Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(2,6-Diphenylpiperidin-4-ylidene)-(phenyl)acetonitrile

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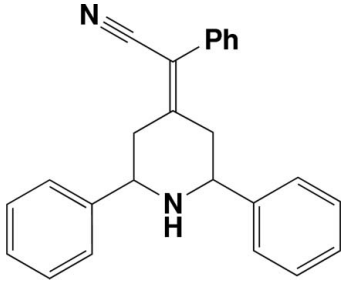
Received 4 May 2007; accepted 7 May 2007

Key indicators: single-crystal X-ray study; T = 160 K; mean σ(C–C) = 0.003 Å; R factor = 0.052; wR factor = 0.144; data-to-parameter ratio = 13.5.

In the title molecule, $C_{25}H_{22}N_2$, the piperidine ring adopts a chair conformation. The two phenyl rings attached to the piperidine ring have equatorial orientations and make a dihedral angle of 17.9 (1)°. The phenylacetonitrile group has a bisectional orientation. Molecules are linked by intramolecular C—H···N interactions, and by N—H···π and C—H···π interactions.

Related literature

For related literature, see: Lavagnino & Shepard (1957); Balamurugan *et al.* (2006, 2007). Balamurugan *et al.* (2006, 2007) have reported crystal structures of di-2-furylpiperidin-4-one derivatives, where the piperidine ring adopts chair and twist–boat conformations.



Experimental

Crystal data

$C_{25}H_{22}N_2$
M_r = 350.45
Triclinic, $P\overline{1}$
a = 7.5687 (3) Å
b = 11.3610 (5) Å
c = 12.1481 (5) Å
α = 111.318 (2)°
β = 92.757 (2)°
γ = 97.920 (2)°
V = 958.36 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 160 (1) K
0.28 × 0.28 × 0.18 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: none
12846 measured reflections
3338 independent reflections
2742 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.144
S = 1.05
3338 reflections
248 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of rings C61–C66 and C411–C416, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C22—H22···N1	0.95	2.56	2.873 (2)	100
C66—H66···N1	0.95	2.50	2.834 (2)	101
N1—H1···*Cg*1^{i}	0.90 (2)	2.68 (2)	3.537 (2)	159.4 (2)
C62—H62···*Cg*2^{ii}	0.95	2.74	3.639	159

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

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

The data collection was carried out by Dr A. Linden of the Institute of Organic Chemistry at the University of Zurich; his help is gratefully acknowledged by AT.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WW2085).

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 doi:10.1107/S1600536807022386

supplementary materials

Acta Cryst. (2007). E**63**, o2903 [**doi:10.1107/S1600536807022386**]

(2,6-Diphenylpiperidin-4-ylidene)(phenyl)acetonitrile

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Comment

In the title compound, (I), (Fig. 1), piperidine ring adopts a chair conformation. Two phenyl rings attached to the piperidine ring in positions 2 and 6 have equatorial orientations and make a dihedral angle of 17.9 (1)°. The phenyl-acetonitrile group at position 4 has a bisectional orientation. Molecules are linked by C22—H22···N1, C66—H66···N1 intramolecular and intermolecular hydrogen bonds: N1—H1···π (1-x, 1-y, 2-z) involving the phenyl ring at position 6 and C62—H62···π (1-x, -y, 2-z) involving the phenyl ring at C41.

Experimental

The title compound was prepared following the general procedure reported by Lavagnino & Shepard (1957). A mixture of r(2),c(6)-diphenylpiperidin-4-one (2.51 g, 0.01 mol), benzylcyanide (1.15 ml, 0.01 mol) and potassium hydroxide (0.66 g, 0.01 mol) in 50 ml of absolute ethanol. The solution was heated on water bath for 2 days. Then diluted with 25 ml water and chilled in an ice bath. The solid mass which separated was filtered off, dried and recrystallized from ethanol. The yield of the isolated product was 2.09 g (60%).

Refinement

The H atom bonded to N1 was located in a difference Fourier map and refined isotropically. The C-bound H atoms were positioned geometrically and allowed to ride on their parent atoms with C—H = 0.95–1.00 Å and U_{iso}(H) = 1.2U_{eq}(parent atom).

