0.0504	0.053*
H3	−0.1399	0.3824	0.0119	0.051*
H4	−0.1555	0.3912	0.2052	0.051*
H5A	−0.0339	0.4024	0.4060	0.060*
H5B	0.0020	0.2522	0.3905	0.060*
H6A	0.1611	0.3500	0.5415	0.056*
H6B	0.1908	0.4703	0.4794	0.056*
H72	0.4770	0.5131	0.6512	0.047*
H73	0.4582	0.5747	0.8446	0.051*

H74	0.3792	0.4239	0.9461	0.052*
H75	0.3161	0.2087	0.8532	0.056*
H76	0.3354	0.1454	0.6588	0.046*
H82A	0.6853	−0.0068	0.6243	0.088*
H82B	0.5905	0.0999	0.6833	0.088*
H82C	0.7424	0.0699	0.7538	0.088*
H83A	0.6752	0.3366	0.7230	0.102*
H83B	0.8161	0.3805	0.6798	0.102*
H83C	0.8294	0.3039	0.7873	0.102*
H84A	0.9598	0.2081	0.5851	0.097*
H84B	0.9085	0.0576	0.5709	0.097*
H84C	0.9667	0.1407	0.6977	0.097*
H102	0.5263	0.1830	0.1055	0.045*
H103	0.6044	0.1080	−0.0673	0.050*
H104	0.8136	−0.0031	−0.0667	0.049*
H105	0.9469	−0.0370	0.1090	0.051*
H106	0.8719	0.0381	0.2836	0.046*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0371 (15)	0.0450 (16)	0.0377 (14)	0.0060 (12)	0.0073 (12)	0.0092 (12)
C2	0.0479 (17)	0.0513 (17)	0.0344 (14)	0.0098 (13)	0.0033 (12)	0.0124 (12)
C3	0.0366 (15)	0.0459 (16)	0.0439 (16)	0.0065 (12)	0.0009 (12)	0.0108 (13)
C4	0.0361 (15)	0.0430 (16)	0.0454 (16)	0.0021 (12)	0.0047 (12)	0.0039 (12)
C4A	0.0343 (14)	0.0382 (14)	0.0368 (14)	0.0020 (11)	0.0079 (11)	0.0068 (11)
C5	0.0390 (16)	0.071 (2)	0.0409 (15)	0.0066 (14)	0.0102 (13)	0.0071 (14)
C6	0.0419 (16)	0.0659 (19)	0.0328 (14)	0.0127 (14)	0.0093 (12)	0.0067 (13)
C6A	0.0341 (14)	0.0350 (14)	0.0308 (13)	0.0050 (11)	0.0103 (11)	0.0055 (10)
C7	0.0343 (14)	0.0318 (13)	0.0306 (13)	−0.0006 (11)	0.0094 (11)	0.0047 (10)
C71	0.0318 (14)	0.0402 (15)	0.0293 (13)	0.0036 (11)	0.0056 (10)	0.0069 (11)
C72	0.0428 (16)	0.0407 (15)	0.0343 (14)	−0.0009 (12)	0.0074 (12)	0.0067 (12)
C73	0.0457 (16)	0.0451 (16)	0.0334 (14)	−0.0008 (13)	0.0040 (12)	0.0005 (12)
C74	0.0433 (16)	0.0543 (18)	0.0307 (13)	0.0014 (13)	0.0064 (12)	0.0035 (13)
C75	0.0506 (17)	0.0535 (18)	0.0381 (15)	−0.0047 (14)	0.0134 (13)	0.0121 (13)
C76	0.0432 (15)	0.0385 (15)	0.0352 (14)	−0.0029 (12)	0.0120 (12)	0.0044 (11)
C7A	0.0356 (14)	0.0352 (14)	0.0272 (12)	0.0023 (11)	0.0085 (10)	0.0078 (10)
C8	0.0327 (13)	0.0355 (14)	0.0336 (13)	0.0014 (11)	0.0051 (11)	0.0106 (11)
C81	0.0362 (14)	0.0455 (15)	0.0311 (13)	0.0060 (12)	0.0044 (11)	0.0122 (11)
C82	0.065 (2)	0.072 (2)	0.0438 (17)	0.0035 (17)	0.0081 (15)	0.0286 (15)
C83	0.074 (2)	0.0517 (19)	0.0589 (19)	0.0055 (16)	−0.0272 (17)	−0.0052 (15)
C84	0.0457 (18)	0.110 (3)	0.0404 (16)	0.0251 (18)	0.0025 (14)	0.0251 (17)
N9	0.0345 (12)	0.0423 (12)	0.0298 (11)	0.0028 (9)	0.0043 (9)	0.0091 (9)
N10	0.0298 (11)	0.0410 (12)	0.0280 (11)	0.0047 (9)	0.0062 (9)	0.0072 (9)
C101	0.0318 (14)	0.0367 (14)	0.0291 (13)	0.0002 (11)	0.0089 (10)	0.0042 (10)
C102	0.0341 (14)	0.0458 (15)	0.0323 (13)	0.0034 (12)	0.0057 (11)	0.0048 (11)
C103	0.0419 (16)	0.0562 (17)	0.0272 (13)	0.0009 (13)	0.0071 (11)	0.0081 (12)
C104	0.0418 (16)	0.0478 (16)	0.0353 (14)	0.0024 (13)	0.0137 (12)	0.0048 (12)

