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10-(4-Chlorophenyl)-9-(4-methoxyphenyl)-3,3,6,6-tetramethyl-3,4,6,7-tetrahydroacridine-1,8(2*H*,5*H*,9*H*,10*H*)-dione

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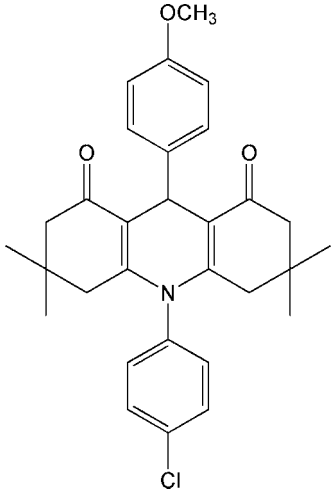
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.056; wR factor = 0.146; data-to-parameter ratio = 14.1.

The title compound, $C_{30}H_{32}ClNO_3$, was synthesized by the reaction of dimedone with 4-methoxybenzaldehyde and 4-chlorobenzenamine in water. The dihydropyridine ring is in a boat conformation. Both cyclohexene rings adopt envelope conformations. The chlorophenyl and methoxyphenyl rings form dihedral angles of 81.31 (11) and 88.84 (12)°, respectively, with the planar part of the dihydropyridine ring. The crystal packing is stabilized by weak C—H···O hydrogen bonds.

Related literature

For related literature, see: Mandi *et al.* (1994); Nasim & Brychey (1979); Reil *et al.* (1994); Thull & Testa (1994); Tu *et al.* (2004); Wysocka-Skrzela & Ledochowski (1976).



Experimental

Crystal data

$C_{30}H_{32}ClNO_3$
M_r = 490.02
Monoclinic, $P2_1/c$
a = 12.227 (2) Å
b = 10.883 (2) Å
c = 20.178 (3) Å
β = 100.788 (2)°
V = 2637.8 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 298 (2) K
0.40 × 0.38 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.933, T_{max} = 0.962
10435 measured reflections
4516 independent reflections
2146 reflections with $I > 2\sigma(I)$
R_{int} = 0.072

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.146
S = 1.02
4516 reflections
321 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15···O2^{i}	0.93	2.48	3.366 (4)	161
C21—H21A···O2^{ii}	0.96	2.53	3.418 (4)	154

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2452).

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supplementary materials

Acta Cryst. (2007). E**63**, o3934 [**doi:10.1107/S1600536807042365**]

10-(4-Chlorophenyl)-9-(4-methoxyphenyl)-3,3,6,6-tetramethyl-3,4,6,7-tetrahydroacridine-1,8(2*H*,5*H*,9*H*,10*H*)-dione

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Comment

Acridine derivatives containing 1,4-dihydropyridine unit belong to a special class of compounds not only because of their interesting chemical and physical properties but also due to their immense utility in pharmaceutical and dye industry, and they are well known atherapeutic agents (Wysocka-Skrzela & Ledochowski, 1976; Nasim & Brychey, 1979; Thull & Testa, 1994; Reil *et al.*, 1994; Mandi *et al.*, 1994). We have reported the synthesis of *N*-hydroxylacridine derivatives, previously, (Tu *et al.*, 2004) and report herein the structure of the title compound.

In the title molecule, the dihydropyridine ring is in a boat conformation, with atoms N1 and C7 deviating from the C1/C6/C8/C13 plane by 0.099 (5) and 0.255 (5) Å, respectively (Fig. 1). Both cyclohexene rings adopt envelope conformations: atom C3 deviaties from the C1/C2/C4/C5/C6 by 0.667 (5) Å and atom C11 deviates from the C8/C9/C10/C12/C13 plane by 0.660 (5) Å. The dihedral angle between the C1/C6/C8/C13 plane and the C14–C29 benzene ring attached at atom N1 is 81.31 (11)° and that between the C1/C6/C8/C13 plane and the C24–C29 benzene ring attached at atom C7 is 88.84 (12)°.

The crystal packing is stabilized by weak C—H···O hydrogen bonds (Table 1).

