

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

N-(Diphenylvinylidene)-2,6-diisopropylaniline

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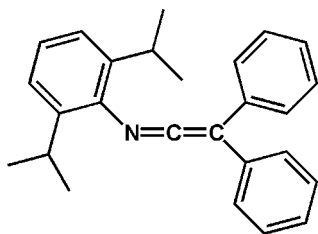
Received 19 November 2008; accepted 1 December 2008

 Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.040; wR factor = 0.103; data-to-parameter ratio = 7.5.

The title compound, $\text{C}_{26}\text{H}_{27}\text{N}$, was prepared by the elimination of water from *N*-(2,6-diisopropylphenyl)-2,2-diphenylacetamide. The angle at the central C atom of the cumulene measures $172.5(4)^\circ$. Molecules are connected into infinite chains by intermolecular $\text{C}-\text{H}\cdots\text{N}$ interactions.

Related literature

For the synthetic procedure, see: Stevens & Singhal (1964). For related structures, see: Naqvi & Wheatley (1970); Jochims *et al.* (1984); Kuipers *et al.* (1989). For general background, see: Imhof (1997*a,b*). For properties of weak hydrogen bonds, see: Desiraju & Steiner (1999).



Experimental

Crystal data

$\text{C}_{26}\text{H}_{27}\text{N}$
 $M_r = 353.49$
 Orthorhombic, $P2_12_12_1$
 $a = 8.082(4)$ Å

$b = 14.308(4)$ Å
 $c = 17.790(2)$ Å
 $V = 2057(1)$ Å³
 $Z = 4$

Mo $K\alpha$ radiation
 $\mu = 0.07$ mm⁻¹

$T = 173(2)$ K
 $0.3 \times 0.2 \times 0.2$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer
 Absorption correction: none
 3554 measured reflections
 1853 independent reflections
 1531 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.065$
 $\theta_{\text{max}} = 24.0^\circ$
 3 standard reflections
 frequency: 120 min
 intensity decay: <0.1%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.103$
 $S = 0.82$
 1853 reflections

248 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.15$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.17$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C5}-\text{H5}\cdots\text{N1}^i$	0.95	2.72	3.554 (4)	146

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *SET4* (de Boer & Duisenberg, 1984); data reduction: *MolEN* (Enraf–Nonius, 1990); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* (Siemens, 1990); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2125).

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supplementary materials

Acta Cryst. (2009). E65, o25 [doi:10.1107/S1600536808040397]

***N*-(Diphenylvinylidene)-2,6-diisopropylaniline**

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Comment

In the course of a study on the organometallic and catalytic chemistry of aromatic imines (Imhof, 1997*a,b*) we became interested in the reactivity of the vinylogous keteneimines. The latter are prepared by the elimination of water from the corresponding acetamides by P₂O₅ in anhydrous pyridine (Stevens & Singhal, 1964).

As expected the molecular structure of the title compound shows an almost linear cumulene system with an angle of 172.5 (4)° at the central C atom. The bonds C1—C2 and C2—N1 show bond lengths of 1.332 (5) and 1.213 (4) Å, respectively. The dihedral angle between the C1—C8—C14 plane and the aromatic substituent at the imine N atom measures to 52.4 (7)° which means that the substituents at the cumulene system do not show the expected orthogonal arrangement. This is most probably caused by the high steric requirements of the two isopropyl groups in *ortho*-position. A comparison with related aromatic diphenylvinylidene amines from the literature shows that the corresponding dihedral angle is close to 90° if there is no or just one *ortho*-substituent present in the aromatic group at nitrogen (*p*-Br-C₆H₄: 85.6°, Naqvi & Wheatley, 1970; *o*-Me-C₆H₄: 88.1°, Jochims *et al.*, 1984; *p*-(N=C=CPh₂)-C₆H₄: 88.4°, Kuipers *et al.*, 1989; *p*-Me-C₆H₄: 83.9°, Naqvi & Wheatley, 1970). If both *ortho*-positions are substituted the conformation is no longer orthogonal (*o*-Me₂-C₆H₃: 51.7°, Jochims *et al.*, 1984) as it is also observed for the title compound. The lone pair at nitrogen is involved in a weak intramolecular hydrogen bond (Desiraju & Steiner, 1999) interaction towards H5 leading to the formation of infinite chains.

