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2,6-Diisopropyl-*N*-[(*Z*)-quinolin-2-ylmethylidene]aniline

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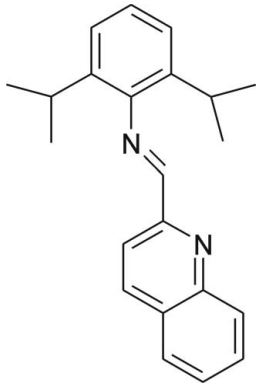
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.003 Å; R factor = 0.053; wR factor = 0.116; data-to-parameter ratio = 15.3.

In the title compound, $C_{22}H_{24}N_2$, all bond lengths and angles are within normal ranges. The molecule is in a non-planar conformation, the dihedral angle between the two aromatic ring systems being 55.01 (8)°. The molecular packing is accomplished by a weak intermolecular C—H···N hydrogen bond.

Related literature

For related literature, see: Yliheikkilä *et al.* (2007); Räisänen, Elo *et al.*, (2007) Räisänen, Leskelä & Repo (2007); Alshahateet *et al.* (2004); Kottke & Stalke (1993).



Experimental

Crystal data

$C_{22}H_{24}N_2$
M_r = 316.43
Monoclinic, $P2_1/c$
a = 13.811 (3) Å
b = 10.971 (2) Å
c = 11.995 (2) Å
β = 93.88 (3)°
V = 1813.3 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 120 (2) K
0.30 × 0.30 × 0.25 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: multi-scan (*XPREP* in *SHELXTL*; Bruker, 1998)
T_{min} = 0.980, T_{max} = 0.983
29862 measured reflections
3384 independent reflections
1994 reflections with $I > 2\sigma(I)$
R_{int} = 0.141

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.116
S = 1.06
3384 reflections
221 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···N1^{i}	0.95	2.61	3.464 (3)	151

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

Data collection: *COLLECT* (Nonius, 1997); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2509).

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supplementary materials

Acta Cryst. (2007). E**63**, o4083 [**doi:10.1107/S1600536807044947**]

2,6-Diisopropyl-*N*-[(*Z*)-quinolin-2-ylmethylidene]aniline

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Comment

The title compound was prepared as a ligand for metal complexes to be studied as catalysts for ethene polymerization. Its structure is a typical example of *N*-aryl Schiff base ligand as it has adopted a non-planar conformation (Fig. 1) and all the bond lengths and angles are within normal ranges (Räisänen, Elo *et al.*, 2007; Räisänen Leskelä, & Repo 2007). The *N*-aryl substituent is twisted along the C—N axis as the C10—N2—C11—C16 torsion angle is 64.9 (3)° whereas the other aromatic ring is practically in plane with the imine bond as the N2—C10—C9—C8 angle deviates from zero only by −9.2 (3)°. The molecular packing of the compound is facilitated by intermolecular C—H···N hydrogen bonds (H···N distance of 2.61 Å) which fall in the range of weak hydrogen bonds (Alshahateet *et al.*, 2004).

Experimental

The title compound was synthesized (Yliheikkilä *et al.*, 2007) by refluxing 2,6-diisopropylaniline (1.6 g, 9.1 mmol) and 2-quinolinecarboxaldehyde (1.3 g, 7.8 mmol) in ethanol (40 ml) for 20 min. The solvent was removed and raw product was purified by a column chromatography on basic alumina using pentane/ethyl acetate (3:1) eluent. Recrystallization from n-pentane yielded yellow crystals. The pale yellow crystals suitable for X-ray analysis were obtained from acetone.

Refinement

Crystal selected for the X-ray measurement at 120 K was mounted on a goniometer head using the oil drop method (Kottke & Stalke, 1993). All H atoms were introduced in their calculated positions (C—H = 0.95 or 0.98 Å, U_{iso} = 1.2 times the U_{eq} of the carrier atom and U_{iso} = 1.5 times the U_{eq} of the carrier atom for methyl H atoms) and refined with fixed geometry with respect to their carrier atoms. The methyl groups were allowed to rotate but not to tip.