Experimental

The title compound was prepared by the reaction of dimedone (2 mmol) with 4-methoxybenzaldehyde (1 mmol) and 4-chlorobenzenamine (1 mmol) at 413 K under microwave irradiation (maximum power 150 W, initial power 100 W) for 12 min (yield 85%; m.p. 542–543 K). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

Refinement

H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms, with C—H distances in the range 0.93–0.98 Å, and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for other H atoms. Owing to the large number of weak high-angle reflections, the ratio of observed to unique reflections is low (48%).

Figures

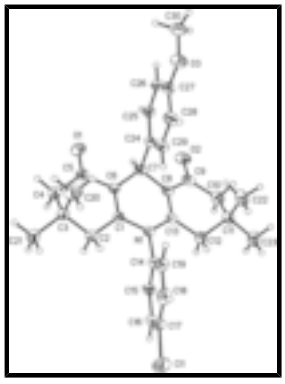


Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

10-(4-Chlorophenyl)-9-(4-methoxyphenyl)-3,3,6,6-tetramethyl-3,4,6,7- tetrahydroacridine-1,8(2*H*,5H,9*H*,10H)-dione

Crystal data

$C_{30}H_{32}ClNO_3$	F_{000} = 1040
M_r = 490.02	D_x = 1.234 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 542-543 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 12.227 (2) Å	Cell parameters from 2397 reflections
b = 10.883 (2) Å	θ = 2.4–25.4º
c = 20.178 (3) Å	μ = 0.18 mm^{-1}
β = 100.788 (2)º	T = 298 (2) K
V = 2637.8 (8) Å^3	Block, yellow
Z = 4	0.40 × 0.38 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer	4516 independent reflections
Radiation source: fine-focus sealed tube	2146 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.072
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −13→14
T_{min} = 0.933, T_{max} = 0.962	k = −12→12
10435 measured reflections	l = −24→18

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.057$

$wR(F^2) = 0.146$

$S = 1.02$

4516 reflections

321 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0416P)^2 + 1.2116P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.19$ e Å^{-3}

$\Delta\rho_{min} = -0.37$ e Å^{-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 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	0.63124 (12)	−0.02238 (10)	0.23800 (6)	0.0953 (5)
N1	0.7981 (2)	0.4467 (2)	0.36849 (14)	0.0383 (7)
O1	0.9443 (2)	0.8361 (2)	0.32608 (14)	0.0679 (8)
O2	0.9300 (2)	0.6883 (2)	0.56080 (13)	0.0635 (8)
O3	0.4979 (2)	1.0176 (2)	0.41504 (13)	0.0618 (8)
C1	0.8330 (3)	0.5342 (3)	0.32568 (17)	0.0358 (8)
C2	0.8322 (3)	0.4956 (3)	0.25370 (17)	0.0445 (9)
H2A	0.7686	0.4424	0.2388	0.053*
H2B	0.8989	0.4484	0.2521	0.053*
C3	0.8266 (3)	0.6043 (3)	0.20498 (18)	0.0458 (10)
C4	0.9179 (3)	0.6935 (3)	0.23476 (19)	0.0538 (11)
H4A	0.9896	0.6548	0.2352	0.065*
H4B	0.9134	0.7653	0.2059	0.065*
C5	0.9121 (3)	0.7340 (3)	0.30488 (19)	0.0456 (10)
C6	0.8679 (3)	0.6463 (3)	0.34922 (17)	0.0372 (9)
C7	0.8619 (3)	0.6884 (3)	0.41955 (17)	0.0397 (9)
H7	0.9316	0.7309	0.4381	0.048*
C8	0.8520 (3)	0.5780 (3)	0.46365 (17)	0.0387 (9)
C9	0.8828 (3)	0.5939 (3)	0.53650 (19)	0.0476 (10)
C10	0.8585 (3)	0.4910 (3)	0.58209 (18)	0.0546 (11)
H10A	0.8375	0.5269	0.6219	0.066*
H10B	0.9264	0.4445	0.5968	0.066*