Experimental

The title compound was prepared following a literature method (Stevens & Singhal, 1964). A sample of 2 g (5.4 mmol) *N*-(2,6-Diisopropyl-phenyl)-2,2-diphenyl-acetamide was dissolved in 50 ml of anhydrous pyridine. To this solution 5 g P₂O₅ were added and the mixture was refluxed for 7 h. After cooling the solution was filtered and pyridine was evaporated resulting in a red oily residue. The oil was transferred to a short chromatography column and light petroleum (b.p. 40–60°C) was used to elute a yellow solution of the title compound. Concentration of the solution and cooling to 4°C led to the formation of crystalline material from which the crystal for the structure analysis described herein was collected (yield: 1.56 g, 82%). MS (EI) [*m/z*, %]: 353 (*M*⁺, 80), 338 (C₂₅H₂₄N⁺, 22), 186 (C₁₃H₁₆N⁺, 100), 165 (C₁₃H₉⁺, 50), 115 (C₉H₇⁺, 19), 91 (C₇H₇⁺, 37), 77 (C₆H₅⁺, 17), 55 (C₄H₇⁺, 11), 41 (C₃H₅⁺, 35). ¹H NMR (CDCl₃, 298 K) [p.p.m.]: 1.11 (12 H, d, ³J_{HH} = 6.8 Hz, CH₃), 3.24 (2 H, h, ³J_{HH} = 6.8 Hz, CH), 7.05–7.34 (15 H, m, CH_{ar}). ¹³C NMR (CDCl₃, 298 K) [p.p.m.]: 22.4 (CH₃), 28.5 (CH), 72.0 (=C), 123.4 (C_{ar}H), 125.9 (C_{ar}H), 126.3 (C_{ar}H), 127.8 (C_{ar}H), 128.7 (C_{ar}H), 134.8 (C_{ar}), 136.2 (C_{ar}), 140.8 (C_{ar}), 183.4 (=C=).

Refinement

H atoms were positioned with idealized geometry at distances of 0.95 Å for aromatic C—H functions, 1.00 Å for aliphatic C—H bonds and 0.98 Å for methyl groups and were refined riding on their parent atoms with isotropic thermal parameters

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of 1.2 times the corresponding values of their parent atoms. In the absence of significant anomalous dispersion effects, Friedel pairs were averaged.

Figures

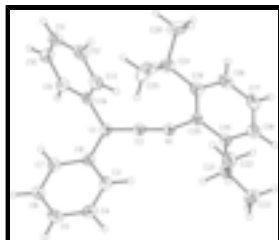


Fig. 1. The molecular structure of the title compound, presenting the labelling scheme and 40% probability displacement ellipsoids for non-H atoms.

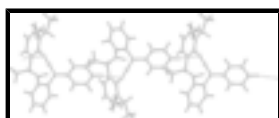


Fig. 2. Infinite chains of the title compound realized by C—H...O hydrogen bonds.

N-(Diphenylvinylidene)-2,6-diisopropylaniline

Crystal data

$C_{26}H_{27}N$

$M_r = 353.49$

Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 8.082$ (4) Å

$b = 14.308$ (4) Å

$c = 17.790$ (2) Å

$V = 2057$ (1) Å³

$Z = 4$

$F_{000} = 760$

$D_x = 1.141$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 25 reflections

$\theta = 20.9$ – 35.5°

$\mu = 0.07$ mm⁻¹

$T = 173$ (2) K

Cube, pale yellow

$0.3 \times 0.2 \times 0.2$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 173$ (2) K

