Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

9-Methyl-2,6-di-*p*-tolyl-2,3,6,7-tetrahydro-1*H*,5*H*-pyrimido[5,6,1-*ij*]quinazoline

Andrew B. Mahon,[a] Donald C. Craig[b] and Andrew C. Try[a]*

[a]Department of Chemistry and Biomolecular Sciences, Building F7B, Macquarie University, Sydney, NSW 2109, Australia, and [b]School of Chemistry, University of New South Wales, Sydney, NSW 2052, Australia
Correspondence e-mail: andrew.try@mq.edu.au

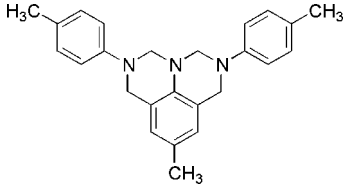
Received 24 September 2007; accepted 8 October 2007

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.006 Å; R factor = 0.058; wR factor = 0.065; data-to-parameter ratio = 8.4.

The title compound, $C_{25}H_{27}N_3$, possesses an essentially planar, fused tricyclic platform, from which two *p*-tolyl rings project on the same face to create a hydrophobic pocket.

Related literature

For related literature, see: Becker *et al.* (1993); Bhuiyan *et al.* (2007); Eisner & Wagner (1934); Farrar (1964); Johnson *et al.* (1993); Maffei (1928, 1929); Smith & Schubert (1948); Walther & Bamberg (1906); Ibers & Hamilton (1974); Wagner & Eisner (1937).



Experimental

Crystal data

$C_{25}H_{27}N_3$
M_r = 369.5
Monoclinic, $P2_1/c$
a = 9.035 (3) Å
b = 20.805 (7) Å
c = 11.790 (3) Å
β = 110.95 (1)°
V = 2070 (1) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 294 K
0.30 × 0.08 × 0.05 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
3813 measured reflections
3628 independent reflections
2127 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
1 standard reflection
frequency: 30 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.065
S = 1.85
2127 reflections
254 parameters
H-atom parameters not refined
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

Data collection: *CAD-4* (Schagen *et al.*, 1989); cell refinement: *CAD-4*; data reduction: local program; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *RAELS* (Rae, 1996); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: local programs.

The authors thank the Australian Research Council for a Discovery Project grant to ACT (DP0345180), and Macquarie University for the award of a Macquarie University Research Development Grant to ACT and the award of a PhD scholarship to ABM.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2304).

References

Altomare, A., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435–436.
Becker, D. P., Finnegan, P. M. & Collins, P. W. (1993). *Tetrahedron Lett.* **34**, 1889–1892.
Bhuiyan, M. D. H., Clegg, J. K. & Try, A. C. (2007). *Acta Cryst.* E**63**, o308–o310.
Eisner, A. & Wagner, E. C. (1934). *J. Am. Chem. Soc.* **56**, 1938–1943.
Farrar, W. V. (1964). *J. Appl. Chem.* **14**, 389–399.
Ibers, J. A. & Hamilton, W. C. (1974). *International Tables for X-Ray Crystallography*, Vol. 4. Birmingham: Kynoch Press. (Present distributor Kluwer Academic Publishers, Dordrecht.)
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Oak Ridge, Tennessee.
Johnson, R. A., Gorman, R. R., Wnuk, R. J., Crittenden, N. J. & Aiken, J. W. (1993). *J. Med. Chem.* **36**, 3202–3206.
Maffei, G. (1928). *Gazz. Chim. Ital.* **58**, 261–269.
Maffei, G. (1929). *Gazz. Chim. Ital.* **59**, 3–9.
Rae, A. D. (1996). *RAELS*. University of New South Wales, Australia.
Schagen, J. D., Straver, L., van Meurs, F. & Williams, G. (1989). *CAD4*. Version 5.0. Delft Instruments X-ray Diffraction, The Netherlands..
Smith, L. I. & Schubert, W. M. (1948). *J. Am. Chem. Soc.* **70**, 2656–2661.
Wagner, E. C. & Eisner, A. (1937). *J. Am. Chem. Soc.* **59**, 879–883.
Walther, R. von & Bamberg, R. (1906). *J. Prakt. Chem.* **73**, 209–228.