C11	0.7674 (3)	0.4030 (3)	0.55013 (17)	0.0471 (10)
C12	0.7937 (3)	0.3617 (3)	0.48203 (17)	0.0446 (10)
H12A	0.8586	0.3087	0.4901	0.054*
H12B	0.7316	0.3139	0.4582	0.054*
C13	0.8154 (3)	0.4675 (3)	0.43802 (17)	0.0365 (8)
C14	0.7567 (3)	0.3295 (3)	0.34056 (17)	0.0373 (9)
C15	0.8265 (3)	0.2303 (3)	0.34167 (17)	0.0423 (9)
H15	0.9005	0.2368	0.3631	0.051*
C16	0.7876 (4)	0.1206 (3)	0.31119 (19)	0.0518 (11)
H16	0.8347	0.0532	0.3127	0.062*
C17	0.6786 (4)	0.1127 (3)	0.27868 (19)	0.0518 (11)
C18	0.6075 (4)	0.2106 (4)	0.27786 (19)	0.0592 (11)
H18	0.5335	0.2039	0.2563	0.071*
C19	0.6465 (3)	0.3196 (3)	0.30932 (19)	0.0508 (10)
H19	0.5985	0.3858	0.3094	0.061*
C20	0.7133 (3)	0.6675 (3)	0.1972 (2)	0.0701 (13)
H20A	0.7027	0.6976	0.2402	0.105*
H20B	0.6556	0.6096	0.1801	0.105*
H20C	0.7104	0.7349	0.1662	0.105*
C21	0.8439 (4)	0.5572 (3)	0.13605 (19)	0.0729 (14)
H21A	0.8441	0.6255	0.1059	0.109*
H21B	0.7847	0.5019	0.1179	0.109*
H21C	0.9139	0.5149	0.1412	0.109*
C22	0.6529 (3)	0.4660 (4)	0.5398 (2)	0.0684 (13)
H22A	0.6355	0.4869	0.5828	0.103*
H22B	0.5972	0.4112	0.5164	0.103*
H22C	0.6546	0.5394	0.5135	0.103*
C23	0.7667 (4)	0.2905 (4)	0.59582 (19)	0.0670 (12)
H23A	0.8377	0.2502	0.6017	0.100*
H23B	0.7095	0.2346	0.5754	0.100*
H23C	0.7526	0.3164	0.6389	0.100*
C24	0.7657 (3)	0.7782 (3)	0.41982 (17)	0.0383 (9)
C25	0.7838 (3)	0.8957 (3)	0.44530 (17)	0.0451 (10)
H25	0.8561	0.9202	0.4632	0.054*
C26	0.6972 (3)	0.9784 (3)	0.44502 (18)	0.0492 (10)
H26	0.7114	1.0567	0.4629	0.059*
C27	0.5906 (3)	0.9430 (3)	0.41801 (18)	0.0465 (10)
C28	0.5696 (3)	0.8255 (3)	0.39276 (19)	0.0536 (11)
H28	0.4971	0.8009	0.3753	0.064*
C29	0.6569 (3)	0.7451 (3)	0.39361 (19)	0.0508 (10)
H29	0.6424	0.6665	0.3761	0.061*
C30	0.5146 (4)	1.1371 (3)	0.4434 (2)	0.0681 (13)
H30A	0.5551	1.1311	0.4889	0.102*
H30B	0.4438	1.1751	0.4434	0.102*
H30C	0.5562	1.1857	0.4171	0.102*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1363 (12)	0.0698 (8)	0.0820 (9)	−0.0530 (8)	0.0264 (8)	−0.0276 (6)
N1	0.047 (2)	0.0310 (15)	0.0380 (18)	−0.0046 (14)	0.0118 (15)	−0.0043 (13)
O1	0.076 (2)	0.0475 (16)	0.083 (2)	−0.0252 (15)	0.0219 (17)	−0.0111 (15)
O2	0.070 (2)	0.0567 (17)	0.0580 (18)	−0.0008 (15)	−0.0039 (15)	−0.0193 (14)
