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2-[2,6-Bis(2-chlorophenyl)piperidin-4-ylidene]malononitrile

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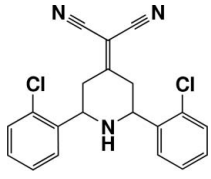
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.124; data-to-parameter ratio = 26.3.

The piperidine ring of the title molecule, $C_{20}H_{15}Cl_2N_3$, is in a chair form. The dihedral angle between the two chlorophenyl rings is 38.4 (1)°. The benzene rings are in equatorial orientations. The malononitrile group is planar. Intramolecular C—H···Cl and C—H···N hydrogen bonds are found in the crystal structure.

Related literature

For applications of piperidines, see: Jayabharathi *et al.* (2007); Manimekalai *et al.* 2000. For a related crystal structure, see: Thiruvalluvar *et al.* (2007).



Experimental

Crystal data

$C_{20}H_{15}Cl_2N_3$
M_r = 368.25
Monoclinic, $P2_1/c$
a = 15.1732 (10) Å
b = 7.5493 (5) Å
c = 16.3452 (12) Å
β = 105.494 (7)°
V = 1804.3 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 200 (2) K
0.51 × 0.44 × 0.21 mm

Data collection

Oxford Diffraction Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.829, T_{max} = 0.926
17148 measured reflections
6044 independent reflections
2122 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.124
S = 0.89
6044 reflections
230 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···Cl1	1.00	2.74	3.0777 (18)	100
C6—H6···Cl2	1.00	2.60	3.0909 (18)	110
C26—H26···N1	0.95	2.45	2.795 (2)	102

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); 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).

RJB acknowledges the NSF–MRI program for funding to purchase the X-ray CCD diffractometer. JJ is grateful to the UGC, New Delhi [F. No. 30-71/2004(SR)], for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2063).

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supplementary materials

Acta Cryst. (2007). E**63**, o4853 [**doi:10.1107/S1600536807060059**]

2-[2,6-Bis(2-chlorophenyl)piperidin-4-ylidene]malononitrile

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Comment

Jayabharathi *et al.* (2007) have reported synthesis, stereochemistry and antimicrobial evaluation of *t*3-benzyl-*r*2,*c*6-diarylpiperidin-4-one and its derivatives. Manimekalai *et al.* (2000) have reported ^{13}C– and ^{1}H-NMR spectral studies of some *t*3-carboxyethyl-*r*2,*c*6-diphenylpiperidine derivatives. Thiruvalluvar *et al.* (2007) have reported a crystal structure of 3-ethyl-2,6-diphenylpiperidin-4-ol wherein the piperidine ring is in chair form. The piperidine ring of the title molecule, $C_{20}H_{15}Cl_2N_3$, is in chair form too. The dihedral angle between the two chlorophenyl rings is 38.4 (1)°. The phenyl rings at 2 and 6 positions are in equatorial orientations. The malononitrile group at position 4 has a coplanar orientation. Weak C—H···Cl and C—H···N intramolecular hydrogen bonds are found in the crystal structure.

Experimental

2,6-bis(*O*-chlorophenyl)piperidin-4-one (3 mmol, 1 g), ammonium acetate (3 mmol, 0.256 g) and basic alumina (3 mmol, 3 g) and malononitrile (3 mmol, 0.02 g) were mixed thoroughly in a mortar. The reaction mixture was placed in a beaker and irradiated using microwave in a microwave oven operating at 2450 Hz (100% power, 850 W) for 3 minutes. The reaction mixture was extracted with dichloromethane followed by water. The product was recrystallized from ethanol. The yield of the isolated product was 0.42 g (60%).

Refinement

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

Figures

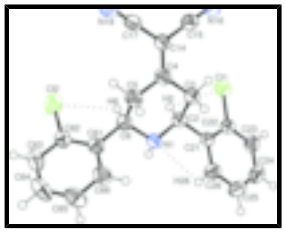


Fig. 1. The molecular structure of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at 50% probability level. H atoms are shown as small spheres of arbitrary radius.