Figures

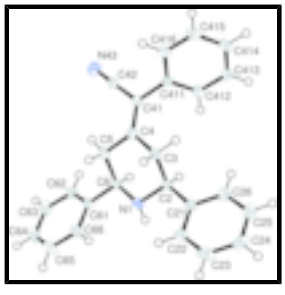


Fig. 1. View of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

(2,6-Diphenylpiperidin-4-ylidene)(phenyl)acetonitrile

Crystal data

$C_{25}H_{22}N_2$	$Z = 2$
$M_r = 350.45$	$F_{000} = 372$

Triclinic, $P\bar{1}$	D_x = 1.214 Mg m^{-3}
Hall symbol: -P 1	Melting point: 441(1) K
a = 7.5687 (3) Å	Mo $K\alpha$ radiation λ = 0.71073 Å
b = 11.3610 (5) Å	Cell parameters from 3245 reflections
c = 12.1481 (5) Å	θ = 2.0–25.0º
α = 111.318 (2)º	μ = 0.07 mm^{-1}
β = 92.757 (2)º	T = 160 (1) K
γ = 97.920 (2)º	Plate-like, yellow
V = 958.36 (7) Å^3	0.28 × 0.28 × 0.18 mm

Data collection

Nonius KappaCCD area-detector diffractometer	3338 independent reflections
Radiation source: Nonius FR590 sealed tube generator	2742 reflections with $I > 2\sigma(I)$
Monochromator: horizontally mounted graphite crystal	R_{int} = 0.055
Detector resolution: 9 pixels mm^{-1}	θ_{max} = 25.0º
T = 160(1) K	θ_{min} = 2.1º
ω scans with κ offsets	h = −8→8
Absorption correction: none	k = −13→13
12846 measured reflections	l = −14→14

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0746P)^2 + 0.3813P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.052	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.144	$\Delta\rho_{max}$ = 0.27 e Å^{-3}
S = 1.05	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
3338 reflections	Extinction correction: none
248 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

Special details

Experimental. Solvent used: ethanol Cooling Device: Oxford Cryosystems Cryostream 700 Crystal mount: glued on a glass fibre Mosaicity (deg.): 0.483 (2) Frames collected: 193 Seconds exposure per frame: 38 Degrees rotation per frame: 2.0 Crystal-Detector distance (mm): 30.0

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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	0.2897 (2)	0.28665 (14)	0.85699 (12)	0.0234 (5)
N43	0.2792 (2)	−0.07061 (15)	1.11208 (13)	0.0337 (5)
C2	0.3019 (2)	0.16655 (15)	0.75950 (14)	0.0221 (5)
C3	0.1698 (2)	0.05895 (16)	0.77310 (15)	0.0245 (5)
C4	0.2102 (2)	0.04948 (16)	0.89088 (15)	0.0247 (5)
C5	0.2147 (3)	0.17506 (16)	0.99182 (15)	0.0259 (5)
C6	0.3418 (2)	0.28366 (16)	0.97355 (14)	0.0228 (5)
C21	0.2547 (2)	0.17135 (16)	0.63899 (15)	0.0231 (5)
C22	0.1527 (3)	0.25663 (17)	0.62196 (16)	0.0305 (6)
C23	0.1094 (3)	0.25267 (18)	0.50784 (17)	0.0351 (6)
C24	0.1656 (3)	0.16411 (19)	0.41083 (16)	0.0334 (6)
C25	0.2624 (3)	0.07576 (19)	0.42646 (16)	0.0326 (6)
C26	0.3064 (3)	0.08000 (18)	0.53961 (15)	0.0289 (6)
C41	0.2409 (2)	−0.05984 (16)	0.90312 (14)	0.0224 (5)
C42	0.2639 (2)	−0.06391 (16)	1.02001 (15)	0.0229 (5)
C61	0.3303 (2)	0.40939 (15)	1.07285 (15)	0.0229 (5)
C62	0.4168 (3)	0.43681 (17)	1.18522 (16)	0.0294 (6)
C63	0.4012 (3)	0.54702 (18)	1.27961 (16)	0.0332 (6)
C64	0.3011 (3)	0.63333 (18)	1.26372 (17)	0.0339 (6)
C65	0.2169 (3)	0.60898 (18)	1.15273 (17)	0.0353 (6)
C66	0.2303 (3)	0.49737 (17)	1.05758 (17)	0.0297 (6)
C411	0.2472 (2)	−0.18250 (16)	0.80123 (14)	0.0219 (5)
C412	0.3720 (2)	−0.18561 (17)	0.72031 (15)	0.0262 (5)
C413	0.3729 (3)	−0.29637 (17)	0.62162 (15)	0.0282 (6)
C414	0.2500 (3)	−0.40591 (17)	0.60354 (16)	0.0280 (5)
C415	0.1280 (3)	−0.40399 (17)	0.68462 (16)	0.0292 (6)
C416	0.1269 (3)	−0.29380 (16)	0.78340 (16)	0.0268 (6)
H1	0.369 (3)	0.349 (2)	0.8489 (18)	0.032 (5)*
H2	0.42655	0.14747	0.76422	0.0265*
H3A	0.04586	0.07614	0.76593	0.0294*
H3B	0.17785	−0.02350	0.70878	0.0294*
H5A	0.25571	0.16749	1.06722	0.0310*
H5B	0.09216	0.19647	0.99775	0.0310*
H6	0.46768	0.26643	0.97639	0.0273*
H22	0.11217	0.31797	0.68822	0.0366*
H23	0.04009	0.31198	0.49694	0.0421*