Figures

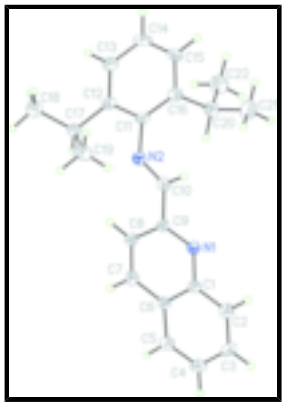


Fig. 1. Perspective view of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

2,6-Diisopropyl-*N*-[(*Z*)-quinolin-2-ylmethylidene]aniline

Crystal data

$C_{22}H_{24}N_2$	$Z = 4$
$M_r = 316.43$	$F_{000} = 680$
Monoclinic, $P2_1/c$	$D_x = 1.159$ Mg m^{-3}
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 13.811$ (3) Å	$\theta = 2.9$–25.5º
$b = 10.971$ (2) Å	$\mu = 0.07$ mm^{-1}
$c = 11.995$ (2) Å	$T = 120$ (2) K
$\beta = 93.88$ (3)º	Block, yellow
$V = 1813.3$ (6) Å^3	0.30 × 0.30 × 0.25 mm

Data collection

Nonius KappaCCD area-detector diffractometer	3384 independent reflections
Radiation source: fine-focus sealed tube	1994 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.141$
$T = 120(2)$ K	$\theta_{max} = 25.5$º
CCD scans	$\theta_{min} = 2.9$º
Absorption correction: multi-scan (XPREP in SHELXTL; Bruker, 1998)	$h = -16 \rightarrow 16$
$T_{min} = 0.980$, $T_{max} = 0.983$	$k = -13 \rightarrow 13$
29862 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.053$	H-atom parameters constrained
$wR(F^2) = 0.116$	$w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} < 0.001$
3384 reflections	$\Delta\rho_{max} = 0.18$ e Å^{-3}
221 parameters	$\Delta\rho_{min} = -0.19$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 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 $F^2 > 2\text{sigma}(F^2)$ 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}
N1	0.33403 (11)	0.31501 (15)	0.32844 (14)	0.0198 (4)
N2	0.17009 (12)	0.55989 (15)	0.28608 (14)	0.0221 (4)
C1	0.38589 (14)	0.23119 (17)	0.27262 (17)	0.0181 (5)
C2	0.45110 (15)	0.15362 (19)	0.33471 (19)	0.0258 (5)
H2	0.4581	0.1603	0.4138	0.031*
C3	0.50408 (15)	0.06922 (19)	0.28154 (19)	0.0285 (6)
H3	0.5480	0.0179	0.3240	0.034*
C4	0.49432 (15)	0.0576 (2)	0.16481 (19)	0.0296 (6)
H4	0.5315	−0.0018	0.1290	0.036*
C5	0.43210 (15)	0.13036 (19)	0.10256 (19)	0.0268 (5)
H5	0.4259	0.1213	0.0236	0.032*
C6	0.37635 (13)	0.21976 (18)	0.15456 (17)	0.0187 (5)
C7	0.31029 (14)	0.29851 (18)	0.09469 (18)	0.0227 (5)
H7	0.3014	0.2931	0.0156	0.027*
C8	0.25974 (14)	0.38189 (18)	0.15135 (17)	0.0199 (5)
H8	0.2155	0.4358	0.1123	0.024*
C9	0.27386 (14)	0.38728 (18)	0.26879 (17)	0.0188 (5)
C10	0.22059 (14)	0.47578 (18)	0.33397 (18)	0.0211 (5)
H10	0.2241	0.4698	0.4132	0.025*
C11	0.12220 (14)	0.64621 (18)	0.35299 (17)	0.0199 (5)
C12	0.02034 (15)	0.64969 (18)	0.33829 (17)	0.0201 (5)
C13	−0.02806 (16)	0.73603 (19)	0.39868 (19)	0.0268 (5)
H13	−0.0969	0.7395	0.3911	0.032*
C14	0.02217 (16)	0.81686 (19)	0.46951 (19)	0.0295 (6)
H14	−0.0122	0.8757	0.5095	0.035*
C15	0.12161 (16)	0.81238 (19)	0.48227 (18)	0.0274 (6)
H15	0.1552	0.8683	0.5315	0.033*
C16	0.17470 (15)	0.72720 (18)	0.42437 (17)	0.0236 (5)
C17	−0.03429 (14)	0.55741 (18)	0.26433 (18)	0.0239 (5)
H17	0.0083	0.5350	0.2033	0.029*
C18	−0.12959 (15)	0.6060 (2)	0.2089 (2)	0.0353 (6)
H18A	−0.1767	0.6169	0.2656	0.053*
H18B	−0.1553	0.5477	0.1525	0.053*
H18C	−0.1179	0.6844	0.1732	0.053*
C19	−0.05266 (17)	0.4411 (2)	0.3303 (2)	0.0366 (6)
H19A	0.0094	0.4072	0.3601	0.055*
H19B	−0.0862	0.3812	0.2808	0.055*
H19C	−0.0930	0.4603	0.3921	0.055*