C105	0.0402 (15)	0.0475 (16)	0.0436 (15)	0.0100 (12)	0.0178 (13)	0.0097 (12)
C106	0.0363 (15)	0.0447 (16)	0.0346 (13)	0.0072 (12)	0.0069 (11)	0.0111 (11)
C10A	0.0317 (13)	0.0287 (13)	0.0315 (13)	0.0003 (10)	0.0062 (11)	0.0051 (10)
N11	0.0308 (11)	0.0341 (11)	0.0289 (10)	0.0041 (9)	0.0052 (9)	0.0061 (9)
C11A	0.0330 (14)	0.0299 (13)	0.0312 (13)	−0.0008 (11)	0.0085 (11)	0.0058 (10)
C11B	0.0313 (14)	0.0332 (13)	0.0300 (13)	0.0003 (11)	0.0016 (10)	0.0069 (10)

Geometric parameters (Å, °)

C1—C2	1.376 (4)	C8—C81	1.521 (3)
C1—C11B	1.400 (3)	C81—C82	1.526 (4)
C1—H1	0.95	C81—C84	1.527 (4)
C2—C3	1.384 (4)	C81—C83	1.528 (4)
C2—H2	0.95	C82—H82A	0.98
C3—C4	1.370 (4)	C82—H82B	0.98
C3—H3	0.95	C82—H82C	0.98
C4—C4A	1.393 (4)	C83—H83A	0.98
C4—H4	0.95	C83—H83B	0.98
C4A—C11B	1.401 (3)	C83—H83C	0.98
C4A—C5	1.482 (4)	C84—H84A	0.98
C5—C6	1.458 (4)	C84—H84B	0.98
C5—H5A	0.99	C84—H84C	0.98
C5—H5B	0.99	N9—N10	1.373 (3)
C6—C6A	1.494 (3)	N10—C10A	1.376 (3)
C6—H6A	0.99	N10—C101	1.422 (3)
C6—H6B	0.99	C101—C106	1.380 (3)
C6A—C7	1.399 (3)	C101—C102	1.386 (3)
C7—C7A	1.415 (3)	C102—C103	1.382 (3)
C7—C71	1.493 (3)	C102—H102	0.95
C71—C76	1.382 (3)	C103—C104	1.381 (4)
C71—C72	1.399 (3)	C103—H103	0.95
C72—C73	1.377 (3)	C104—C105	1.370 (4)
C72—H72	0.95	C104—H104	0.95
C73—C74	1.369 (4)	C105—C106	1.388 (3)
C73—H73	0.95	C105—H105	0.95
C74—C75	1.386 (4)	C106—H106	0.95
C74—H74	0.95	C10A—N11	1.332 (3)
C75—C76	1.387 (3)	N11—C11A	1.352 (3)
C75—H75	0.95	C11A—C6A	1.414 (3)
C76—H76	0.95	C7A—C10A	1.410 (3)
C7A—C8	1.446 (3)	C11A—C11B	1.464 (3)
C8—N9	1.322 (3)		
C2—C1—C11B	120.8 (2)	C8—C81—C82	108.7 (2)
C2—C1—H1	119.6	C8—C81—C84	110.0 (2)
C11B—C1—H1	119.6	C82—C81—C84	107.9 (2)
C1—C2—C3	120.0 (2)	C8—C81—C83	112.2 (2)
C1—C2—H2	120.0	C82—C81—C83	109.8 (2)
C3—C2—H2	120.0	C84—C81—C83	108.1 (2)
C4—C3—C2	119.9 (2)	C81—C82—H82A	109.5