H24	0.13807	0.16362	0.33352	0.0401*
H25	0.29848	0.01237	0.35966	0.0391*
H26	0.37339	0.01920	0.54979	0.0346*
H62	0.48774	0.37882	1.19713	0.0353*
H63	0.45969	0.56346	1.35593	0.0399*
H64	0.29037	0.70903	1.32881	0.0407*
H65	0.14914	0.66877	1.14112	0.0424*
H66	0.17080	0.48112	0.98158	0.0356*
H412	0.45739	−0.11123	0.73267	0.0314*
H413	0.45778	−0.29715	0.56637	0.0338*
H414	0.24992	−0.48166	0.53582	0.0336*
H415	0.04390	−0.47891	0.67264	0.0351*
H416	0.04356	−0.29416	0.83935	0.0322*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0313 (9)	0.0161 (8)	0.0203 (8)	0.0036 (6)	0.0011 (6)	0.0044 (6)
N43	0.0441 (10)	0.0307 (9)	0.0234 (9)	0.0011 (7)	0.0014 (7)	0.0088 (7)
C2	0.0261 (9)	0.0177 (9)	0.0196 (9)	0.0061 (7)	0.0003 (7)	0.0031 (7)
C3	0.0293 (10)	0.0179 (9)	0.0223 (9)	0.0030 (7)	−0.0005 (7)	0.0036 (7)
C4	0.0291 (10)	0.0202 (9)	0.0214 (9)	0.0004 (7)	0.0026 (7)	0.0053 (7)
C5	0.0338 (10)	0.0213 (9)	0.0200 (9)	0.0040 (7)	0.0045 (7)	0.0047 (7)
C6	0.0271 (9)	0.0194 (9)	0.0193 (9)	0.0058 (7)	0.0022 (7)	0.0037 (7)
C21	0.0265 (9)	0.0182 (9)	0.0227 (9)	0.0010 (7)	0.0001 (7)	0.0069 (7)
C22	0.0407 (11)	0.0204 (9)	0.0279 (10)	0.0066 (8)	−0.0028 (8)	0.0064 (8)
C23	0.0438 (12)	0.0251 (10)	0.0355 (11)	0.0032 (8)	−0.0125 (9)	0.0133 (9)
C24	0.0385 (11)	0.0355 (11)	0.0243 (10)	−0.0091 (9)	−0.0092 (8)	0.0158 (9)
C25	0.0358 (11)	0.0370 (11)	0.0217 (9)	0.0019 (8)	0.0029 (8)	0.0087 (8)
C26	0.0329 (10)	0.0312 (10)	0.0240 (9)	0.0099 (8)	0.0053 (8)	0.0102 (8)
C41	0.0272 (9)	0.0183 (9)	0.0191 (8)	0.0010 (7)	0.0028 (7)	0.0051 (7)
C42	0.0269 (9)	0.0172 (9)	0.0208 (9)	0.0005 (7)	0.0028 (7)	0.0038 (7)
C61	0.0257 (9)	0.0161 (9)	0.0231 (9)	0.0010 (7)	0.0028 (7)	0.0039 (7)
C62	0.0361 (11)	0.0243 (10)	0.0248 (9)	0.0077 (8)	0.0007 (8)	0.0049 (8)
C63	0.0380 (11)	0.0312 (10)	0.0220 (9)	0.0036 (8)	0.0011 (8)	0.0011 (8)
C64	0.0356 (11)	0.0223 (10)	0.0305 (10)	0.0025 (8)	0.0063 (8)	−0.0052 (8)
C65	0.0367 (11)	0.0238 (10)	0.0399 (12)	0.0121 (8)	0.0017 (9)	0.0032 (8)
C66	0.0321 (10)	0.0230 (9)	0.0288 (10)	0.0065 (8)	−0.0021 (8)	0.0037 (8)
C411	0.0288 (10)	0.0173 (9)	0.0183 (8)	0.0039 (7)	0.0007 (7)	0.0053 (7)
C412	0.0310 (10)	0.0220 (9)	0.0215 (9)	−0.0007 (7)	0.0017 (7)	0.0054 (7)
C413	0.0334 (10)	0.0284 (10)	0.0199 (9)	0.0050 (8)	0.0060 (7)	0.0055 (7)
C414	0.0363 (10)	0.0199 (9)	0.0232 (9)	0.0084 (8)	−0.0015 (8)	0.0019 (7)
C415	0.0332 (10)	0.0166 (9)	0.0348 (10)	−0.0001 (7)	0.0002 (8)	0.0079 (8)
C416	0.0312 (10)	0.0211 (9)	0.0288 (10)	0.0052 (7)	0.0079 (8)	0.0092 (8)