2-[2,6-Bis(2-chlorophenyl)piperidin-4-ylidene]malononitrile

Crystal data

$C_{20}H_{15}Cl_2N_3$ F_{000} = 760

M_r = 368.25	D_x = 1.356 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 452 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 15.1732 (10) Å	Cell parameters from 3546 reflections
b = 7.5493 (5) Å	θ = 4.7–32.8º
c = 16.3452 (12) Å	μ = 0.37 mm^{-1}
β = 105.494 (7)º	T = 200 (2) K
V = 1804.3 (2) Å^3	Plate, pale yellow
Z = 4	0.51 × 0.44 × 0.21 mm

Data collection

Oxford Diffraction Gemini diffractometer	6044 independent reflections
Radiation source: fine–focus sealed tube	2122 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.050
T = 200(2) K	θ_{max} = 32.8º
φ and ω scans	θ_{min} = 4.7º
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	h = −22→21
T_{min} = 0.829, T_{max} = 0.926	k = −11→11
17148 measured reflections	l = −17→24

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.041	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.124	$w = 1/[\sigma^2(F_o^2) + (0.0517P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.89	$(\Delta/\sigma)_{max}$ = <0.002
6044 reflections	$\Delta\rho_{max}$ = 0.22 e Å^{-3}
230 parameters	$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All s.u.'s are estimated from the variances of the (full) variance–covariance matrix. The cell s.u.'s 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 $F^2 > 2\sigma(F^2)$ 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}
Cl1	0.51594 (3)	0.83403 (7)	0.09858 (4)	0.0614 (2)
Cl2	0.20649 (5)	0.40648 (8)	0.32315 (5)	0.0862 (3)
N1	0.27010 (10)	0.8856 (2)	0.19991 (11)	0.0415 (5)
N16	0.32725 (12)	0.4937 (3)	−0.09216 (11)	0.0692 (7)
N18	0.12217 (15)	0.2456 (3)	0.01170 (14)	0.0857 (9)
C2	0.33512 (11)	0.8643 (2)	0.14911 (11)	0.0391 (6)
C3	0.28114 (13)	0.8191 (2)	0.05805 (12)	0.0459 (6)
C4	0.22329 (11)	0.6593 (3)	0.05782 (12)	0.0432 (6)
C5	0.16425 (12)	0.6703 (3)	0.11789 (12)	0.0517 (7)
C6	0.22218 (11)	0.7209 (2)	0.20674 (11)	0.0416 (6)
C14	0.22543 (11)	0.5155 (3)	0.01047 (11)	0.0434 (6)
C15	0.28311 (13)	0.5028 (3)	−0.04622 (12)	0.0486 (7)
C17	0.16823 (14)	0.3631 (3)	0.01110 (13)	0.0554 (8)
C21	0.39066 (11)	1.0311 (2)	0.15015 (10)	0.0374 (6)
C22	0.47250 (12)	1.0308 (3)	0.12742 (11)	0.0429 (6)
C23	0.52285 (13)	1.1825 (3)	0.12783 (12)	0.0508 (7)
C24	0.49203 (13)	1.3408 (3)	0.15060 (13)	0.0547 (7)
C25	0.41203 (14)	1.3466 (3)	0.17392 (14)	0.0559 (7)
C26	0.36109 (12)	1.1931 (2)	0.17297 (12)	0.0476 (7)
C61	0.16153 (11)	0.7413 (3)	0.26566 (11)	0.0414 (6)
C62	0.14843 (12)	0.6070 (3)	0.31873 (12)	0.0472 (7)
C63	0.08924 (13)	0.6248 (3)	0.36937 (12)	0.0599 (8)
C64	0.04183 (13)	0.7797 (4)	0.36721 (13)	0.0651 (9)