 doi:10.1107/S1600536807049173

supplementary materials

Acta Cryst. (2007). E**63**, o4311 [**doi:10.1107/S1600536807049173**]

9-Methyl-2,6-di-*p*-tolyl-2,3,6,7-tetrahydro-1*H*,5*H*-pyrimido[5,6,1-*ij*]quinazoline

A. B. Mahon, D. C. Craig and A. C. Try

Comment

Compound (I) was first reported as one of several products formed in the reaction of *p*-toluidine with aqueous formaldehyde solution in hydrochloric acid, in approximately 3% yield (Farrar, 1964). An analogous compound, with methoxy groups in place of the methyl groups, was proposed when *p*-anisidine was used instead of *p*-toluidine. Compound (I) was also obtained 26% yield from a 1:1 reaction of hexamethylene tetraamine and *p*-toluidine in trifluoroacetic acid (Johnson *et al.*, 1993). These compounds are related to 3-phenyl-3,4-dihydroquinazolines that have been isolated as impurities in the synthesis of numerous Tröger's base analogues (von Walther & Bamberg, 1906; Eisner & Wagner, 1934; Maffei, 1928; Maffei, 1929; Wagner & Eisner, 1937; Smith, 1948; Becker *et al.*, 1993; Bhuiyan *et al.*, 2007).

The *x*-ray crystal structure reported here (Fig. 1) confirms the earlier stuctural assignments that have been proposed for compound (I). The tetrasubstituted aromatic ring forms the base of a cavity, with the 'walls' provided by the two *p*-di-substituted benzene rings.

Experimental

The title compound (I) was isolated as a minor impurity in the synthesis of Tröger's base, using *p*-toluidine and paraformaldehyde in trifluoroacetic acid (TFA). *p*-Toluidine (30 g, 280 mmol) and *p*-formaldehyde (13.5 g,489 mmol) were dissolved in trifluoroacetic acid (300 ml) and stirred in the dark under an atmosphere of argon for 3 days before pouring the red reaction mixture over ice (200 g) and basifying the mixture with 26% ammonia solution (300 ml). The resultant yellow mixture was extracted with dichloromethane (3 *x* 80 ml) and the organic layers were combined before washing with saturated sodium carbonate solution (2 *x* 100 ml), brine (100 ml) and then drying over anhydrous sodium sulfate. The solvent was removed under reduced pressure and the crude material was purified by column chromatography (silica gel, dichloromethane) to afford (I) as a white solid (1.55 g, 5%). Crystals of (I) were produced by slow evaporation of a methanol solution.

Refinement

Refinement on F was by full-matrix least squares (RAELS) using anisotropic thermal parameters for non-hydrogen atoms. Hydrogen atoms were included in geometrically idealized positions calculated each cycle, with C—H distances of 1.00 Å, and were assigned thermal parameters equal to those of the parent atom.

Figures

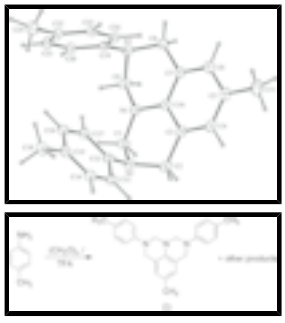


Figure 1. *ORTEPII* (Johnson, 1976) plot of the title compound, with ellipsoids at the 10% probability level. H atoms are drawn as spheres of arbitrary radius.

9-Methyl-2,6-di-*p*-tolyl-2,3,6,7-tetrahydro-1*H*,5*H*- pyrimido[5,6,1-*ij*]quinazoline

Crystal data

$C_{25}H_{27}N_3$	$D_x = 1.19$ Mg m^{-3}
$M_r = 369.5$	Melting point: 421 K
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.035$ (3) Å	Cell parameters from 11 reflections
$b = 20.805$ (7) Å	$\theta = 10$–11º
$c = 11.790$ (3) Å	$\mu = 0.07$ mm^{-1}
$\beta = 110.95$ (1)º	$T = 294$ K
$V = 2070$ (1) Å^3	Prism, colourless
$Z = 4$	0.30 × 0.08 × 0.05 mm
$F_{000} = 792.0$	