O3	0.0567 (19)	0.0575 (17)	0.070 (2)	0.0176 (15)	0.0086 (15)	−0.0048 (14)
C1	0.036 (2)	0.0319 (19)	0.041 (2)	0.0021 (16)	0.0116 (17)	−0.0006 (16)
C2	0.059 (3)	0.0316 (19)	0.046 (2)	−0.0010 (18)	0.0175 (19)	−0.0008 (16)
C3	0.060 (3)	0.035 (2)	0.044 (2)	−0.0015 (19)	0.013 (2)	−0.0003 (17)
C4	0.064 (3)	0.045 (2)	0.055 (3)	−0.008 (2)	0.017 (2)	0.0015 (19)
C5	0.040 (2)	0.039 (2)	0.059 (3)	−0.0022 (19)	0.011 (2)	−0.0027 (19)
C6	0.037 (2)	0.0328 (19)	0.043 (2)	−0.0005 (17)	0.0107 (18)	−0.0047 (16)
C7	0.036 (2)	0.037 (2)	0.046 (2)	−0.0039 (17)	0.0060 (18)	−0.0081 (17)
C8	0.035 (2)	0.041 (2)	0.039 (2)	0.0012 (18)	0.0050 (18)	−0.0076 (17)
C9	0.041 (3)	0.049 (2)	0.052 (3)	0.010 (2)	0.004 (2)	−0.016 (2)
C10	0.056 (3)	0.063 (3)	0.043 (2)	0.011 (2)	0.004 (2)	−0.002 (2)
C11	0.048 (3)	0.057 (2)	0.037 (2)	0.004 (2)	0.0087 (19)	−0.0037 (19)
C12	0.045 (2)	0.042 (2)	0.047 (2)	0.0017 (18)	0.0105 (19)	−0.0033 (18)
C13	0.036 (2)	0.039 (2)	0.035 (2)	0.0034 (17)	0.0069 (17)	−0.0060 (17)
C14	0.040 (3)	0.0314 (19)	0.041 (2)	−0.0039 (18)	0.0104 (19)	−0.0031 (16)
C15	0.042 (2)	0.038 (2)	0.047 (2)	−0.0031 (19)	0.0085 (19)	−0.0060 (17)
C16	0.063 (3)	0.037 (2)	0.058 (3)	−0.001 (2)	0.020 (2)	−0.0095 (19)
C17	0.070 (3)	0.045 (2)	0.043 (2)	−0.020 (2)	0.017 (2)	−0.0098 (19)
C18	0.046 (3)	0.078 (3)	0.051 (3)	−0.023 (2)	0.002 (2)	−0.006 (2)
C19	0.050 (3)	0.048 (2)	0.054 (3)	0.000 (2)	0.008 (2)	0.001 (2)
C20	0.072 (3)	0.059 (3)	0.071 (3)	0.007 (2)	−0.005 (3)	0.001 (2)
C21	0.127 (4)	0.049 (2)	0.046 (3)	−0.006 (3)	0.026 (3)	0.0022 (19)
C22	0.047 (3)	0.091 (3)	0.072 (3)	0.011 (2)	0.023 (2)	0.000 (2)
C23	0.077 (3)	0.073 (3)	0.053 (3)	0.000 (3)	0.015 (2)	0.012 (2)
C24	0.041 (3)	0.035 (2)	0.041 (2)	0.0040 (17)	0.0114 (19)	−0.0045 (16)
C25	0.045 (3)	0.039 (2)	0.051 (2)	−0.0023 (19)	0.0093 (19)	−0.0066 (18)
C26	0.063 (3)	0.0286 (19)	0.057 (3)	0.001 (2)	0.015 (2)	−0.0072 (17)
C27	0.049 (3)	0.044 (2)	0.048 (2)	0.011 (2)	0.012 (2)	0.0019 (18)
C28	0.039 (3)	0.061 (3)	0.060 (3)	−0.001 (2)	0.008 (2)	−0.016 (2)
C29	0.043 (3)	0.046 (2)	0.064 (3)	0.001 (2)	0.011 (2)	−0.0189 (19)
C30	0.080 (3)	0.053 (3)	0.072 (3)	0.020 (2)	0.015 (3)	−0.006 (2)