C65	0.05376 (13)	0.9164 (3)	0.31606 (14)	0.0636 (8)
C66	0.11242 (12)	0.8965 (3)	0.26533 (13)	0.0535 (7)
H1	0.2970 (12)	0.917 (3)	0.2470 (12)	0.049 (6)*
H2	0.37742	0.76416	0.17265	0.0469*
H3A	0.24184	0.92063	0.03298	0.0550*
H3B	0.32408	0.79641	0.02306	0.0550*
H5A	0.13441	0.55450	0.12023	0.0620*
H5B	0.11581	0.76006	0.09739	0.0620*
H6	0.26803	0.62538	0.22874	0.0499*
H23	0.57886	1.17760	0.11236	0.0610*
H24	0.52616	1.44608	0.15019	0.0656*
H25	0.39118	1.45574	0.19082	0.0671*
H26	0.30499	1.19933	0.18823	0.0571*
H63	0.08152	0.53052	0.40532	0.0719*
H64	0.00043	0.79258	0.40135	0.0781*
H65	0.02166	1.02463	0.31559	0.0763*
H66	0.11943	0.99116	0.22929	0.0642*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0679 (3)	0.0520 (3)	0.0765 (4)	0.0007 (2)	0.0403 (3)	−0.0093 (3)
Cl2	0.1155 (5)	0.0572 (4)	0.1071 (5)	0.0202 (3)	0.0665 (4)	0.0268 (4)
N1	0.0461 (9)	0.0446 (10)	0.0375 (9)	−0.0067 (7)	0.0176 (8)	−0.0067 (9)
N16	0.0757 (12)	0.0742 (14)	0.0707 (12)	−0.0104 (10)	0.0422 (10)	−0.0109 (11)
N18	0.1039 (15)	0.0733 (14)	0.1018 (16)	−0.0402 (12)	0.0655 (13)	−0.0354 (13)
C2	0.0453 (10)	0.0367 (10)	0.0371 (10)	−0.0036 (8)	0.0143 (8)	−0.0019 (9)
C3	0.0547 (10)	0.0442 (11)	0.0428 (11)	−0.0087 (9)	0.0202 (9)	−0.0059 (10)
C4	0.0426 (10)	0.0504 (12)	0.0376 (10)	−0.0071 (8)	0.0123 (8)	−0.0057 (10)
C5	0.0494 (10)	0.0574 (13)	0.0557 (12)	−0.0130 (9)	0.0269 (10)	−0.0140 (11)
C6	0.0415 (9)	0.0411 (10)	0.0468 (11)	−0.0012 (8)	0.0197 (8)	−0.0005 (10)
C14	0.0467 (10)	0.0477 (12)	0.0376 (10)	−0.0066 (8)	0.0146 (8)	−0.0035 (10)
C15	0.0532 (11)	0.0473 (12)	0.0478 (11)	−0.0081 (9)	0.0179 (9)	−0.0096 (11)
C17	0.0639 (12)	0.0575 (14)	0.0542 (13)	−0.0150 (10)	0.0319 (10)	−0.0207 (12)
C21	0.0460 (10)	0.0353 (10)	0.0319 (9)	−0.0002 (8)	0.0123 (8)	0.0017 (9)
C22	0.0518 (10)	0.0400 (11)	0.0399 (10)	−0.0045 (8)	0.0176 (9)	−0.0044 (10)
C23	0.0515 (11)	0.0539 (13)	0.0493 (12)	−0.0107 (10)	0.0173 (9)	0.0012 (11)
C24	0.0613 (12)	0.0424 (12)	0.0571 (13)	−0.0134 (10)	0.0101 (10)	0.0045 (11)
C25	0.0664 (13)	0.0360 (11)	0.0638 (14)	−0.0008 (10)	0.0148 (10)	−0.0037 (11)
C26	0.0491 (10)	0.0413 (11)	0.0537 (13)	0.0024 (8)	0.0160 (9)	0.0010 (10)
C61	0.0369 (9)	0.0475 (11)	0.0411 (11)	−0.0007 (8)	0.0126 (8)	−0.0017 (10)
C62	0.0478 (10)	0.0481 (12)	0.0492 (12)	−0.0017 (9)	0.0191 (9)	0.0014 (11)
C63	0.0563 (12)	0.0814 (16)	0.0459 (12)	−0.0101 (11)	0.0202 (10)	0.0072 (13)
C64	0.0463 (12)	0.105 (2)	0.0506 (13)	0.0043 (12)	0.0242 (10)	−0.0030 (15)
C65	0.0535 (12)	0.0791 (17)	0.0619 (14)	0.0208 (11)	0.0220 (10)	−0.0030 (14)
C66	0.0526 (11)	0.0568 (13)	0.0553 (12)	0.0118 (10)	0.0215 (10)	0.0070 (12)

Geometric parameters (Å, °)