C4—C3—H3	120.0	C81—C82—H82B	109.5
C2—C3—H3	120.0	H82A—C82—H82B	109.5
C3—C4—C4A	121.2 (2)	C81—C82—H82C	109.5
C3—C4—H4	119.4	H82A—C82—H82C	109.5
C4A—C4—H4	119.4	H82B—C82—H82C	109.5
C4—C4A—C11B	119.2 (2)	C81—C83—H83A	109.5
C4—C4A—C5	121.8 (2)	C81—C83—H83B	109.5
C11B—C4A—C5	119.0 (2)	H83A—C83—H83B	109.5
C6—C5—C4A	114.5 (2)	C81—C83—H83C	109.5
C6—C5—H5A	108.6	H83A—C83—H83C	109.5
C4A—C5—H5A	108.6	H83B—C83—H83C	109.5
C6—C5—H5B	108.6	C81—C84—H84A	109.5
C4A—C5—H5B	108.6	C81—C84—H84B	109.5
H5A—C5—H5B	107.6	H84A—C84—H84B	109.5
C5—C6—C6A	114.7 (2)	C81—C84—H84C	109.5
C5—C6—H6A	108.6	H84A—C84—H84C	109.5
C6A—C6—H6A	108.6	H84B—C84—H84C	109.5
C5—C6—H6B	108.6	C8—N9—N10	108.3 (2)
C6A—C6—H6B	108.6	N9—N10—C10A	109.87 (18)
H6A—C6—H6B	107.6	N9—N10—C101	118.18 (19)
C7—C6A—C11A	120.5 (2)	C10A—N10—C101	131.9 (2)
C7—C6A—C6	121.7 (2)	C106—C101—C102	120.0 (2)
C11A—C6A—C6	117.7 (2)	C106—C101—N10	118.6 (2)
C6A—C7—C7A	117.8 (2)	C102—C101—N10	121.3 (2)
C6A—C7—C71	117.4 (2)	C103—C102—C101	119.1 (2)
C7A—C7—C71	124.7 (2)	C103—C102—H102	120.4
C76—C71—C72	118.6 (2)	C101—C102—H102	120.4
C76—C71—C7	122.2 (2)	C104—C103—C102	121.3 (2)
C72—C71—C7	119.1 (2)	C104—C103—H103	119.3
C73—C72—C71	120.5 (2)	C102—C103—H103	119.3
C73—C72—H72	119.7	C105—C104—C103	118.9 (2)
C71—C72—H72	119.7	C105—C104—H104	120.5
C74—C73—C72	120.4 (3)	C103—C104—H104	120.5
C74—C73—H73	119.8	C104—C105—C106	120.8 (2)
C72—C73—H73	119.8	C104—C105—H105	119.6
C73—C74—C75	120.0 (2)	C106—C105—H105	119.6
C73—C74—H74	120.0	C101—C106—C105	119.7 (2)
C75—C74—H74	120.0	C101—C106—H106	120.1
C74—C75—C76	119.8 (2)	C105—C106—H106	120.1
C74—C75—H75	120.1	N11—C10A—N10	124.4 (2)
C76—C75—H75	120.1	N11—C10A—C7A	128.1 (2)
C71—C76—C75	120.7 (2)	N10—C10A—C7A	107.5 (2)
C71—C76—H76	119.7	C10A—N11—C11A	115.07 (19)
C75—C76—H76	119.7	N11—C11A—C6A	122.7 (2)
C10A—C7A—C7	115.7 (2)	N11—C11A—C11B	116.8 (2)
C10A—C7A—C8	104.4 (2)	C6A—C11A—C11B	120.4 (2)
C7—C7A—C8	139.8 (2)	C1—C11B—C4A	118.9 (2)
N9—C8—C7A	109.9 (2)	C1—C11B—C11A	121.4 (2)
N9—C8—C81	116.1 (2)	C4A—C11B—C11A	119.6 (2)