Geometric parameters (Å, °)

Cl1—C17	1.730 (4)	C14—C15	1.374 (4)
N1—C13	1.398 (4)	C14—C19	1.380 (5)
N1—C1	1.405 (4)	C15—C16	1.385 (4)
N1—C14	1.447 (4)	C15—H15	0.93
O1—C5	1.228 (4)	C16—C17	1.374 (5)
O2—C9	1.234 (4)	C16—H16	0.93
O3—C27	1.387 (4)	C17—C18	1.373 (5)

O3—C30	1.420 (4)	C18—C19	1.387 (5)
C1—C6	1.349 (4)	C18—H18	0.93
C1—C2	1.510 (4)	C19—H19	0.93
C2—C3	1.532 (4)	C20—H20A	0.96
C2—H2A	0.97	C20—H20B	0.96
C2—H2B	0.97	C20—H20C	0.96
C3—C4	1.517 (5)	C21—H21A	0.96
C3—C20	1.528 (5)	C21—H21B	0.96
C3—C21	1.534 (5)	C21—H21C	0.96
C4—C5	1.496 (5)	C22—H22A	0.96
C4—H4A	0.97	C22—H22B	0.96
C4—H4B	0.97	C22—H22C	0.96
C5—C6	1.478 (5)	C23—H23A	0.96
C6—C7	1.506 (4)	C23—H23B	0.96
C7—C8	1.513 (4)	C23—H23C	0.96
C7—C24	1.530 (4)	C24—C25	1.381 (4)
C7—H7	0.98	C24—C29	1.384 (5)
C8—C13	1.352 (4)	C25—C26	1.388 (4)
C8—C9	1.458 (5)	C25—H25	0.93
C9—C10	1.513 (5)	C26—C27	1.370 (5)
C10—C11	1.519 (5)	C26—H26	0.93
C10—H10A	0.97	C27—C28	1.383 (5)
C10—H10B	0.97	C28—C29	1.377 (5)
C11—C23	1.533 (5)	C28—H28	0.93
C11—C12	1.536 (5)	C29—H29	0.93
C11—C22	1.537 (5)	C30—H30A	0.96
C12—C13	1.508 (4)	C30—H30B	0.96
C12—H12A	0.97	C30—H30C	0.96
C12—H12B	0.97		
C13—N1—C1	120.1 (3)	C15—C14—N1	121.0 (3)
C13—N1—C14	120.6 (3)	C19—C14—N1	119.2 (3)
C1—N1—C14	118.8 (3)	C14—C15—C16	120.6 (4)
C27—O3—C30	117.6 (3)	C14—C15—H15	119.7
C6—C1—N1	120.6 (3)	C16—C15—H15	119.7
C6—C1—C2	122.4 (3)	C17—C16—C15	119.1 (4)
N1—C1—C2	117.0 (3)	C17—C16—H16	120.4
C1—C2—C3	113.2 (3)	C15—C16—H16	120.4
C1—C2—H2A	108.9	C18—C17—C16	120.9 (3)
C3—C2—H2A	108.9	C18—C17—Cl1	119.9 (3)
C1—C2—H2B	108.9	C16—C17—Cl1	119.2 (3)
C3—C2—H2B	108.9	C17—C18—C19	119.7 (4)
H2A—C2—H2B	107.8	C17—C18—H18	120.2
C4—C3—C20	109.8 (3)	C19—C18—H18	120.2
C4—C3—C2	107.4 (3)	C14—C19—C18	119.9 (4)
C20—C3—C2	110.2 (3)	C14—C19—H19	120.0
C4—C3—C21	110.9 (3)	C18—C19—H19	120.0
C20—C3—C21	109.5 (3)	C3—C20—H20A	109.5
C2—C3—C21	109.1 (3)	C3—C20—H20B	109.5
C5—C4—C3	113.7 (3)	H20A—C20—H20B	109.5