$\omega/2\theta$ scans

Absorption correction: none

3554 measured reflections

1853 independent reflections

1531 reflections with $I > 2\sigma(I)$

$R_{int} = 0.065$

$\theta_{max} = 24.0^\circ$

$\theta_{min} = 1.8^\circ$

$h = -9 \rightarrow 0$

$k = -16 \rightarrow 16$

$l = 0 \rightarrow 20$

3 standard reflections

every 120 min

intensity decay: $<0.1\%$

Refinement

Refinement on F^2

Secondary atom site location: difference Fourier map

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.040$$

$$wR(F^2) = 0.103$$

$$S = 0.82$$

1853 reflections

248 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.1319P)^2 + 0.5946P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} < 0.001$$

$$\Delta\rho_{\max} = 0.15 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.17 \text{ e } \text{\AA}^{-3}$$

Extinction correction: none

Special details

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 on F^2 for ALL reflections except for 9 with very negative F^2 or flagged by the user for potential systematic errors. Weighted R -factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating `_R_factor_obs` 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.1809 (3)	0.90928 (16)	0.93459 (13)	0.0304 (6)
C1	0.2195 (4)	1.06100 (19)	1.00668 (17)	0.0303 (7)
C2	0.1892 (4)	0.98254 (19)	0.96930 (15)	0.0306 (7)
C3	0.1148 (4)	0.9958 (2)	1.12860 (17)	0.0363 (7)
H3	0.0626	0.9470	1.1012	0.044*
C4	0.1008 (4)	0.9981 (2)	1.20605 (18)	0.0421 (8)
H4	0.0401	0.9508	1.2314	0.051*
C5	0.1749 (4)	1.0691 (2)	1.24668 (18)	0.0414 (8)
H5	0.1636	1.0717	1.2998	0.050*
C6	0.2652 (4)	1.1358 (2)	1.20919 (18)	0.0408 (8)
H6	0.3178	1.1841	1.2370	0.049*
C7	0.2810 (4)	1.1341 (2)	1.13188 (16)	0.0339 (7)
H7	0.3444	1.1807	1.1071	0.041*
C8	0.2041 (4)	1.06391 (18)	1.09007 (17)	0.0289 (6)
C9	0.1828 (5)	1.2310 (2)	0.97473 (17)	0.0404 (8)
H9	0.1050	1.2370	1.0144	0.049*
C10	0.2210 (5)	1.3071 (2)	0.9299 (2)	0.0494 (9)
H10	0.1695	1.3656	0.9395	0.059*
C11	0.3325 (6)	1.2993 (3)	0.87148 (19)	0.0569 (11)
H11	0.3577	1.3521	0.8411	0.068*
C12	0.4071 (5)	1.2144 (3)	0.85749 (19)	0.0544 (10)