Geometric parameters (Å, °)

N1—C2	1.464 (2)	C3—H3A	0.9900
N1—C6	1.465 (2)	C3—H3B	0.9900

N43—C42	1.150 (2)	C5—H5B	0.9900
N1—H1	0.90 (2)	C5—H5A	0.9900
C2—C3	1.532 (3)	C6—H6	1.0000
C2—C21	1.512 (2)	C22—H22	0.9500
C3—C4	1.494 (2)	C23—H23	0.9500
C4—C5	1.500 (3)	C24—H24	0.9500
C4—C41	1.352 (3)	C25—H25	0.9500
C5—C6	1.546 (3)	C26—H26	0.9500
C6—C61	1.515 (2)	C62—H62	0.9500
C21—C22	1.384 (3)	C63—H63	0.9500
C21—C26	1.391 (3)	C64—H64	0.9500
C22—C23	1.392 (3)	C65—H65	0.9500
C23—C24	1.373 (3)	C66—H66	0.9500
C24—C25	1.381 (3)	C411—C416	1.393 (3)
C25—C26	1.381 (3)	C411—C412	1.390 (2)
C41—C411	1.499 (2)	C412—C413	1.388 (3)
C41—C42	1.441 (2)	C413—C414	1.387 (3)
C61—C62	1.392 (3)	C414—C415	1.379 (3)
C61—C66	1.392 (3)	C415—C416	1.385 (3)
C62—C63	1.381 (3)	C412—H412	0.9500
C63—C64	1.379 (3)	C413—H413	0.9500
C64—C65	1.378 (3)	C414—H414	0.9500
C65—C66	1.391 (3)	C415—H415	0.9500
C2—H2	1.0000	C416—H416	0.9500
N1···H22	2.5600	H3A···C25^{v}	3.0500
N1···H66	2.5000	H3B···C26	2.8600
N43···H25^{i}	2.8000	H3B···C411	2.5500
N43···H3A^{ii}	2.9400	H3B···C412	2.5500
N43···H412^{iii}	2.7300	H3B···H412	2.5100
C2···C64^{iv}	3.598 (3)	H3B···C24^{v}	2.8700
C3···C412	3.232 (3)	H3B···H24^{v}	2.6000
C3···C24^{v}	3.380 (3)	H5A···C42	2.4900
C24···C3^{v}	3.380 (3)	H5A···C62	2.9200
C64···C2^{iv}	3.598 (3)	H5B···C42^{ii}	2.8600
C3···H412	3.0500	H5B···H416^{ii}	2.2600
C3···H24^{v}	3.0300	H6···H2	2.4200
C4···H412	3.0400	H6···H62	2.5000
C5···H416^{ii}	2.9900	H22···N1	2.5600
C22···H1	2.89 (2)	H22···H1	2.5800
C22···H415^{vi}	3.0800	H22···H415^{vi}	2.5000
C23···H414^{vi}	2.9500	H23···H414^{vi}	2.5200
C24···H3B^{v}	2.8700	H23···H415^{vi}	2.5500
C24···H413^{vii}	2.9900	H23···C414^{v}	2.9600
C24···H3A^{v}	2.9700	H23···C415^{v}	3.0600
C25···H3A^{v}	3.0500	H24···C3^{v}	3.0300