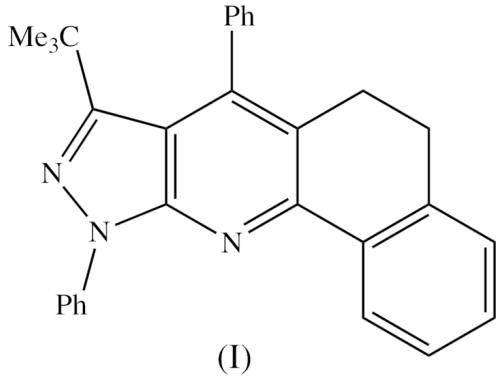
C7A—C8—C81	133.9 (2)		
C11B—C1—C2—C3	0.0 (4)	C81—C8—N9—N10	178.42 (19)
C1—C2—C3—C4	0.4 (4)	C8—N9—N10—C10A	−1.2 (3)
C2—C3—C4—C4A	−0.6 (4)	C8—N9—N10—C101	−179.43 (19)
C3—C4—C4A—C11B	0.3 (4)	N9—N10—C101—C106	6.9 (3)
C3—C4—C4A—C5	−177.1 (2)	C10A—N10—C101—C106	−170.9 (2)
C4—C4A—C5—C6	−151.3 (3)	N9—N10—C101—C102	−172.6 (2)
C11B—C4A—C5—C6	31.3 (4)	C10A—N10—C101—C102	9.5 (4)
C4A—C5—C6—C6A	−44.5 (4)	C106—C101—C102—C103	1.0 (4)
C5—C6—C6A—C7	−152.8 (2)	N10—C101—C102—C103	−179.4 (2)
C5—C6—C6A—C11A	30.8 (4)	C101—C102—C103—C104	−0.2 (4)
C11A—C6A—C7—C7A	−0.3 (3)	C102—C103—C104—C105	−0.4 (4)
C6—C6A—C7—C7A	−176.6 (2)	C103—C104—C105—C106	0.3 (4)
C11A—C6A—C7—C71	178.8 (2)	C102—C101—C106—C105	−1.2 (4)
C6—C6A—C7—C71	2.5 (4)	N10—C101—C106—C105	179.2 (2)
C6A—C7—C71—C76	92.4 (3)	C104—C105—C106—C101	0.5 (4)
C7A—C7—C71—C76	−88.6 (3)	N9—N10—C10A—N11	−179.3 (2)
C6A—C7—C71—C72	−83.3 (3)	C101—N10—C10A—N11	−1.4 (4)
C7A—C7—C71—C72	95.7 (3)	N9—N10—C10A—C7A	0.9 (3)
C76—C71—C72—C73	1.3 (4)	C101—N10—C10A—C7A	178.9 (2)
C7—C71—C72—C73	177.1 (2)	C7—C7A—C10A—N11	−0.3 (4)
C71—C72—C73—C74	−0.5 (4)	C8—C7A—C10A—N11	179.9 (2)
C72—C73—C74—C75	−0.4 (4)	C7—C7A—C10A—N10	179.4 (2)
C73—C74—C75—C76	0.5 (4)	C8—C7A—C10A—N10	−0.4 (2)
C72—C71—C76—C75	−1.1 (4)	N10—C10A—N11—C11A	−179.4 (2)
C7—C71—C76—C75	−176.9 (2)	C7A—C10A—N11—C11A	0.3 (3)
C74—C75—C76—C71	0.3 (4)	C10A—N11—C11A—C6A	−0.3 (3)
C6A—C7—C7A—C10A	0.3 (3)	C10A—N11—C11A—C11B	179.1 (2)
C71—C7—C7A—C10A	−178.7 (2)	C7—C6A—C11A—N11	0.3 (4)
C6A—C7—C7A—C8	179.9 (3)	C6—C6A—C11A—N11	176.7 (2)
C71—C7—C7A—C8	0.9 (5)	C7—C6A—C11A—C11B	−179.1 (2)
C10A—C7A—C8—N9	−0.3 (3)	C6—C6A—C11A—C11B	−2.7 (3)
C7—C7A—C8—N9	−180.0 (3)	C2—C1—C11B—C4A	−0.3 (4)
C10A—C7A—C8—C81	−177.2 (3)	C2—C1—C11B—C11A	−179.5 (2)
C7—C7A—C8—C81	3.1 (5)	C4—C4A—C11B—C1	0.1 (4)
N9—C8—C81—C82	−108.9 (3)	C5—C4A—C11B—C1	177.6 (2)
C7A—C8—C81—C82	67.9 (3)	C4—C4A—C11B—C11A	179.3 (2)
N9—C8—C81—C84	9.1 (3)	C5—C4A—C11B—C11A	−3.2 (4)
C7A—C8—C81—C84	−174.1 (3)	N11—C11A—C11B—C1	−11.7 (3)
N9—C8—C81—C83	129.5 (3)	C6A—C11A—C11B—C1	167.7 (2)
C7A—C8—C81—C83	−53.8 (4)	N11—C11A—C11B—C4A	169.1 (2)
C7A—C8—N9—N10	0.9 (3)	C6A—C11A—C11B—C4A	−11.5 (3)