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H12	0.4830	1.2085	0.8170	0.065*
C13	0.3720 (4)	1.1378 (2)	0.90200 (17)	0.0408 (8)
H13	0.4248	1.0797	0.8923	0.049*
C14	0.2595 (4)	1.1454 (2)	0.96113 (15)	0.0314 (6)
C15	0.0304 (4)	0.7690 (2)	0.90761 (15)	0.0300 (7)
C16	-0.1020 (4)	0.7236 (2)	0.87388 (17)	0.0374 (7)
H16	-0.1141	0.6580	0.8796	0.045*
C17	-0.2159 (4)	0.7728 (2)	0.83219 (19)	0.0432 (8)
H17	-0.3071	0.7409	0.8103	0.052*
C18	-0.1993 (4)	0.8682 (2)	0.82167 (17)	0.0406 (7)
H18	-0.2781	0.9007	0.7918	0.049*
C19	-0.0683 (4)	0.9176 (2)	0.85429 (16)	0.0335 (7)
C20	0.0419 (4)	0.8665 (2)	0.89897 (14)	0.0282 (6)
C21	0.1642 (4)	0.7162 (2)	0.95050 (17)	0.0364 (7)
H21	0.1917	0.7540	0.9961	0.044*
C22	0.3218 (5)	0.7091 (2)	0.9033 (2)	0.0461 (8)
H22A	0.3554	0.7716	0.8869	0.055*
H22B	0.3008	0.6698	0.8592	0.055*
H22C	0.4103	0.6812	0.9336	0.055*
C23	0.1115 (6)	0.6197 (2)	0.9776 (2)	0.0545 (10)
H23A	0.1997	0.5926	1.0085	0.065*
H23B	0.0906	0.5793	0.9342	0.065*
H23C	0.0103	0.6252	1.0076	0.065*
C24	-0.0519 (4)	1.0221 (2)	0.84131 (18)	0.0396 (8)
H24	0.0658	1.0392	0.8521	0.048*
C25	-0.1593 (5)	1.0765 (2)	0.8963 (3)	0.0586 (10)
H25A	-0.1315	1.0581	0.9478	0.070*
H25B	-0.2761	1.0628	0.8865	0.070*
H25C	-0.1394	1.1436	0.8899	0.070*
C26	-0.0872 (5)	1.0502 (3)	0.7602 (2)	0.0623 (11)
H26A	-0.2043	1.0392	0.7488	0.075*
H26B	-0.0183	1.0129	0.7262	0.075*
H26C	-0.0618	1.1167	0.7534	0.075*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0354 (14)	0.0255 (12)	0.0303 (12)	0.0015 (11)	-0.0040 (11)	-0.0019 (10)
C1	0.0340 (16)	0.0248 (14)	0.0322 (14)	-0.0013 (14)	-0.0016 (13)	-0.0040 (12)
C2	0.0334 (15)	0.0293 (15)	0.0291 (13)	0.0027 (13)	-0.0018 (13)	0.0026 (13)
C3	0.0431 (17)	0.0271 (13)	0.0387 (15)	-0.0057 (15)	-0.0027 (15)	-0.0019 (13)
C4	0.0489 (18)	0.0383 (16)	0.0391 (16)	-0.0007 (17)	0.0021 (16)	0.0087 (14)
C5	0.0473 (19)	0.0491 (18)	0.0279 (14)	0.0042 (17)	-0.0023 (15)	0.0052 (14)
C6	0.0512 (18)	0.0367 (16)	0.0347 (15)	-0.0019 (17)	-0.0147 (15)	-0.0037 (13)
C7	0.0391 (16)	0.0298 (14)	0.0329 (15)	-0.0042 (15)	-0.0033 (13)	0.0013 (12)
C8	0.0297 (14)	0.0254 (13)	0.0315 (14)	0.0021 (13)	-0.0019 (13)	-0.0005 (11)
C9	0.0502 (19)	0.0352 (16)	0.0358 (16)	-0.0024 (16)	-0.0036 (16)	0.0020 (13)
C10	0.065 (2)	0.0340 (16)	0.0491 (19)	-0.0055 (18)	-0.0197 (19)	0.0057 (15)

C11	0.079 (3)	0.059 (2)	0.0328 (17)	-0.040 (2)	-0.0121 (19)	0.0129 (17)
C12	0.067 (2)	0.063 (2)	0.0333 (17)	-0.031 (2)	-0.0003 (18)	-0.0005 (16)
C13	0.0444 (18)	0.0420 (16)	0.0360 (15)	-0.0120 (16)	0.0041 (14)	-0.0062 (15)
C14	0.0365 (15)	0.0316 (14)	0.0260 (13)	-0.0075 (15)	-0.0038 (12)	-0.0018 (12)
C15	0.0369 (16)	0.0290 (14)	0.0242 (13)	0.0021 (13)	-0.0013 (14)	-0.0039 (12)
C16	0.0438 (18)	0.0333 (15)	0.0351 (15)	-0.0013 (15)	-0.0010 (15)	-0.0049 (14)
C17	0.0385 (18)	0.0483 (18)	0.0427 (17)	-0.0083 (16)	-0.0062 (16)	-0.0083 (16)
C18	0.0399 (17)	0.0486 (18)	0.0334 (15)	0.0025 (17)	-0.0105 (14)	-0.0015 (14)
C19	0.0338 (16)	0.0365 (16)	0.0303 (14)	0.0024 (14)	0.0029 (13)	-0.0040 (13)
C20	0.0319 (14)	0.0284 (13)	0.0242 (13)	0.0035 (13)	0.0007 (12)	-0.0048 (11)
C21	0.0454 (18)	0.0283 (14)	0.0354 (15)	0.0048 (14)	-0.0075 (15)	-0.0029 (13)
C22	0.0431 (18)	0.0409 (17)	0.054 (2)	0.0099 (16)	-0.0056 (17)	-0.0066 (16)
C23	0.065 (2)	0.0357 (17)	0.063 (2)	0.0021 (19)	-0.015 (2)	0.0084 (17)
C24	0.0386 (17)	0.0363 (16)	0.0438 (17)	0.0075 (15)	-0.0028 (15)	0.0061 (14)
C25	0.055 (2)	0.0350 (17)	0.086 (3)	0.0103 (18)	0.011 (2)	-0.0023 (19)
C26	0.060 (2)	0.064 (2)	0.064 (2)	0.000 (2)	-0.010 (2)	0.030 (2)