Data collection

Enraf–Nonius CAD-4 diffractometer	$\theta_{max} = 25$º
ω–2θ scans	$h = -10 \rightarrow 10$
Absorption correction: none	$k = 0 \rightarrow 24$
3813 measured reflections	$l = 0 \rightarrow 14$
3628 independent reflections	1 standard reflections
2127 reflections with $I > 2\sigma(I)$	every 30 min
$R_{int} = 0.023$	intensity decay: none

Refinement

Refinement on F	H-atom parameters not refined
$R[F^2 > 2\sigma(F^2)] = 0.058$	$w = 1/[\sigma^2(F) + 0.0004F^2]$
$wR(F^2) = 0.065$	$(\Delta/\sigma)_{max} = 0.002$
$S = 1.85$	$\Delta\rho_{max} = 0.33$ e Å^{-3}
2127 reflections	$\Delta\rho_{min} = -0.34$ e Å^{-3}
254 parameters	Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.1834 (3)	0.2545 (1)	0.5530 (2)	0.0630 (8)
N2	−0.0410 (3)	0.2116 (2)	0.3932 (2)	0.0674 (8)
N3	0.4565 (3)	0.2671 (1)	0.6746 (2)	0.0629 (8)
C1	0.0391 (4)	0.2186 (2)	0.5239 (3)	0.072 (1)
C2	−0.0829 (4)	0.2753 (2)	0.3394 (3)	0.075 (1)
C3	0.0602 (4)	0.3184 (2)	0.3720 (3)	0.0606 (9)
C4	0.0696 (5)	0.3696 (2)	0.2992 (3)	0.072 (1)
C5	0.2015 (6)	0.4082 (2)	0.3281 (3)	0.078 (1)
C6	0.3297 (5)	0.3954 (2)	0.4353 (4)	0.075 (1)
C7	0.3221 (4)	0.3454 (2)	0.5114 (3)	0.0623 (9)
C8	0.4565 (4)	0.3331 (2)	0.6317 (3)	0.072 (1)
C9	0.2996 (4)	0.2530 (2)	0.6763 (3)	0.070 (1)
C10	0.1887 (4)	0.3065 (2)	0.4799 (3)	0.0572 (8)
C11	0.2124 (6)	0.4629 (2)	0.2461 (4)	0.118 (2)
C12	0.0224 (4)	0.1667 (2)	0.3334 (3)	0.0596 (9)
C13	−0.0610 (4)	0.1534 (2)	0.2092 (3)	0.074 (1)
C14	−0.0068 (5)	0.1074 (2)	0.1496 (3)	0.076 (1)
C15	0.1288 (5)	0.0722 (2)	0.2063 (3)	0.070 (1)
C16	0.2110 (4)	0.0861 (2)	0.3282 (3)	0.071 (1)
C17	0.1597 (4)	0.1323 (2)	0.3897 (3)	0.0645 (9)
C18	0.1839 (5)	0.0208 (2)	0.1407 (3)	0.092 (1)
C19	0.5173 (3)	0.2185 (2)	0.6180 (3)	0.0554 (8)
C20	0.5351 (4)	0.1567 (2)	0.6634 (3)	0.0643 (9)
C21	0.5978 (4)	0.1086 (2)	0.6143 (3)	0.071 (1)
C22	0.6484 (4)	0.1206 (2)	0.5163 (3)	0.0671 (9)
C23	0.6312 (4)	0.1823 (2)	0.4732 (3)	0.0620 (9)
C24	0.5658 (4)	0.2311 (2)	0.5200 (3)	0.0573 (9)
C25	0.7166 (5)	0.0679 (2)	0.4629 (4)	0.099 (1)
H1C1	−0.0330	0.2414	0.5580	0.072
H2C1	0.0644	0.1749	0.5613	0.072
H1C2	−0.1625	0.2951	0.3698	0.075
H2C2	−0.1300	0.2709	0.2490	0.075
HC4	−0.0227	0.3787	0.2233	0.072
HC6	0.4274	0.4225	0.4573	0.075
H1C8	0.4449	0.3632	0.6941	0.072
H2C8	0.5596	0.3414	0.6208	0.072
H1C9	0.2709	0.2859	0.7268	0.070
H2C9	0.2999	0.2094	0.7119	0.070
H1C11	0.2273	0.5044	0.2916	0.118
H2C11	0.3044	0.4555	0.2196	0.118
H3C11	0.1125	0.4648	0.1732	0.118
HC13	−0.1603	0.1777	0.1642	0.074
HC14	−0.0683	0.0992	0.0618	0.076
HC16	0.3104	0.0618	0.3727	0.071
HC17	0.2234	0.1410	0.4771	0.064