C25···H413^{vii}	3.0300	H24···H3B^{v}	2.6000
C25···H412^{vii}	3.0200	H25···N43^{viii}	2.8000
C26···H3B	2.8600	H25···H412^{vii}	2.5500
C26···H26^{vii}	2.9100	H26···H2	2.4600
C42···H416	2.9500	H26···C26^{vii}	2.9100
C42···H5B^{ii}	2.8600	H26···H26^{vii}	2.3200
C42···H5A	2.4900	H62···H6	2.5000
C62···H1^{iv}	2.90 (2)	H62···C412^{iii}	3.0200
C62···H5A	2.9200	H62···C413^{iii}	2.9000
C63···H1^{iv}	2.81 (2)	H62···C414^{iii}	2.9500
C64···H1^{iv}	2.92 (2)	H63···H413^{ix}	2.4700
C66···H1	2.83 (2)	H66···N1	2.5000
C412···C3	3.232 (3)	H66···H1	2.4900
C411···H3B	2.5500	H412···C3	3.0500
C412···H3B	2.5500	H412···C4	3.0400
C412···H62^{iii}	3.0200	H412···H3B	2.5100
C413···H62^{iii}	2.9000	H412···N43^{iii}	2.7300
C414···H23^{v}	2.9600	H412···C25^{vii}	3.0200
C414···H62^{iii}	2.9500	H412···H25^{vii}	2.5500
C415···H23^{v}	3.0600	H413···H63^{x}	2.4700
H1···C22	2.89 (2)	H413···C24^{vii}	2.9900
H1···C66	2.83 (2)	H413···C25^{vii}	3.0300
H1···H22	2.5800	H414···C23^{xi}	2.9500
H1···H66	2.4900	H414···H23^{xi}	2.5200
H1···C62^{iv}	2.90 (2)	H415···C22^{xi}	3.0800
H1···C63^{iv}	2.81 (2)	H415···H22^{xi}	2.5000
H1···C64^{iv}	2.92 (2)	H415···H23^{xi}	2.5500
H2···H6	2.4200	H416···C42	2.9500
H2···H26	2.4600	H416···C5^{ii}	2.9900
H3A···N43^{ii}	2.9400	H416···H5B^{ii}	2.2600
H3A···C24^{v}	2.9700		
C2—N1—C6	112.35 (14)	C6—C5—H5A	109.00
C2—N1—H1	107.7 (14)	C6—C5—H5B	109.00
C6—N1—H1	106.2 (13)	H5A—C5—H5B	108.00
N1—C2—C3	108.33 (13)	C61—C6—H6	109.00
C3—C2—C21	108.25 (13)	N1—C6—H6	109.00
N1—C2—C21	112.35 (15)	C5—C6—H6	109.00
C2—C3—C4	110.66 (14)	C21—C22—H22	120.00
C3—C4—C5	111.94 (16)	C23—C22—H22	120.00
C3—C4—C41	123.22 (16)	C24—C23—H23	120.00
C5—C4—C41	124.83 (16)	C22—C23—H23	120.00
C4—C5—C6	111.10 (15)	C25—C24—H24	120.00
C5—C6—C61	108.78 (13)	C23—C24—H24	120.00
N1—C6—C61	111.40 (15)	C26—C25—H25	120.00