Geometric parameters (Å, °)

N1—C2	1.218 (4)	C15—C20	1.406 (4)
N1—C20	1.428 (4)	C15—C21	1.523 (4)
C1—C2	1.328 (4)	C16—C17	1.376 (5)
C1—C14	1.490 (4)	C16—H16	0.9500
C1—C8	1.489 (4)	C17—C18	1.385 (5)
C3—C8	1.393 (4)	C17—H17	0.9500
C3—C4	1.383 (4)	C18—C19	1.399 (5)
C3—H3	0.9500	C18—H18	0.9500
C4—C5	1.384 (5)	C19—C20	1.400 (4)
C4—H4	0.9500	C19—C24	1.519 (4)
C5—C6	1.374 (5)	C21—C23	1.523 (5)
C5—H5	0.9500	C21—C22	1.529 (5)
C6—C7	1.381 (4)	C21—H21	1.0000
C6—H6	0.9500	C22—H22A	0.9800
C7—C8	1.395 (4)	C22—H22B	0.9800
C7—H7	0.9500	C22—H22C	0.9800
C9—C10	1.385 (5)	C23—H23A	0.9800
C9—C14	1.393 (5)	C23—H23B	0.9800
C9—H9	0.9500	C23—H23C	0.9800
C10—C11	1.380 (6)	C24—C26	1.525 (5)
C10—H10	0.9500	C24—C25	1.521 (5)
C11—C12	1.379 (6)	C24—H24	1.0000
C11—H11	0.9500	C25—H25A	0.9800
C12—C13	1.381 (5)	C25—H25B	0.9800
C12—H12	0.9500	C25—H25C	0.9800
C13—C14	1.395 (4)	C26—H26A	0.9800
C13—H13	0.9500	C26—H26B	0.9800
C15—C16	1.388 (5)	C26—H26C	0.9800
C2—N1—C20	129.6 (3)	C16—C17—H17	119.6
C2—C1—C14	116.9 (3)	C18—C17—H17	119.6