Cl1—C22	1.741 (2)	C25—C26	1.391 (3)
Cl2—C62	1.743 (2)	C61—C66	1.388 (3)
N1—C2	1.458 (2)	C61—C62	1.383 (3)
N1—C6	1.460 (2)	C62—C63	1.381 (3)
N16—C15	1.134 (3)	C63—C64	1.368 (4)
N18—C17	1.131 (3)	C64—C65	1.370 (3)
N1—H1	0.81 (2)	C65—C66	1.377 (3)
C2—C21	1.513 (2)	C2—H2	1.0000
C2—C3	1.533 (3)	C3—H3A	0.9900
C3—C4	1.491 (3)	C3—H3B	0.9900
C4—C14	1.339 (3)	C5—H5A	0.9900
C4—C5	1.498 (3)	C5—H5B	0.9900
C5—C6	1.532 (3)	C6—H6	1.0000
C6—C61	1.507 (2)	C23—H23	0.9500
C14—C17	1.443 (3)	C24—H24	0.9500
C14—C15	1.438 (3)	C25—H25	0.9500
C21—C22	1.388 (3)	C26—H26	0.9500

C21—C26	1.388 (2)	C63—H63	0.9500
C22—C23	1.376 (3)	C64—H64	0.9500
C23—C24	1.371 (3)	C65—H65	0.9500
C24—C25	1.367 (3)	C66—H66	0.9500
Cl1···C3	3.447 (2)	C65···C63^{xi}	3.586 (3)
Cl1···C25^{i}	3.586 (2)	C66···C15^{x}	3.537 (3)
Cl1···N16^{ii}	3.454 (2)	C15···H3B	2.4900
Cl1···C23^{iii}	3.591 (2)	C17···H5A	2.4500
Cl1···H2	2.7400	C22···H3B	3.0100
Cl1···H3B	2.8600	C24···H2^{viii}	3.0900
Cl1···H24^{iv}	3.0400	C26···H1	2.72 (2)
Cl2···H6	2.6000	C62···H65^{vi}	2.9700
N16···C24^{iii}	3.375 (3)	C63···H3A^{x}	3.0500
N16···Cl1^{ii}	3.454 (2)	C66···H1	2.899 (19)
N1···H66	2.5800	C66···H5B	2.9500
N1···H26	2.4500	H1···C26	2.72 (2)
N16···H23^{iii}	2.9200	H1···C66	2.899 (19)
N16···H24^{iii}	2.6800	H1···H26	2.3500
N16···H1^{v}	2.633 (19)	H1···N16^{x}	2.633 (19)
N18···H5A	2.9100	H2···Cl1	2.7400
N18···H64^{vi}	2.6500	H2···H6	2.3500
N18···H63^{vii}	2.6800	H2···H25^{iv}	2.3500
C3···Cl1	3.447 (2)	H2···C24^{i}	3.0900
C4···C63^{v}	3.596 (3)	H3A···C63^{v}	3.0500
C4···C64^{v}	3.594 (3)	H3B···Cl1	2.8600
C14···C25^{iv}	3.569 (3)	H3B···C15	2.4900
C14···C64^{v}	3.486 (3)	H3B···C22	3.0100
C14···C65^{v}	3.567 (3)	H5A···N18	2.9100
C15···C66^{v}	3.537 (3)	H5A···C17	2.4500
C21···C24^{i}	3.570 (3)	H5B···C66	2.9500
C22···C25^{i}	3.537 (3)	H6···Cl2	2.6000
C23···Cl1^{iii}	3.591 (2)	H6···H2	2.3500
C24···N16^{iii}	3.375 (3)	H6···H25^{iv}	2.4800
C24···C21^{viii}	3.570 (3)	H23···N16^{iii}	2.9200
C25···Cl1^{viii}	3.586 (2)	H24···Cl1^{ix}	3.0400
C25···C14^{ix}	3.569 (3)	H24···N16^{iii}	2.6800
C25···C22^{viii}	3.537 (3)	H25···H2^{ix}	2.3500
C62···C65^{vi}	3.567 (3)	H25···H6^{ix}	2.4800
C63···C4^{x}	3.596 (3)	H26···N1	2.4500
C63···C65^{vi}	3.586 (3)	H26···H1	2.3500
C64···C4^{x}	3.594 (3)	H63···N18^{xii}	2.6800
C64···C14^{x}	3.486 (3)	H64···N18^{xi}	2.6500