Hydrogen-bond geometry (Å, °)

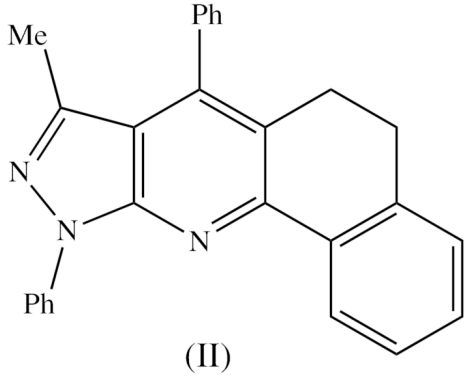
D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C72—H72···Cg^{i}	0.95	2.70	3.607 (3)	159

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

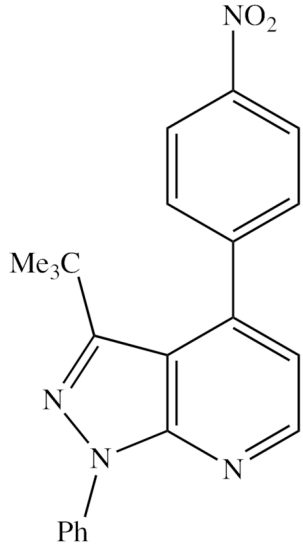
Fig. 1



(I)



(II)



(III)