H1C18	0.1362	−0.0214	0.1499	0.092
H2C18	0.1500	0.0319	0.0526	0.092
H3C18	0.3021	0.0176	0.1760	0.092
HC20	0.5017	0.1466	0.7337	0.064
HC21	0.6077	0.0642	0.6488	0.071
HC23	0.6676	0.1927	0.4046	0.062
HC24	0.5533	0.2752	0.4839	0.057
H1C25	0.7710	0.0358	0.5275	0.099
H2C25	0.6295	0.0463	0.3960	0.099
H3C25	0.7948	0.0866	0.4298	0.099

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.060 (2)	0.093 (2)	0.037 (2)	−0.004 (2)	0.018 (1)	0.007 (1)
N2	0.060 (2)	0.103 (2)	0.044 (2)	−0.001 (2)	0.023 (1)	0.005 (2)
N3	0.065 (2)	0.080 (2)	0.044 (2)	0.002 (2)	0.019 (1)	−0.010 (1)
C1	0.066 (2)	0.114 (3)	0.045 (2)	−0.011 (2)	0.032 (2)	−0.002 (2)
C2	0.063 (2)	0.111 (3)	0.053 (2)	0.014 (2)	0.024 (2)	0.002 (2)
C3	0.062 (2)	0.084 (3)	0.042 (2)	0.012 (2)	0.027 (2)	−0.001 (2)
C4	0.093 (3)	0.088 (3)	0.046 (2)	0.025 (2)	0.040 (2)	0.009 (2)
C5	0.110 (3)	0.076 (3)	0.069 (3)	0.021 (3)	0.059 (3)	0.011 (2)
C6	0.088 (3)	0.074 (3)	0.080 (3)	0.005 (2)	0.049 (2)	−0.001 (2)
C7	0.070 (2)	0.070 (2)	0.055 (2)	0.005 (2)	0.031 (2)	−0.004 (2)
C8	0.072 (3)	0.076 (3)	0.067 (2)	−0.001 (2)	0.022 (2)	−0.018 (2)
C9	0.067 (2)	0.110 (3)	0.036 (2)	0.007 (2)	0.022 (2)	−0.002 (2)
C10	0.062 (2)	0.075 (2)	0.044 (2)	0.008 (2)	0.030 (2)	0.002 (2)
C11	0.177 (5)	0.099 (3)	0.102 (3)	0.023 (3)	0.081 (3)	0.031 (3)
C12	0.052 (2)	0.086 (3)	0.045 (2)	−0.010 (2)	0.022 (2)	0.006 (2)
C13	0.062 (2)	0.106 (3)	0.046 (2)	−0.010 (2)	0.009 (2)	0.006 (2)
C14	0.086 (3)	0.097 (3)	0.042 (2)	−0.015 (2)	0.020 (2)	−0.003 (2)
C15	0.085 (3)	0.078 (3)	0.050 (2)	−0.014 (2)	0.028 (2)	0.002 (2)
C16	0.076 (3)	0.080 (3)	0.054 (2)	−0.009 (2)	0.020 (2)	0.001 (2)
C17	0.066 (2)	0.086 (3)	0.039 (2)	−0.005 (2)	0.015 (2)	0.005 (2)
C18	0.133 (4)	0.082 (3)	0.068 (2)	−0.008 (3)	0.045 (3)	−0.004 (2)
C19	0.049 (2)	0.077 (2)	0.037 (2)	0.001 (2)	0.011 (2)	−0.002 (2)
C20	0.071 (2)	0.079 (2)	0.045 (2)	0.002 (2)	0.023 (2)	0.006 (2)
C21	0.083 (3)	0.072 (3)	0.058 (2)	0.006 (2)	0.024 (2)	0.010 (2)
C22	0.067 (2)	0.077 (3)	0.057 (2)	0.003 (2)	0.022 (2)	−0.007 (2)
C23	0.060 (2)	0.081 (3)	0.047 (2)	−0.001 (2)	0.022 (2)	−0.003 (2)
C24	0.057 (2)	0.072 (2)	0.044 (2)	0.002 (2)	0.020 (2)	0.005 (2)
C25	0.119 (4)	0.096 (3)	0.094 (3)	0.017 (3)	0.051 (3)	−0.014 (2)