C65···C14^{x}	3.567 (3)	H65···C62^{xi}	2.9700
C65···C62^{xi}	3.567 (3)	H66···N1	2.5800
C2—N1—C6	112.10 (14)	C63—C64—C65	120.34 (19)
C6—N1—H1	108.3 (15)	C64—C65—C66	119.8 (2)
C2—N1—H1	109.3 (13)	C61—C66—C65	121.5 (2)
N1—C2—C21	111.19 (13)	N1—C2—H2	109.00
N1—C2—C3	108.06 (15)	C3—C2—H2	109.00
C3—C2—C21	110.34 (14)	C21—C2—H2	109.00
C2—C3—C4	110.11 (15)	C2—C3—H3A	110.00
C3—C4—C5	114.09 (18)	C2—C3—H3B	110.00
C5—C4—C14	122.35 (19)	C4—C3—H3A	110.00
C3—C4—C14	123.53 (17)	C4—C3—H3B	110.00
C4—C5—C6	110.07 (15)	H3A—C3—H3B	108.00
N1—C6—C61	111.32 (15)	C4—C5—H5A	110.00
C5—C6—C61	109.74 (14)	C4—C5—H5B	110.00
N1—C6—C5	108.14 (15)	C6—C5—H5A	110.00
C15—C14—C17	114.98 (19)	C6—C5—H5B	110.00
C4—C14—C15	122.66 (19)	H5A—C5—H5B	108.00
C4—C14—C17	122.34 (17)	N1—C6—H6	109.00
N16—C15—C14	178.7 (2)	C5—C6—H6	109.00
N18—C17—C14	178.8 (2)	C61—C6—H6	109.00
C2—C21—C26	121.17 (15)	C22—C23—H23	120.00
C2—C21—C22	122.08 (16)	C24—C23—H23	120.00
C22—C21—C26	116.75 (16)	C23—C24—H24	120.00
Cl1—C22—C23	117.51 (15)	C25—C24—H24	120.00
Cl1—C22—C21	120.30 (16)	C24—C25—H25	120.00
C21—C22—C23	122.19 (19)	C26—C25—H25	120.00
C22—C23—C24	119.86 (19)	C21—C26—H26	119.00
C23—C24—C25	119.8 (2)	C25—C26—H26	119.00
C24—C25—C26	120.2 (2)	C62—C63—H63	120.00
C21—C26—C25	121.25 (18)	C64—C63—H63	120.00
C62—C61—C66	117.03 (17)	C63—C64—H64	120.00
C6—C61—C62	122.72 (18)	C65—C64—H64	120.00
C6—C61—C66	120.18 (17)	C64—C65—H65	120.00
C61—C62—C63	122.0 (2)	C66—C65—H65	120.00
Cl2—C62—C61	120.46 (15)	C61—C66—H66	119.00
Cl2—C62—C63	117.52 (17)	C65—C66—H66	119.00
C62—C63—C64	119.3 (2)		
C6—N1—C2—C3	64.46 (17)	C5—C6—C61—C66	−80.5 (2)
C6—N1—C2—C21	−174.30 (14)	C2—C21—C22—Cl1	−1.4 (2)
C2—N1—C6—C5	−64.40 (18)	C2—C21—C22—C23	179.60 (16)
C2—N1—C6—C61	174.98 (14)	C26—C21—C22—Cl1	179.49 (13)
N1—C2—C3—C4	−55.69 (18)	C26—C21—C22—C23	0.5 (3)
C21—C2—C3—C4	−177.45 (15)	C2—C21—C26—C25	−179.97 (17)
N1—C2—C21—C22	161.78 (16)	C22—C21—C26—C25	−0.8 (3)
N1—C2—C21—C26	−19.1 (2)	Cl1—C22—C23—C24	−179.57 (15)
C3—C2—C21—C22	−78.3 (2)	C21—C22—C23—C24	−0.5 (3)
C3—C2—C21—C26	100.77 (19)	C22—C23—C24—C25	0.9 (3)