C20	0.28494 (15)	0.7276 (2)	0.44076 (19)	0.0303 (6)
H20	0.3102	0.6653	0.3892	0.036*
C21	0.31763 (18)	0.6906 (2)	0.5603 (2)	0.0457 (7)
H21A	0.2943	0.7507	0.6126	0.069*
H21B	0.3887	0.6870	0.5683	0.069*
H21C	0.2908	0.6103	0.5765	0.069*
C22	0.32809 (17)	0.8514 (2)	0.4114 (2)	0.0411 (7)
H22A	0.3058	0.8735	0.3347	0.062*
H22B	0.3991	0.8461	0.4174	0.062*
H22C	0.3069	0.9135	0.4631	0.062*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0197 (9)	0.0174 (9)	0.0222 (10)	0.0002 (8)	0.0019 (8)	−0.0019 (8)
N2	0.0209 (10)	0.0195 (10)	0.0255 (11)	0.0002 (8)	0.0000 (8)	−0.0019 (8)
C1	0.0162 (10)	0.0149 (11)	0.0232 (12)	−0.0019 (9)	0.0016 (9)	−0.0001 (10)
C2	0.0258 (12)	0.0271 (13)	0.0242 (13)	0.0020 (10)	−0.0003 (10)	0.0001 (11)
C3	0.0246 (12)	0.0252 (13)	0.0351 (15)	0.0086 (10)	−0.0015 (11)	0.0012 (11)
C4	0.0283 (13)	0.0273 (13)	0.0334 (15)	0.0071 (11)	0.0041 (11)	−0.0069 (11)
C5	0.0283 (13)	0.0263 (13)	0.0261 (13)	0.0040 (10)	0.0028 (11)	−0.0051 (11)
C6	0.0192 (11)	0.0148 (11)	0.0222 (13)	−0.0031 (9)	0.0014 (10)	−0.0013 (9)
C7	0.0235 (11)	0.0246 (12)	0.0196 (12)	−0.0025 (10)	−0.0009 (10)	0.0020 (10)
C8	0.0197 (11)	0.0180 (12)	0.0218 (12)	0.0008 (9)	0.0007 (10)	0.0012 (10)
C9	0.0187 (11)	0.0148 (11)	0.0227 (13)	0.0001 (9)	−0.0003 (10)	0.0012 (10)
C10	0.0220 (11)	0.0197 (12)	0.0218 (12)	−0.0007 (10)	0.0026 (10)	−0.0014 (10)
C11	0.0246 (12)	0.0135 (11)	0.0218 (12)	0.0039 (9)	0.0037 (10)	−0.0006 (9)
C12	0.0224 (11)	0.0163 (11)	0.0216 (12)	0.0022 (9)	0.0025 (10)	0.0027 (10)
C13	0.0236 (12)	0.0234 (12)	0.0333 (14)	0.0038 (10)	0.0022 (11)	−0.0014 (11)
C14	0.0340 (14)	0.0187 (12)	0.0364 (15)	0.0064 (11)	0.0078 (11)	−0.0064 (11)
C15	0.0355 (14)	0.0177 (12)	0.0286 (13)	0.0017 (10)	0.0001 (11)	−0.0068 (10)
C16	0.0268 (12)	0.0180 (11)	0.0258 (13)	−0.0004 (10)	−0.0005 (10)	0.0010 (10)
C17	0.0236 (12)	0.0217 (12)	0.0266 (13)	0.0006 (10)	0.0025 (10)	−0.0035 (10)
C18	0.0278 (13)	0.0379 (15)	0.0396 (16)	0.0019 (11)	−0.0023 (12)	−0.0067 (12)
C19	0.0426 (14)	0.0249 (13)	0.0422 (16)	−0.0066 (11)	0.0027 (12)	−0.0034 (12)
C20	0.0270 (12)	0.0246 (13)	0.0387 (15)	0.0000 (10)	−0.0028 (11)	−0.0063 (11)
C21	0.0402 (15)	0.0378 (15)	0.0565 (19)	−0.0018 (13)	−0.0151 (13)	0.0062 (14)
C22	0.0322 (14)	0.0359 (15)	0.0551 (18)	−0.0058 (11)	0.0022 (13)	−0.0027 (13)