C5—C4—H4A	108.8	C3—C20—H20C	109.5
C3—C4—H4A	108.8	H20A—C20—H20C	109.5
C5—C4—H4B	108.8	H20B—C20—H20C	109.5
C3—C4—H4B	108.8	C3—C21—H21A	109.5
H4A—C4—H4B	107.7	C3—C21—H21B	109.5
O1—C5—C6	120.2 (3)	H21A—C21—H21B	109.5
O1—C5—C4	121.8 (3)	C3—C21—H21C	109.5
C6—C5—C4	118.0 (3)	H21A—C21—H21C	109.5
C1—C6—C5	119.9 (3)	H21B—C21—H21C	109.5
C1—C6—C7	122.6 (3)	C11—C22—H22A	109.5
C5—C6—C7	117.5 (3)	C11—C22—H22B	109.5
C6—C7—C8	109.6 (3)	H22A—C22—H22B	109.5
C6—C7—C24	111.8 (3)	C11—C22—H22C	109.5
C8—C7—C24	111.0 (3)	H22A—C22—H22C	109.5
C6—C7—H7	108.1	H22B—C22—H22C	109.5
C8—C7—H7	108.1	C11—C23—H23A	109.5
C24—C7—H7	108.1	C11—C23—H23B	109.5
C13—C8—C9	119.7 (3)	H23A—C23—H23B	109.5
C13—C8—C7	122.6 (3)	C11—C23—H23C	109.5
C9—C8—C7	117.7 (3)	H23A—C23—H23C	109.5
O2—C9—C8	120.8 (4)	H23B—C23—H23C	109.5
O2—C9—C10	120.3 (3)	C25—C24—C29	117.3 (3)
C8—C9—C10	118.8 (3)	C25—C24—C7	121.6 (3)
C9—C10—C11	114.9 (3)	C29—C24—C7	121.2 (3)
C9—C10—H10A	108.6	C24—C25—C26	122.0 (4)
C11—C10—H10A	108.6	C24—C25—H25	119.0
C9—C10—H10B	108.6	C26—C25—H25	119.0
C11—C10—H10B	108.6	C27—C26—C25	119.1 (3)
H10A—C10—H10B	107.5	C27—C26—H26	120.4
C10—C11—C23	109.5 (3)	C25—C26—H26	120.4
C10—C11—C12	107.7 (3)	C26—C27—C28	120.3 (4)
C23—C11—C12	109.3 (3)	C26—C27—O3	124.2 (3)
C10—C11—C22	110.7 (3)	C28—C27—O3	115.6 (4)
C23—C11—C22	109.4 (3)	C29—C28—C27	119.5 (4)
C12—C11—C22	110.3 (3)	C29—C28—H28	120.3
C13—C12—C11	113.1 (3)	C27—C28—H28	120.3
C13—C12—H12A	109.0	C28—C29—C24	121.8 (3)
C11—C12—H12A	109.0	C28—C29—H29	119.1
C13—C12—H12B	109.0	C24—C29—H29	119.1
C11—C12—H12B	109.0	O3—C30—H30A	109.5
H12A—C12—H12B	107.8	O3—C30—H30B	109.5
C8—C13—N1	120.3 (3)	H30A—C30—H30B	109.5
C8—C13—C12	122.4 (3)	O3—C30—H30C	109.5
N1—C13—C12	117.2 (3)	H30A—C30—H30C	109.5
C15—C14—C19	119.7 (3)	H30B—C30—H30C	109.5
C13—N1—C1—C6	−10.0 (5)	C22—C11—C12—C13	69.6 (4)
C14—N1—C1—C6	177.3 (3)	C9—C8—C13—N1	−172.4 (3)
C13—N1—C1—C2	168.5 (3)	C7—C8—C13—N1	8.0 (5)
C14—N1—C1—C2	−4.2 (4)	C9—C8—C13—C12	6.4 (5)