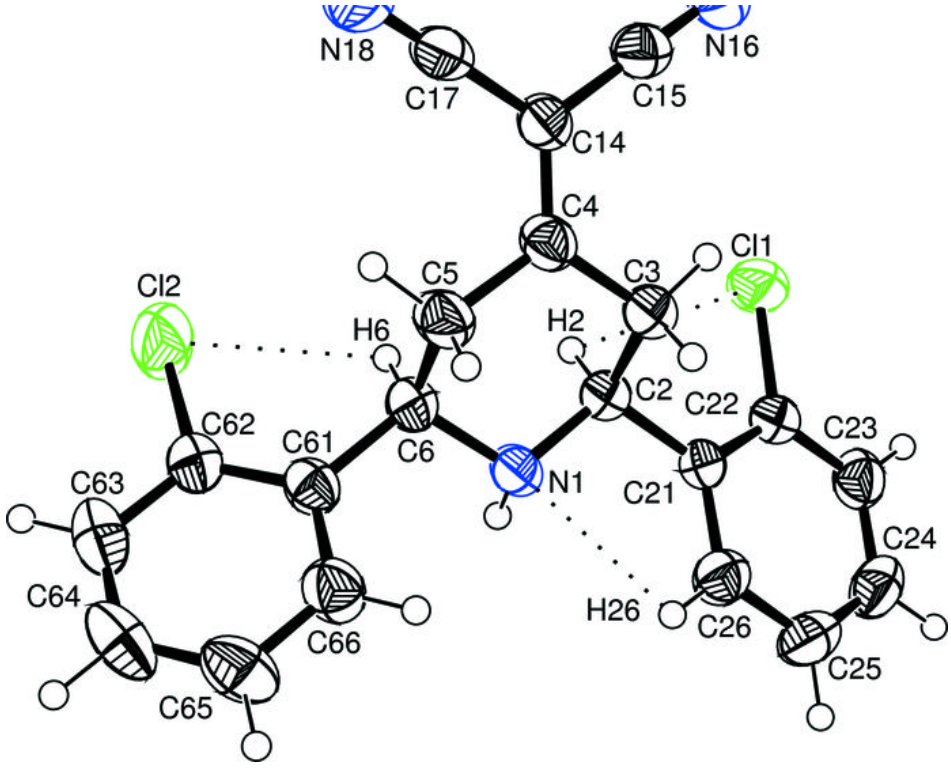
C2—C3—C4—C5	51.7 (2)	C23—C24—C25—C26	−1.3 (3)
C2—C3—C4—C14	−126.22 (19)	C24—C25—C26—C21	1.2 (3)
C3—C4—C5—C6	−51.6 (2)	C6—C61—C62—Cl2	2.7 (3)
C14—C4—C5—C6	126.36 (19)	C6—C61—C62—C63	−176.83 (18)
C3—C4—C14—C15	−1.1 (3)	C66—C61—C62—Cl2	179.61 (15)
C3—C4—C14—C17	−179.60 (18)	C66—C61—C62—C63	0.1 (3)
C5—C4—C14—C15	−178.89 (18)	C6—C61—C66—C65	177.46 (18)
C5—C4—C14—C17	2.6 (3)	C62—C61—C66—C65	0.5 (3)
C4—C5—C6—N1	55.4 (2)	Cl2—C62—C63—C64	−179.49 (16)
C4—C5—C6—C61	176.97 (17)	C61—C62—C63—C64	0.1 (3)
N1—C6—C61—C62	−144.01 (18)	C62—C63—C64—C65	−0.7 (3)
N1—C6—C61—C66	39.2 (2)	C63—C64—C65—C66	1.3 (3)
C5—C6—C61—C62	96.3 (2)	C64—C65—C66—C61	−1.2 (3)

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) −*x*+1, −*y*+1, −*z*; (iii) −*x*+1, −*y*+2, −*z*; (iv) *x*, *y*−1, *z*; (v) *x*, −*y*+3/2, *z*−1/2; (vi) −*x*, *y*−1/2, −*z*+1/2; (vii) *x*, −*y*+1/2, *z*−1/2; (viii) −*x*+1, *y*+1/2, −*z*+1/2; (ix) *x*, *y*+1, *z*; (x) *x*, −*y*+3/2, *z*+1/2; (xi) −*x*, *y*+1/2, −*z*+1/2; (xii) *x*, −*y*+1/2, *z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···Cl1	1.00	2.74	3.0777 (18)	100.00
C6—H6···Cl2	1.00	2.60	3.0909 (18)	110.00
C26—H26···N1	0.95	2.45	2.795 (2)	102.00

Fig. 1


N18
C17
C15
N16
C14
C4
Cl1
C5
C3
Cl2
H6
H2
C2
C22
C62
C61
C6
C23
C63
N1
C21
C24
C64
H26
C26
C66
C25
C65