Geometric parameters (Å, °)

N1—C9	1.323 (2)	C13—C14	1.382 (3)
N1—C1	1.368 (2)	C13—H13	0.9500
N2—C10	1.270 (2)	C14—C15	1.372 (3)
N2—C11	1.432 (2)	C14—H14	0.9500
C1—C2	1.414 (3)	C15—C16	1.401 (3)
C1—C6	1.419 (3)	C15—H15	0.9500
C2—C3	1.365 (3)	C16—C20	1.522 (3)
C2—H2	0.9500	C17—C18	1.530 (3)

C3—C4	1.403 (3)	C17—C19	1.532 (3)
C3—H3	0.9500	C17—H17	1.0000
C4—C5	1.359 (3)	C18—H18A	0.9800
C4—H4	0.9500	C18—H18B	0.9800
C5—C6	1.417 (3)	C18—H18C	0.9800
C5—H5	0.9500	C19—H19A	0.9800
C6—C7	1.416 (3)	C19—H19B	0.9800
C7—C8	1.360 (3)	C19—H19C	0.9800
C7—H7	0.9500	C20—C21	1.528 (3)
C8—C9	1.410 (3)	C20—C22	1.534 (3)
C8—H8	0.9500	C20—H20	1.0000
C9—C10	1.474 (3)	C21—H21A	0.9800
C10—H10	0.9500	C21—H21B	0.9800
C11—C16	1.402 (3)	C21—H21C	0.9800
C11—C12	1.406 (3)	C22—H22A	0.9800
C12—C13	1.391 (3)	C22—H22B	0.9800
C12—C17	1.514 (3)	C22—H22C	0.9800
C9—N1—C1	117.94 (17)	C13—C14—H14	119.9
C10—N2—C11	119.16 (18)	C14—C15—C16	121.5 (2)
N1—C1—C2	118.85 (19)	C14—C15—H15	119.3
N1—C1—C6	122.11 (18)	C16—C15—H15	119.3
C2—C1—C6	119.04 (18)	C15—C16—C11	117.35 (19)
C3—C2—C1	120.3 (2)	C15—C16—C20	119.13 (19)
C3—C2—H2	119.8	C11—C16—C20	123.52 (18)
C1—C2—H2	119.8	C12—C17—C18	113.70 (17)
C2—C3—C4	120.6 (2)	C12—C17—C19	110.37 (18)
C2—C3—H3	119.7	C18—C17—C19	110.30 (18)
C4—C3—H3	119.7	C12—C17—H17	107.4
C5—C4—C3	120.6 (2)	C18—C17—H17	107.4
C5—C4—H4	119.7	C19—C17—H17	107.4
C3—C4—H4	119.7	C17—C18—H18A	109.5
C4—C5—C6	120.5 (2)	C17—C18—H18B	109.5
C4—C5—H5	119.8	H18A—C18—H18B	109.5
C6—C5—H5	119.8	C17—C18—H18C	109.5
C7—C6—C5	123.33 (19)	H18A—C18—H18C	109.5
C7—C6—C1	117.73 (18)	H18B—C18—H18C	109.5
C5—C6—C1	118.93 (19)	C17—C19—H19A	109.5
C8—C7—C6	119.5 (2)	C17—C19—H19B	109.5
C8—C7—H7	120.3	H19A—C19—H19B	109.5
C6—C7—H7	120.3	C17—C19—H19C	109.5
C7—C8—C9	119.10 (19)	H19A—C19—H19C	109.5
C7—C8—H8	120.5	H19B—C19—H19C	109.5
C9—C8—H8	120.5	C16—C20—C21	110.49 (18)
N1—C9—C8	123.67 (18)	C16—C20—C22	111.93 (18)
N1—C9—C10	115.18 (19)	C21—C20—C22	110.86 (19)
C8—C9—C10	121.14 (19)	C16—C20—H20	107.8
N2—C10—C9	121.1 (2)	C21—C20—H20	107.8
N2—C10—H10	119.4	C22—C20—H20	107.8
C9—C10—H10	119.4	C20—C21—H21A	109.5