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C2—C1—C8	120.5 (3)	C17—C18—C19	121.0 (3)
C14—C1—C8	122.5 (2)	C17—C18—H18	119.5
N1—C2—C1	172.5 (3)	C19—C18—H18	119.5
C8—C3—C4	121.1 (3)	C18—C19—C20	117.0 (3)
C8—C3—H3	119.5	C18—C19—C24	120.0 (3)
C4—C3—H3	119.5	C20—C19—C24	123.0 (3)
C5—C4—C3	120.2 (3)	C15—C20—C19	122.6 (3)
C5—C4—H4	119.9	C15—C20—N1	115.4 (2)
C3—C4—H4	119.9	C19—C20—N1	121.9 (3)
C6—C5—C4	119.1 (3)	C23—C21—C15	114.2 (3)
C6—C5—H5	120.4	C23—C21—C22	110.3 (3)
C4—C5—H5	120.4	C15—C21—C22	110.4 (3)
C5—C6—C7	121.3 (3)	C23—C21—H21	107.2
C5—C6—H6	119.4	C15—C21—H21	107.2
C7—C6—H6	119.4	C22—C21—H21	107.2
C6—C7—C8	120.2 (3)	C21—C22—H22A	109.5
C6—C7—H7	119.9	C21—C22—H22B	109.5
C8—C7—H7	119.9	H22A—C22—H22B	109.5
C3—C8—C7	118.1 (3)	C21—C22—H22C	109.5
C3—C8—C1	120.9 (3)	H22A—C22—H22C	109.5
C7—C8—C1	120.9 (3)	H22B—C22—H22C	109.5
C10—C9—C14	119.5 (3)	C21—C23—H23A	109.5
C10—C9—H9	120.3	C21—C23—H23B	109.5
C14—C9—H9	120.3	H23A—C23—H23B	109.5
C11—C10—C9	121.0 (3)	C21—C23—H23C	109.5
C11—C10—H10	119.5	H23A—C23—H23C	109.5
C9—C10—H10	119.5	H23B—C23—H23C	109.5
C12—C11—C10	119.5 (3)	C19—C24—C26	112.8 (3)
C12—C11—H11	120.2	C19—C24—C25	110.8 (3)
C10—C11—H11	120.2	C26—C24—C25	111.5 (3)
C13—C12—C11	120.4 (3)	C19—C24—H24	107.1
C13—C12—H12	119.8	C26—C24—H24	107.1
C11—C12—H12	119.8	C25—C24—H24	107.1
C12—C13—C14	120.3 (3)	C24—C25—H25A	109.5
C12—C13—H13	119.9	C24—C25—H25B	109.5
C14—C13—H13	119.9	H25A—C25—H25B	109.5
C9—C14—C13	119.3 (3)	C24—C25—H25C	109.5
C9—C14—C1	121.4 (3)	H25A—C25—H25C	109.5
C13—C14—C1	119.2 (3)	H25B—C25—H25C	109.5
C16—C15—C20	117.8 (3)	C24—C26—H26A	109.5
C16—C15—C21	122.1 (3)	C24—C26—H26B	109.5
C20—C15—C21	120.0 (3)	H26A—C26—H26B	109.5
C17—C16—C15	120.7 (3)	C24—C26—H26C	109.5
C17—C16—H16	119.7	H26A—C26—H26C	109.5
C15—C16—H16	119.7	H26B—C26—H26C	109.5
C16—C17—C18	120.8 (3)		
C20—N1—C2—C1	-169 (2)	C8—C1—C14—C13	137.9 (3)
C14—C1—C2—N1	82 (2)	C20—C15—C16—C17	1.3 (4)
C8—C1—C2—N1	-101 (2)	C21—C15—C16—C17	-176.5 (3)