Geometric parameters (Å, °)

N1—C1	1.434 (4)	C11—H3C11	1.000
N1—C9	1.458 (4)	C12—C13	1.414 (4)
N1—C10	1.393 (4)	C12—C17	1.380 (4)
N2—C1	1.457 (4)	C13—C14	1.377 (5)

N2—C2	1.460 (4)	C13—HC13	1.000
N2—C12	1.409 (4)	C14—C15	1.378 (5)
N3—C8	1.463 (4)	C14—HC14	1.000
N3—C9	1.455 (4)	C15—C16	1.392 (4)
N3—C19	1.425 (4)	C15—C18	1.505 (5)
C1—H1C1	1.000	C16—C17	1.380 (4)
C1—H2C1	1.000	C16—HC16	1.000
C2—C3	1.506 (5)	C17—HC17	1.000
C2—H1C2	1.000	C18—H1C18	1.000
C2—H2C2	1.000	C18—H2C18	1.000
C3—C4	1.389 (4)	C18—H3C18	1.000
C3—C10	1.404 (4)	C19—C20	1.381 (4)
C4—C5	1.375 (5)	C19—C24	1.399 (4)
C4—HC4	1.000	C20—C21	1.376 (4)
C5—C6	1.401 (5)	C20—HC20	1.000
C5—C11	1.519 (5)	C21—C22	1.408 (4)
C6—C7	1.392 (4)	C21—HC21	1.000
C6—HC6	1.000	C22—C23	1.369 (4)
C7—C8	1.523 (5)	C22—C25	1.502 (5)
C7—C10	1.388 (4)	C23—C24	1.384 (4)
C8—H1C8	1.000	C23—HC23	1.000
C8—H2C8	1.000	C24—HC24	1.000
C9—H1C9	1.000	C25—H1C25	1.000
C9—H2C9	1.000	C25—H2C25	1.000
C11—H1C11	1.000	C25—H3C25	1.000
C11—H2C11	1.000		
C1—N1—C9	119.7 (3)	C5—C11—H3C11	109.5
C1—N1—C10	119.1 (3)	H1C11—C11—H2C11	109.5
C9—N1—C10	117.5 (3)	H1C11—C11—H3C11	109.5
C1—N2—C2	108.8 (3)	H2C11—C11—H3C11	109.5
C1—N2—C12	117.3 (3)	N2—C12—C13	119.1 (3)
C2—N2—C12	118.2 (2)	N2—C12—C17	124.1 (3)
C8—N3—C9	108.3 (3)	C13—C12—C17	116.8 (3)
C8—N3—C19	117.1 (3)	C12—C13—C14	120.6 (3)
C9—N3—C19	113.8 (3)	C12—C13—HC13	119.7
N1—C1—N2	111.8 (2)	C14—C13—HC13	119.7
N1—C1—H1C1	108.9	C13—C14—C15	122.6 (3)
N1—C1—H2C1	108.9	C13—C14—HC14	118.7
N2—C1—H1C1	108.9	C15—C14—HC14	118.7
N2—C1—H2C1	108.9	C14—C15—C16	116.4 (3)
H1C1—C1—H2C1	109.5	C14—C15—C18	121.9 (3)
N2—C2—C3	111.4 (3)	C16—C15—C18	121.7 (4)
N2—C2—H1C2	109.0	C15—C16—C17	122.1 (3)
N2—C2—H2C2	109.0	C15—C16—HC16	118.9
C3—C2—H1C2	109.0	C17—C16—HC16	118.9
C3—C2—H2C2	109.0	C12—C17—C16	121.5 (3)
H1C2—C2—H2C2	109.5	C12—C17—HC17	119.3
C2—C3—C4	122.4 (3)	C16—C17—HC17	119.3
C2—C3—C10	118.8 (3)	C15—C18—H1C18	109.5