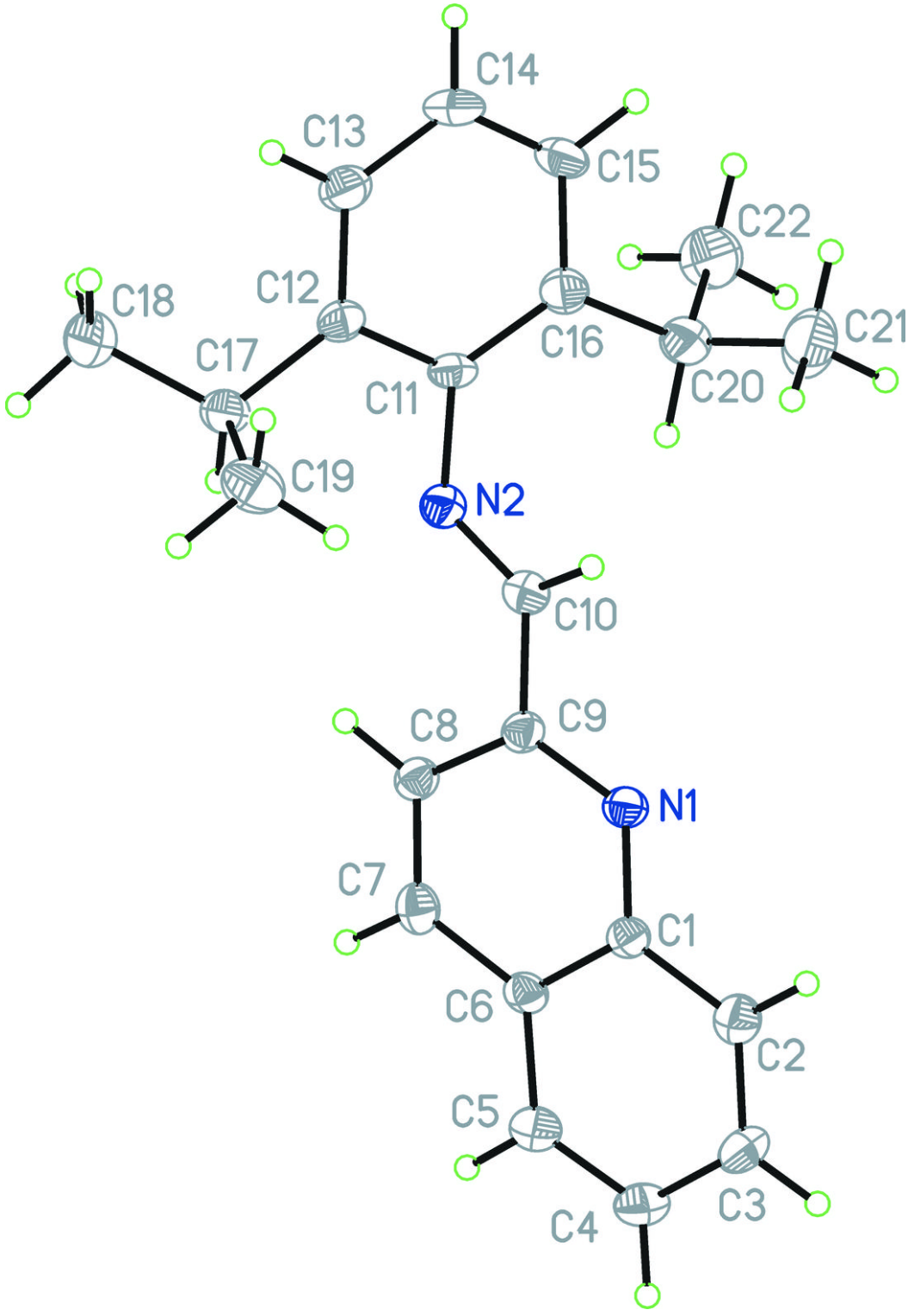
C16—C11—C12	122.09 (18)	C20—C21—H21B	109.5
C16—C11—N2	121.48 (18)	H21A—C21—H21B	109.5
C12—C11—N2	116.34 (18)	C20—C21—H21C	109.5
C13—C12—C11	117.71 (19)	H21A—C21—H21C	109.5
C13—C12—C17	121.52 (18)	H21B—C21—H21C	109.5
C11—C12—C17	120.67 (17)	C20—C22—H22A	109.5
C14—C13—C12	121.2 (2)	C20—C22—H22B	109.5
C14—C13—H13	119.4	H22A—C22—H22B	109.5
C12—C13—H13	119.4	C20—C22—H22C	109.5
C15—C14—C13	120.17 (19)	H22A—C22—H22C	109.5
C15—C14—H14	119.9	H22B—C22—H22C	109.5
C9—N1—C1—C2	179.57 (18)	C10—N2—C11—C12	−118.6 (2)
C9—N1—C1—C6	−0.4 (3)	C16—C11—C12—C13	−0.9 (3)
N1—C1—C2—C3	−179.84 (19)	N2—C11—C12—C13	−177.40 (17)
C6—C1—C2—C3	0.1 (3)	C16—C11—C12—C17	−177.39 (19)
C1—C2—C3—C4	−0.4 (3)	N2—C11—C12—C17	6.1 (3)
C2—C3—C4—C5	0.2 (3)	C11—C12—C13—C14	0.9 (3)
C3—C4—C5—C6	0.3 (3)	C17—C12—C13—C14	177.4 (2)
C4—C5—C6—C7	180.0 (2)	C12—C13—C14—C15	−0.6 (3)
C4—C5—C6—C1	−0.6 (3)	C13—C14—C15—C16	0.3 (3)