C8—C3—C4—C5	0.5 (5)	C15—C16—C17—C18	1.3 (5)
C3—C4—C5—C6	-1.4 (5)	C16—C17—C18—C19	-1.3 (5)
C4—C5—C6—C7	1.0 (5)	C17—C18—C19—C20	-1.3 (5)
C5—C6—C7—C8	0.3 (5)	C17—C18—C19—C24	179.4 (3)
C4—C3—C8—C7	0.8 (5)	C16—C15—C20—C19	-4.1 (4)
C4—C3—C8—C1	179.7 (3)	C21—C15—C20—C19	173.8 (3)
C6—C7—C8—C3	-1.2 (4)	C16—C15—C20—N1	-179.8 (2)
C6—C7—C8—C1	179.9 (3)	C21—C15—C20—N1	-1.9 (4)
C2—C1—C8—C3	-18.4 (5)	C18—C19—C20—C15	4.0 (4)
C14—C1—C8—C3	158.0 (3)	C24—C19—C20—C15	-176.7 (3)
C2—C1—C8—C7	160.5 (3)	C18—C19—C20—N1	179.5 (3)
C14—C1—C8—C7	-23.1 (4)	C24—C19—C20—N1	-1.3 (4)
C14—C9—C10—C11	0.7 (5)	C2—N1—C20—C15	-139.4 (3)
C9—C10—C11—C12	0.1 (5)	C2—N1—C20—C19	44.9 (4)
C10—C11—C12—C13	-0.7 (6)	C16—C15—C21—C23	-21.2 (4)
C11—C12—C13—C14	0.6 (5)	C20—C15—C21—C23	161.0 (3)
C10—C9—C14—C13	-0.7 (5)	C16—C15—C21—C22	103.7 (3)
C10—C9—C14—C1	-178.5 (3)	C20—C15—C21—C22	-74.0 (3)
C12—C13—C14—C9	0.1 (5)	C18—C19—C24—C26	-41.8 (4)
C12—C13—C14—C1	178.0 (3)	C20—C19—C24—C26	139.0 (3)
C2—C1—C14—C9	132.2 (3)	C18—C19—C24—C25	84.0 (4)
C8—C1—C14—C9	-44.3 (4)	C20—C19—C24—C25	-95.2 (4)
C2—C1—C14—C13	-45.6 (4)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C5—H5 \cdots N1 ⁱ	0.95	2.72	3.554 (4)	146

Symmetry codes: (i) $-x+1/2, -y+2, z+1/2$.

Fig. 1

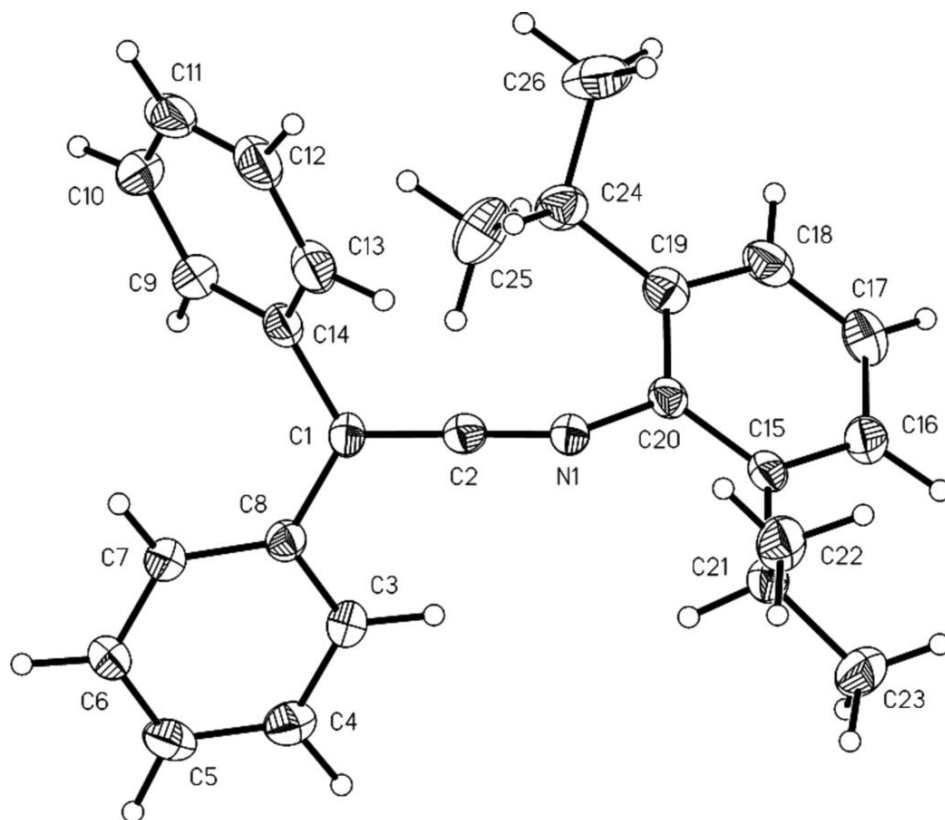


Fig. 2

