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9-(1,3-Benzodioxol-5-yl)-10-(4-chlorophenyl)-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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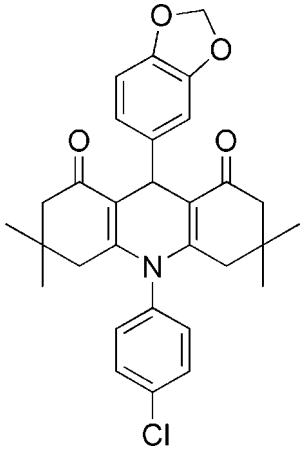
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.069; wR factor = 0.200; data-to-parameter ratio = 14.0.

The title compound, $C_{30}H_{30}ClNO_4$, was synthesized by the reaction of dimedone with 1,3-benzodioxole-5-carbaldehyde and 4-chlorobenzenamine in water. The dihydropyridine ring adopts a boat conformation, while the two cyclohexenone rings have envelope conformations.

Related literature

For related literature, see: Wysocka-Skrzela & Ledochowski (1976); Reil *et al.* (1994); Mandi *et al.* (1994); Thull & Testa (1994); Khurana *et al.* (1990); Popielarz *et al.* (1997); Srividya *et al.* (1996); Tu *et al.* (2004, 2006). For general background, see: Cremer & Pople (1975). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{30}H_{30}ClNO_4$
M_r = 504.00
Monoclinic, $P2_1/c$
a = 12.339 (2) Å
b = 10.991 (2) Å
c = 19.753 (3) Å
β = 102.054 (2)°
V = 2619.8 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 298 (2) K
0.21 × 0.18 × 0.15 mm

Data collection

Bruker CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.963, T_{max} = 0.973
10447 measured reflections
4537 independent reflections
2041 reflections with $I > 2\sigma(I)$
R_{int} = 0.061

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.200
S = 1.03
4537 reflections
325 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); 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, 1999); 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: HK2316).

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supplementary materials

Acta Cryst. (2007). E**63**, o3924 [**doi:10.1107/S160053680704175X**]

9-(1,3-Benzodioxol-5-yl)-10-(4-chlorophenyl)-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

Many of the natural and synthetic compounds containing the acridine skeleton display interesting biological and physical activities, such as antimalaria (Wysocka-Skrzela & Ledochowski, 1976; Reil *et al.*, 1994; Mandi *et al.*, 1994; Thull & Testa, 1994) and antitumor agents (Khurana *et al.*, 1990), and multi- hydroacridineone derivatives have been reported to have high fluorescence efficiency and can be used as fluorescent molecular probes for monitoring of polymerization process (Popielarz *et al.*, 1997). They are also increasingly receiving attention, due to their likeness in properties with those of 1,4-dihydropyridines, which have similarities in structure to the biologically important compounds such as NADH and NADPH (Srividya *et al.*, 1996). As a consequence, the interest of organic chemists in the synthesis or structure modifications of acridinedione derivatives remains high (Tu *et al.*, 2004; 2006). We report herein the structure of the title compound, (I).

In the molecule of the title compound, (I), (Fig. 1) the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987).

Rings A (C1—C6), B (N1/C1/C6—C8/C13) and C (C8—C13) are not planar, having total puckering amplitudes, Q_T, of 0.490 (3), 0.226 (2) and 0.486 (2) Å, respectively. Ring B adopts boat conformation [φ = -2.14 (3)° and θ = 104.81 (3)°] (Cremer & Pople, 1975). Rings A and C have envelope conformations with atoms C3 and C11 displaced by 0.678 (2) Å and 0.668 (2) Å from the planes of the other ring atoms, respectively. Rings D (C14—C19), E (C24—C29) and F (O3/O4/C26/C27/C30) are, of course, planar and rings E and F are also coplanar with a dihedral angle of 0.76 (2)° and ring D is oriented with respect to the coplanar rings system at a dihedral angle of 11.06 (3)°.

In the crystal structure, the molecules are elongated along the *c* axis (Fig. 2).