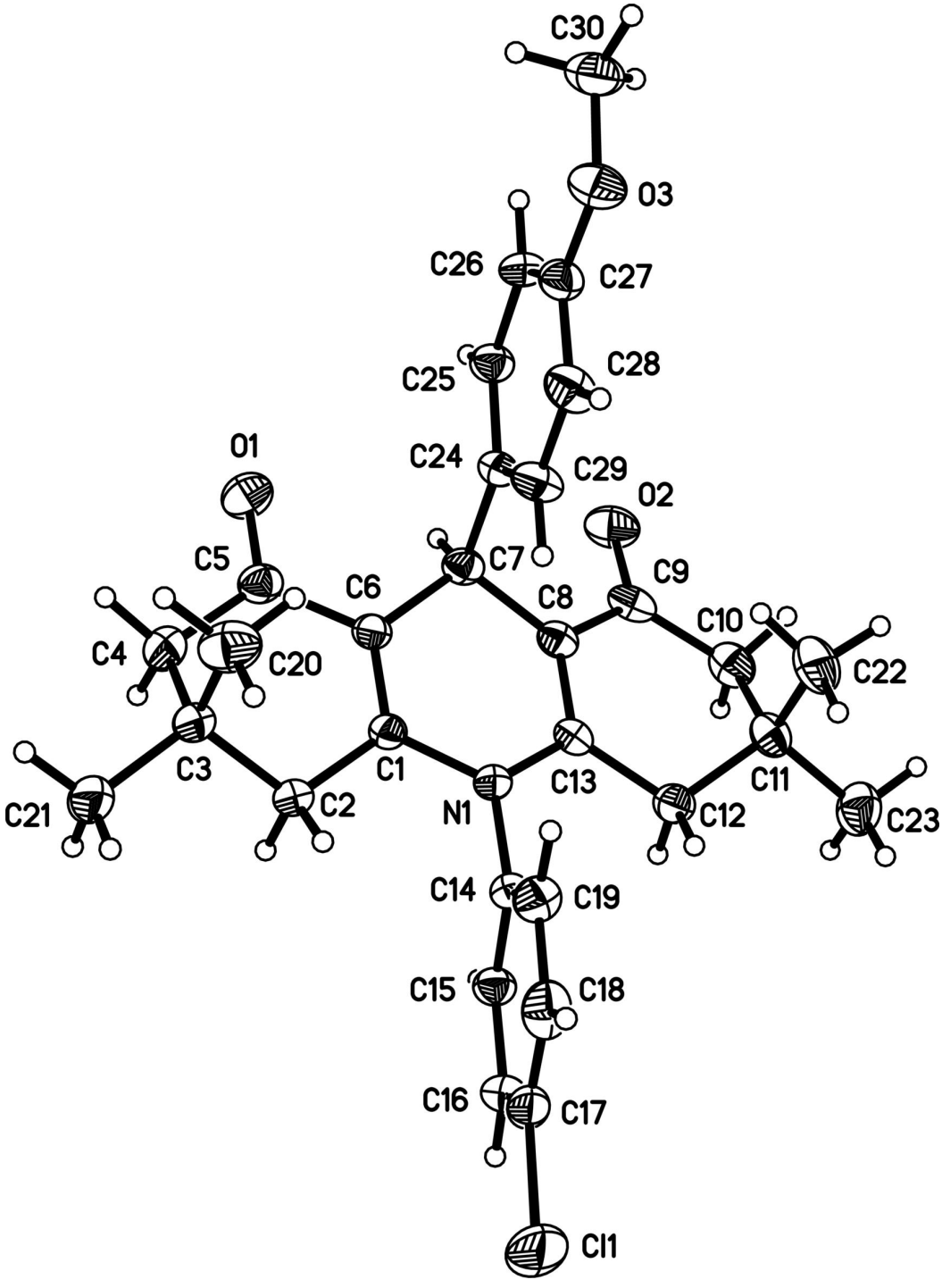
C6—C1—C2—C3	−23.9 (5)	C7—C8—C13—C12	−173.2 (3)
N1—C1—C2—C3	157.6 (3)	C1—N1—C13—C8	8.8 (5)
C1—C2—C3—C4	51.3 (4)	C14—N1—C13—C8	−178.7 (3)
C1—C2—C3—C20	−68.3 (4)	C1—N1—C13—C12	−170.0 (3)
C1—C2—C3—C21	171.5 (3)	C14—N1—C13—C12	2.5 (5)
C20—C3—C4—C5	64.3 (4)	C11—C12—C13—C8	25.0 (5)
C2—C3—C4—C5	−55.5 (4)	C11—C12—C13—N1	−156.2 (3)
C21—C3—C4—C5	−174.6 (3)	C13—N1—C14—C15	−79.9 (4)
C3—C4—C5—O1	−149.3 (4)	C1—N1—C14—C15	92.7 (4)
C3—C4—C5—C6	31.8 (5)	C13—N1—C14—C19	103.4 (4)
N1—C1—C6—C5	175.5 (3)	C1—N1—C14—C19	−84.0 (4)
C2—C1—C6—C5	−2.9 (5)	C19—C14—C15—C16	0.6 (5)
N1—C1—C6—C7	−5.7 (5)	N1—C14—C15—C16	−176.0 (3)
C2—C1—C6—C7	175.9 (3)	C14—C15—C16—C17	1.1 (5)
O1—C5—C6—C1	−179.8 (3)	C15—C16—C17—C18	−2.0 (6)
C4—C5—C6—C1	−0.9 (5)	C15—C16—C17—Cl1	177.7 (3)
O1—C5—C6—C7	1.4 (5)	C16—C17—C18—C19	1.0 (6)
C4—C5—C6—C7	−179.7 (3)	Cl1—C17—C18—C19	−178.6 (3)
C1—C6—C7—C8	19.8 (5)	C15—C14—C19—C18	−1.5 (5)
C5—C6—C7—C8	−161.5 (3)	N1—C14—C19—C18	175.2 (3)
C1—C6—C7—C24	−103.8 (4)	C17—C18—C19—C14	0.7 (6)
C5—C6—C7—C24	75.0 (4)	C6—C7—C24—C25	−120.9 (4)