N1—C6—C5	109.03 (14)	C24—C25—H25	120.00
C2—C21—C26	118.25 (16)	C21—C26—H26	119.00
C22—C21—C26	118.37 (17)	C25—C26—H26	119.00
C2—C21—C22	123.24 (15)	C63—C62—H62	119.00
C21—C22—C23	120.08 (18)	C61—C62—H62	119.00
C22—C23—C24	120.8 (2)	C62—C63—H63	120.00
C23—C24—C25	119.54 (18)	C64—C63—H63	120.00
C24—C25—C26	119.69 (18)	C65—C64—H64	120.00
C21—C26—C25	121.4 (2)	C63—C64—H64	120.00
C4—C41—C411	124.24 (15)	C64—C65—H65	120.00
C4—C41—C42	119.75 (16)	C66—C65—H65	120.00
C42—C41—C411	115.97 (16)	C65—C66—H66	120.00
N43—C42—C41	178.0 (2)	C61—C66—H66	120.00
C6—C61—C62	119.30 (16)	C41—C411—C412	119.85 (16)
C62—C61—C66	118.17 (17)	C41—C411—C416	121.41 (15)
C6—C61—C66	122.48 (15)	C412—C411—C416	118.71 (17)
C61—C62—C63	121.02 (19)	C411—C412—C413	120.62 (18)
C62—C63—C64	120.37 (18)	C412—C413—C414	120.12 (18)
C63—C64—C65	119.49 (19)	C413—C414—C415	119.49 (18)
C64—C65—C66	120.4 (2)	C414—C415—C416	120.60 (19)
C61—C66—C65	120.51 (18)	C411—C416—C415	120.43 (18)
N1—C2—H2	109.00	C411—C412—H412	120.00
C3—C2—H2	109.00	C413—C412—H412	120.00
C21—C2—H2	109.00	C412—C413—H413	120.00
C4—C3—H3A	109.00	C414—C413—H413	120.00
C2—C3—H3A	110.00	C413—C414—H414	120.00
C2—C3—H3B	110.00	C415—C414—H414	120.00
C4—C3—H3B	110.00	C414—C415—H415	120.00
H3A—C3—H3B	108.00	C416—C415—H415	120.00
C4—C5—H5A	109.00	C411—C416—H416	120.00
C4—C5—H5B	109.00	C415—C416—H416	120.00
C6—N1—C2—C3	62.57 (17)	C2—C21—C26—C25	177.69 (19)
C6—N1—C2—C21	−177.90 (13)	C22—C21—C26—C25	1.9 (3)
C2—N1—C6—C5	−60.63 (18)	C21—C22—C23—C24	0.5 (3)
C2—N1—C6—C61	179.31 (13)	C22—C23—C24—C25	1.7 (3)
N1—C2—C3—C4	−58.01 (17)	C23—C24—C25—C26	−2.0 (3)
C21—C2—C3—C4	179.91 (13)	C24—C25—C26—C21	0.3 (3)
N1—C2—C21—C22	−21.6 (2)	C4—C41—C411—C412	59.5 (2)
N1—C2—C21—C26	162.77 (16)	C4—C41—C411—C416	−118.7 (2)
C3—C2—C21—C22	98.0 (2)	C42—C41—C411—C412	−122.58 (17)
C3—C2—C21—C26	−77.65 (19)	C42—C41—C411—C416	59.2 (2)
C2—C3—C4—C5	54.50 (19)	C6—C61—C62—C63	−176.33 (18)
C2—C3—C4—C41	−124.73 (17)	C66—C61—C62—C63	1.2 (3)
C3—C4—C5—C6	−52.5 (2)	C6—C61—C66—C65	177.04 (18)
C41—C4—C5—C6	126.76 (17)	C62—C61—C66—C65	−0.4 (3)
C3—C4—C41—C42	−174.76 (14)	C61—C62—C63—C64	−0.9 (3)
C3—C4—C41—C411	3.1 (3)	C62—C63—C64—C65	−0.2 (3)
C5—C4—C41—C42	6.1 (3)	C63—C64—C65—C66	0.9 (3)
C5—C4—C41—C411	−176.04 (16)	C64—C65—C66—C61	−0.6 (3)

C4—C5—C6—N1	54.1 (2)	C41—C411—C412—C413	−176.23 (17)
C4—C5—C6—C61	175.76 (14)	C416—C411—C412—C413	2.0 (3)
N1—C6—C61—C62	−163.58 (16)	C41—C411—C416—C415	176.03 (18)
N1—C6—C61—C66	19.0 (2)	C412—C411—C416—C415	−2.2 (3)
C5—C6—C61—C62	76.2 (2)	C411—C412—C413—C414	−0.8 (3)
C5—C6—C61—C66	−101.3 (2)	C412—C413—C414—C415	−0.4 (3)
C2—C21—C22—C23	−177.83 (18)	C413—C414—C415—C416	0.2 (3)
C26—C21—C22—C23	−2.2 (3)	C414—C415—C416—C411	1.1 (3)