C4—C3—C10	118.8 (3)	C15—C18—H2C18	109.5
C3—C4—C5	122.3 (3)	C15—C18—H3C18	109.5
C3—C4—HC4	118.9	H1C18—C18—H2C18	109.5
C5—C4—HC4	118.9	H1C18—C18—H3C18	109.5
C4—C5—C6	118.5 (3)	H2C18—C18—H3C18	109.5
C4—C5—C11	121.8 (4)	N3—C19—C20	119.3 (3)
C6—C5—C11	119.7 (4)	N3—C19—C24	122.8 (3)
C5—C6—C7	120.5 (4)	C20—C19—C24	117.8 (3)
C5—C6—HC6	119.7	C19—C20—C21	121.5 (3)
C7—C6—HC6	119.7	C19—C20—HC20	119.2
C6—C7—C8	121.3 (3)	C21—C20—HC20	119.2
C6—C7—C10	120.1 (3)	C20—C21—C22	121.3 (3)
C8—C7—C10	118.6 (3)	C20—C21—HC21	119.4
N3—C8—C7	112.4 (3)	C22—C21—HC21	119.4
N3—C8—H1C8	108.7	C21—C22—C23	116.4 (3)
N3—C8—H2C8	108.7	C21—C22—C25	121.0 (3)
C7—C8—H1C8	108.7	C23—C22—C25	122.6 (3)
C7—C8—H2C8	108.7	C22—C23—C24	123.2 (3)
H1C8—C8—H2C8	109.5	C22—C23—HC23	118.4
N1—C9—N3	109.9 (3)	C24—C23—HC23	118.4
N1—C9—H1C9	109.4	C19—C24—C23	119.8 (3)
N1—C9—H2C9	109.4	C19—C24—HC24	120.1
N3—C9—H1C9	109.4	C23—C24—HC24	120.1
N3—C9—H2C9	109.4	C22—C25—H1C25	109.5
H1C9—C9—H2C9	109.5	C22—C25—H2C25	109.5
N1—C10—C3	119.8 (3)	C22—C25—H3C25	109.5
N1—C10—C7	120.4 (3)	H1C25—C25—H2C25	109.5
C3—C10—C7	119.8 (3)	H1C25—C25—H3C25	109.5
C5—C11—H1C11	109.5	H2C25—C25—H3C25	109.5
C5—C11—H2C11	109.5		
C9—N1—C1—N2	−164.5 (3)	C6—C5—C11—H3C11	178.8
C9—N1—C1—H1C1	75.1	C5—C6—C7—C8	−176.6 (3)
C9—N1—C1—H2C1	−44.2	C5—C6—C7—C10	1.9 (5)
C10—N1—C1—N2	37.7 (4)	HC6—C6—C7—C8	3.4
C10—N1—C1—H1C1	−82.7	HC6—C6—C7—C10	−178.1
C10—N1—C1—H2C1	158.0	C6—C7—C8—N3	−158.0 (3)
C1—N1—C9—N3	155.0 (3)	C6—C7—C8—H1C8	81.5
C1—N1—C9—H1C9	−84.9	C6—C7—C8—H2C8	−37.6
C1—N1—C9—H2C9	35.0	C10—C7—C8—N3	23.5 (4)
C10—N1—C9—N3	−46.8 (4)	C10—C7—C8—H1C8	−97.0
C10—N1—C9—H1C9	73.3	C10—C7—C8—H2C8	143.9
C10—N1—C9—H2C9	−166.9	C6—C7—C10—N1	177.1 (3)
C1—N1—C10—C3	−7.2 (4)	C6—C7—C10—C3	−1.2 (4)
C1—N1—C10—C7	174.6 (3)	C8—C7—C10—N1	−4.4 (4)
C9—N1—C10—C3	−165.5 (3)	C8—C7—C10—C3	177.4 (3)
C9—N1—C10—C7	16.3 (4)	N2—C12—C13—C14	−176.5 (3)
C2—N2—C1—N1	−61.7 (3)	N2—C12—C13—HC13	3.5
C2—N2—C1—H1C1	58.7	C17—C12—C13—C14	0.9 (5)
C2—N2—C1—H2C1	178.0	C17—C12—C13—HC13	−179.1