Fig. 2

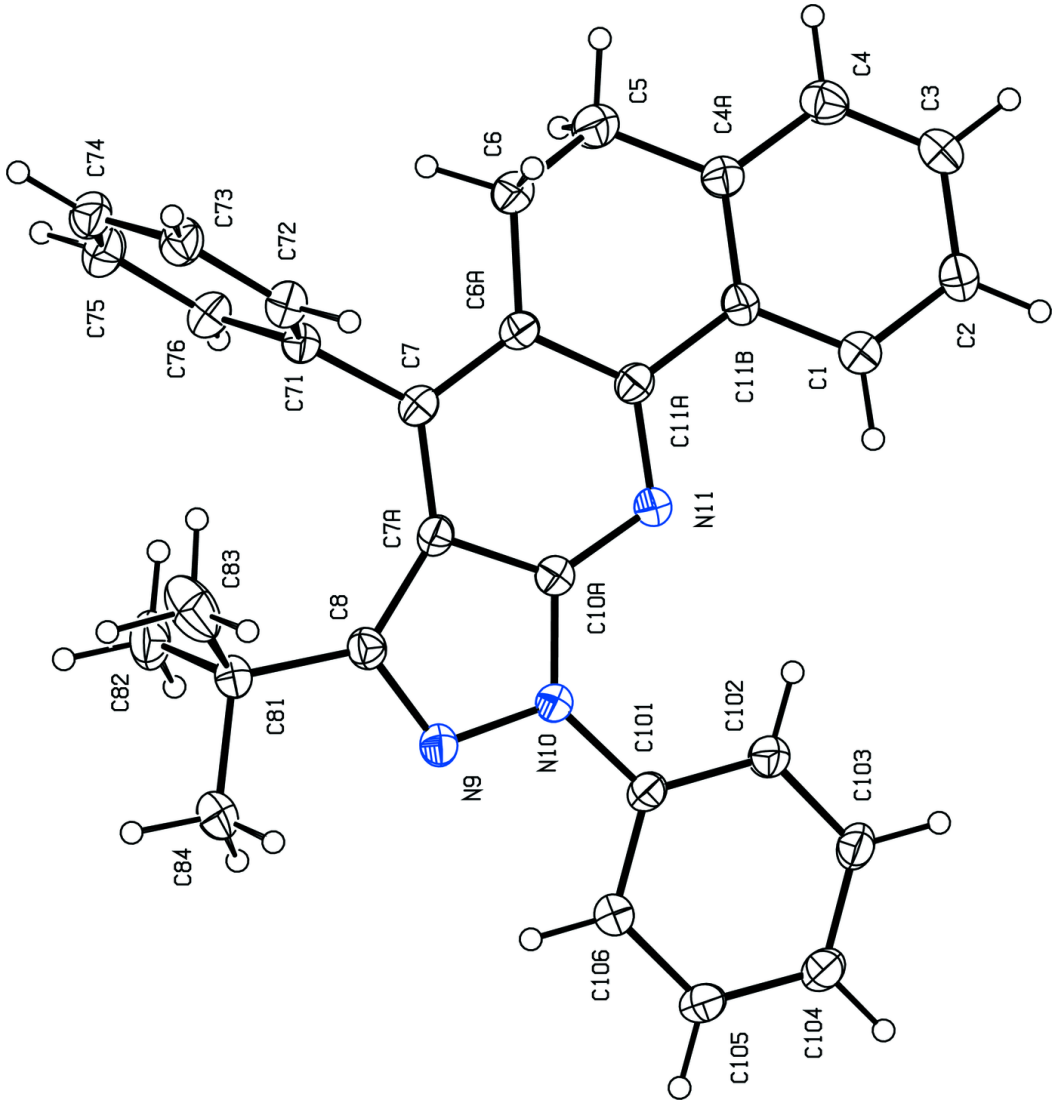

C74
C73
C72
C75
C76
C71
C6
C5
C4A
C4
C3
C6A
C7
C11A
C11B
C1
C2
N11
C7A
C10A
C83
C8
C82
C81
N9
N10
C101
C102
C103
C84
C106
C105
C104

Fig. 3