C6—C7—C8—C13	−21.0 (5)	C8—C7—C24—C25	116.4 (4)
C24—C7—C8—C13	103.0 (4)	C6—C7—C24—C29	58.3 (4)
C6—C7—C8—C9	159.5 (3)	C8—C7—C24—C29	−64.5 (4)
C24—C7—C8—C9	−76.5 (4)	C29—C24—C25—C26	0.0 (5)
C13—C8—C9—O2	170.4 (3)	C7—C24—C25—C26	179.2 (3)
C7—C8—C9—O2	−10.1 (5)	C24—C25—C26—C27	−0.7 (5)
C13—C8—C9—C10	−8.1 (5)	C25—C26—C27—C28	1.4 (5)
C7—C8—C9—C10	171.5 (3)	C25—C26—C27—O3	180.0 (3)
O2—C9—C10—C11	159.4 (3)	C30—O3—C27—C26	−1.7 (5)
C8—C9—C10—C11	−22.2 (5)	C30—O3—C27—C28	177.0 (3)
C9—C10—C11—C23	168.9 (3)	C26—C27—C28—C29	−1.4 (6)
C9—C10—C11—C12	50.2 (4)	O3—C27—C28—C29	179.9 (3)
C9—C10—C11—C22	−70.4 (4)	C27—C28—C29—C24	0.7 (6)
C10—C11—C12—C13	−51.3 (4)	C25—C24—C29—C28	0.0 (5)
C23—C11—C12—C13	−170.2 (3)	C7—C24—C29—C28	−179.2 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···O2^{i}	0.93	2.48	3.366 (4)	161
C21—H21A···O2^{ii}	0.96	2.53	3.418 (4)	154

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) *x*, −*y*+3/2, *z*−1/2.

Fig. 1


C30
O3
C26
C27
C25
C28
O1
C24
C29
O2
C5
C7
C9
C6
C8
C10
C4
C20
C22
C3
C1
C13
C11
C21
C2
N1
C12
C23
C14
C19
C15
C18
C16
C17
Cl1