C12—N2—C1—N1	75.8 (4)	N2—C12—C17—C16	175.9 (3)
C12—N2—C1—H1C1	−163.9	N2—C12—C17—HC17	−4.1
C12—N2—C1—H2C1	−44.6	C13—C12—C17—C16	−1.3 (5)
C1—N2—C2—C3	55.2 (3)	C13—C12—C17—HC17	178.7
C1—N2—C2—H1C2	−65.1	C12—C13—C14—C15	0.2 (5)
C1—N2—C2—H2C2	175.4	C12—C13—C14—HC14	−179.8
C12—N2—C2—C3	−81.8 (3)	HC13—C13—C14—C15	−179.8
C12—N2—C2—H1C2	157.9	HC13—C13—C14—HC14	0.2
C12—N2—C2—H2C2	38.4	C13—C14—C15—C16	−0.8 (5)
C1—N2—C12—C13	173.3 (3)	C13—C14—C15—C18	178.3 (3)
C1—N2—C12—C17	−3.9 (4)	HC14—C14—C15—C16	179.2
C2—N2—C12—C13	−53.2 (4)	HC14—C14—C15—C18	−1.7
C2—N2—C12—C17	129.6 (3)	C14—C15—C16—C17	0.3 (5)
C9—N3—C8—C7	−52.9 (3)	C14—C15—C16—HC16	−179.7
C9—N3—C8—H1C8	67.6	C18—C15—C16—C17	−178.7 (3)
C9—N3—C8—H2C8	−173.3	C18—C15—C16—HC16	1.3
C19—N3—C8—C7	77.5 (3)	C14—C15—C18—H1C18	−90.0
C19—N3—C8—H1C8	−162.1	C14—C15—C18—H2C18	30.0
C19—N3—C8—H2C8	−43.0	C14—C15—C18—H3C18	150.0
C8—N3—C9—N1	64.6 (3)	C16—C15—C18—H1C18	89.0
C8—N3—C9—H1C9	−55.5	C16—C15—C18—H2C18	−151.0
C8—N3—C9—H2C9	−175.4	C16—C15—C18—H3C18	−31.0
C19—N3—C9—N1	−67.5 (4)	C15—C16—C17—C12	0.8 (5)
C19—N3—C9—H1C9	172.4	C15—C16—C17—HC17	−179.2
C19—N3—C9—H2C9	52.5	HC16—C16—C17—C12	−179.2
C8—N3—C19—C20	173.4 (3)	HC16—C16—C17—HC17	0.8
C8—N3—C19—C24	−4.2 (4)	N3—C19—C20—C21	−178.0 (3)
C9—N3—C19—C20	−58.9 (4)	N3—C19—C20—HC20	2.0
C9—N3—C19—C24	123.5 (3)	C24—C19—C20—C21	−0.3 (5)
N2—C2—C3—C4	153.9 (3)	C24—C19—C20—HC20	179.7
N2—C2—C3—C10	−26.3 (4)	N3—C19—C24—C23	176.7 (3)
H1C2—C2—C3—C4	−85.8	N3—C19—C24—HC24	−3.3
H1C2—C2—C3—C10	94.0	C20—C19—C24—C23	−0.9 (4)
H2C2—C2—C3—C4	33.6	C20—C19—C24—HC24	179.1
H2C2—C2—C3—C10	−146.5	C19—C20—C21—C22	0.8 (5)
C2—C3—C4—C5	−178.9 (3)	C19—C20—C21—HC21	−179.2
C2—C3—C4—HC4	1.1	HC20—C20—C21—C22	−179.2
C10—C3—C4—C5	1.3 (5)	HC20—C20—C21—HC21	0.8
C10—C3—C4—HC4	−178.7	C20—C21—C22—C23	−0.2 (5)
C2—C3—C10—N1	1.5 (4)	C20—C21—C22—C25	−179.9 (3)
C2—C3—C10—C7	179.8 (3)	HC21—C21—C22—C23	179.8
C4—C3—C10—N1	−178.6 (3)	HC21—C21—C22—C25	0.1
C4—C3—C10—C7	−0.4 (4)	C21—C22—C23—C24	−1.0 (5)
C3—C4—C5—C6	−0.6 (5)	C21—C22—C23—HC23	179.0
C3—C4—C5—C11	178.2 (3)	C25—C22—C23—C24	178.7 (3)
HC4—C4—C5—C6	179.4	C25—C22—C23—HC23	−1.3
HC4—C4—C5—C11	−1.8	C21—C22—C25—H1C25	−30.0
C4—C5—C6—C7	−1.0 (5)	C21—C22—C25—H2C25i	90.0
C4—C5—C6—HC6	179.0	C21i—C22i—C25i—H3C25i	−150.0