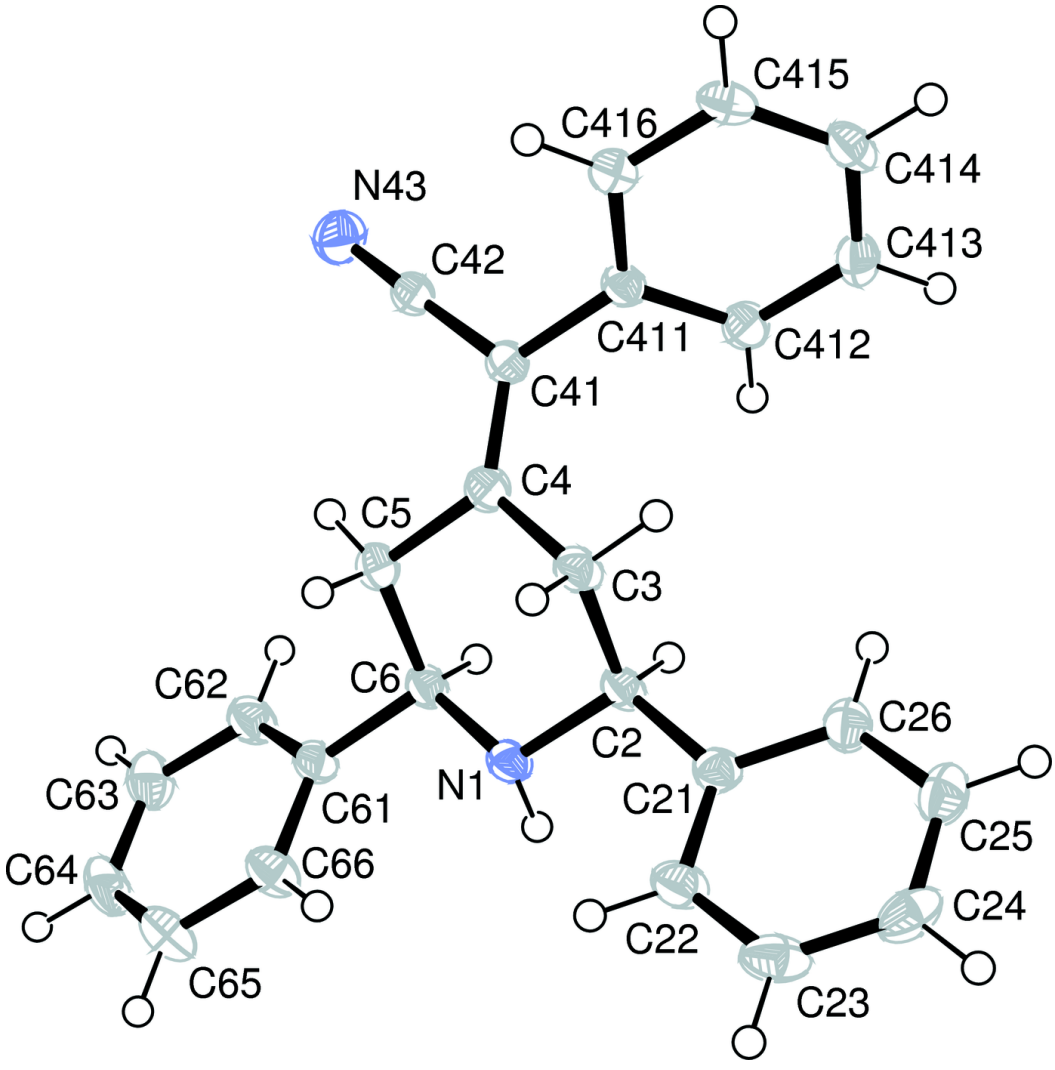
Symmetry codes: (i) *x*, *y*, *z*+1; (ii) −*x*, −*y*, −*z*+2; (iii) −*x*+1, −*y*, −*z*+2; (iv) −*x*+1, −*y*+1, −*z*+2; (v) −*x*, −*y*, −*z*+1; (vi) *x*, *y*+1, *z*; (vii) −*x*+1, −*y*, −*z*+1; (viii) *x*, *y*, *z*−1; (ix) *x*, *y*+1, *z*+1; (x) *x*, *y*−1, *z*−1; (xi) *x*, *y*−1, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C22—H22···N1	0.95	2.56	2.873 (2)	100
C66—H66···N1	0.95	2.50	2.834 (2)	101
N1—H1···Cg^{iv}	0.90 (2)	2.68 (2)	3.537 (2)	159.4 (2)
C62—H62···Cg^{iii}	0.95	2.74	3.639	159

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

Fig. 1


C415
C416
C414
N43
C42
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C411
C412
C41
C4
C5
C3
C62
C6
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C2
C63
N1
C21
C61
C25
C64
C66
C24
C22
C65
C23