N1—C1—C6—C7	−0.2 (3)	C14—C15—C16—C11	−0.2 (3)
C2—C1—C6—C7	179.85 (18)	C14—C15—C16—C20	179.2 (2)
N1—C1—C6—C5	−179.68 (17)	C12—C11—C16—C15	0.6 (3)
C2—C1—C6—C5	0.4 (3)	N2—C11—C16—C15	176.88 (18)
C5—C6—C7—C8	−179.93 (19)	C12—C11—C16—C20	−178.88 (19)
C1—C6—C7—C8	0.6 (3)	N2—C11—C16—C20	−2.6 (3)
C6—C7—C8—C9	−0.5 (3)	C13—C12—C17—C18	33.5 (3)
C1—N1—C9—C8	0.6 (3)	C11—C12—C17—C18	−150.12 (19)
C1—N1—C9—C10	−179.74 (16)	C13—C12—C17—C19	−91.0 (2)
C7—C8—C9—N1	−0.1 (3)	C11—C12—C17—C19	85.3 (2)
C7—C8—C9—C10	−179.82 (18)	C15—C16—C20—C21	66.5 (2)
C11—N2—C10—C9	−177.95 (17)	C11—C16—C20—C21	−114.1 (2)
N1—C9—C10—N2	171.13 (18)	C15—C16—C20—C22	−57.6 (3)
C8—C9—C10—N2	−9.2 (3)	C11—C16—C20—C22	121.8 (2)
C10—N2—C11—C16	64.9 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···N1^{i}	0.95	2.61	3.464 (3)	151

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

Fig. 1


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