C11—C5—C6—C7	−179.9 (3)	C23i—C22i—C25i—H1C25i	150.3
C11—C5—C6—HC6	0.1	C23i—C22i—C25i—H2C25i	−89.7
C4—C5—C11—H1C11	120.0	C23i—C22i—C25i—H3C25i	30.3
C4—C5—C11—H2C11	−120.0	C22i—C23i—C24i—C19i	1.6 (5)
C4—C5—C11—H3C11	0.0	C22i—C23i—C24i—HC24i	−178.4
C6—C5—C11—H1C11	−61.2	HC23i—C23i—C24i—C19i	−178.4
C6—C5—C11—H2C11	58.8	HC23i—C23i—C24i—HC24i	1.6

Fig. 1

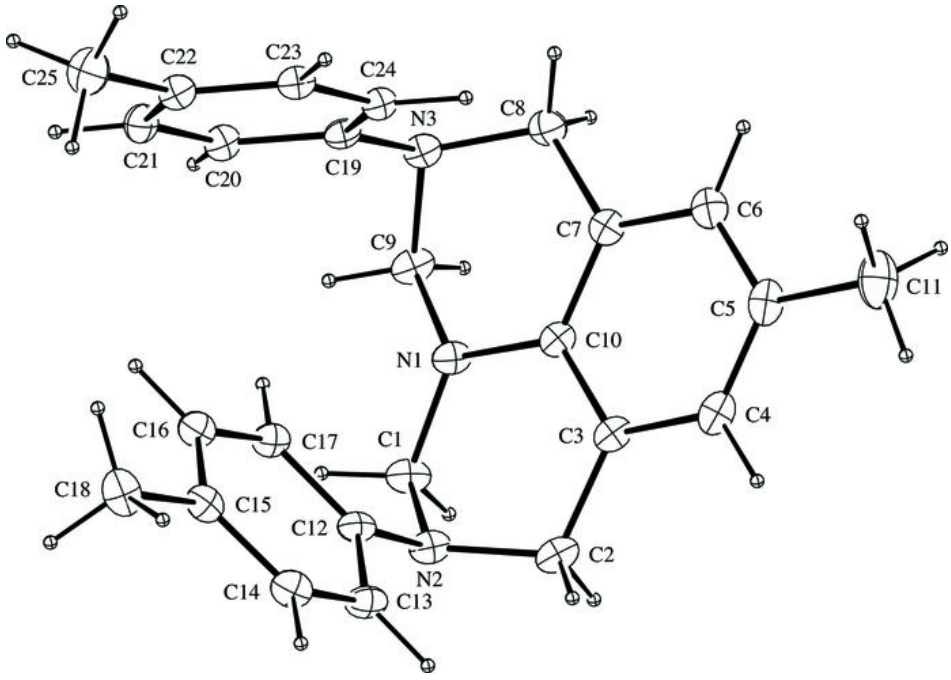
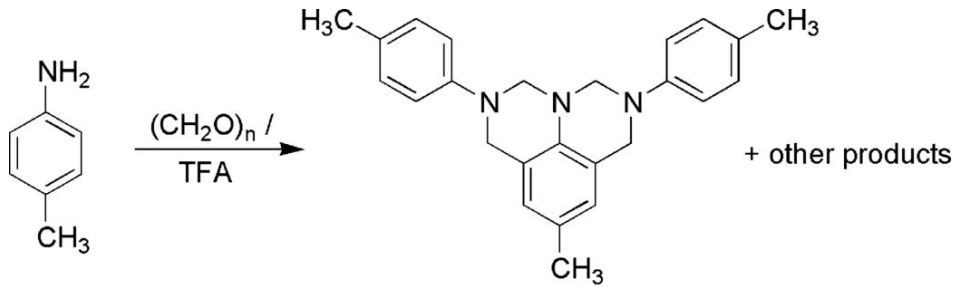

C25
C22
C23
C24
N3
C8
C21
C20
C19
C6
C7
C9
C11
C5
C10
N1
C4
C16
C17
C1
C3
C18
C15
C12
C2
N2
C14
C13

Fig. 2



(I)