Experimental

The title compound was prepared by the reaction of dimedone (280 mg, 2 mmol) with 1,3-benzodioxole-5-carbaldehyde (150 mg, 1 mmol) and 4-chlorobenzen- amine (130 mg, 1 mmol) at 413 K under microwave irradiation (maximum power 150 W, initial power 100 W) for 10 min. Single crystals suitable for X-ray diffraction were obtained from an ethanol solution by slow evaporation (yield; 440 mg, 86%; m.p. 560–561 K).

Refinement

H atoms were positioned geometrically with C—H = 0.93, 0.98, 0.97 and 0.96 Å for aromatic, methine, methylene and methyl H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl H and x = 1.2 for all other H atoms.

Figures

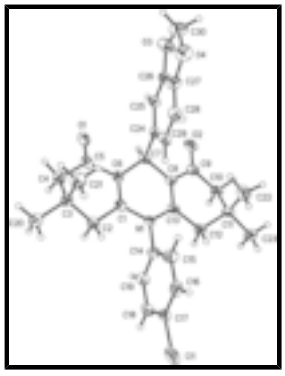

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Fig. 2. A packing diagram for (I). Hydrogen atoms are omitted for clarity.

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Crystal data

$C_{30}H_{30}ClNO_4$	F_{000} = 1064
M_r = 504.00	D_x = 1.278 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point = 560–561 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 12.339 (2) Å	Cell parameters from 2146 reflections
b = 10.991 (2) Å	θ = 2.4–27.8º
c = 19.753 (3) Å	μ = 0.18 mm^{-1}
β = 102.054 (2)º	T = 298 (2) K
V = 2619.8 (8) Å^3	Block, pale yellow
Z = 4	0.21 × 0.18 × 0.15 mm

Data collection

Bruker CCD area-detector diffractometer	4537 independent reflections
Radiation source: fine-focus sealed tube	2041 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.061
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −13→14
T_{min} = 0.963, T_{max} = 0.973	k = −13→12
10447 measured reflections	l = −20→23

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.069$	H-atom parameters constrained
$wR(F^2) = 0.200$	$w = 1/[\sigma^2(F_o^2) + (0.078P)^2 + 0.7779P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
4537 reflections	$\Delta\rho_{max} = 0.32$ e Å^{-3}
325 parameters	$\Delta\rho_{min} = -0.37$ 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 $F^2 > \sigma(F^2)$ 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	0.63239 (16)	1.52738 (15)	0.23984 (8)	0.0964 (7)
N1	0.7985 (3)	1.0541 (3)	0.36537 (18)	0.0380 (9)
O1	0.9268 (3)	0.8116 (3)	0.56215 (17)	0.0621 (10)
O2	0.9340 (3)	0.6660 (3)	0.32234 (18)	0.0641 (11)
O3	0.6752 (3)	0.4195 (3)	0.4549 (2)	0.0705 (11)
O4	0.4981 (3)	0.4951 (3)	0.41699 (19)	0.0687 (11)
C1	0.8183 (4)	1.0340 (4)	0.4368 (2)	0.0373 (11)
C2	0.8007 (4)	1.1398 (4)	0.4815 (2)	0.0465 (13)
H2A	0.7405	1.1896	0.4566	0.056*
H2B	0.8671	1.1895	0.4909	0.056*
C3	0.7732 (4)	1.0995 (4)	0.5509 (2)	0.0445 (12)
C4	0.8625 (4)	1.0098 (4)	0.5835 (2)	0.0542 (14)
H4A	0.9313	1.0541	0.5985	0.065*
H4B	0.8423	0.9756	0.6244	0.065*
C5	0.8830 (4)	0.9069 (4)	0.5377 (2)	0.0422 (12)
C6	0.8509 (4)	0.9237 (4)	0.4620 (2)	0.0367 (11)
C7	0.8551 (4)	0.8137 (4)	0.4177 (2)	0.0395 (12)
H7	0.9226	0.7681	0.4372	0.047*

C8	0.8617 (4)	0.8552 (4)	0.3454 (2)	0.0352 (11)
C9	0.9045 (4)	0.7688 (4)	0.3016 (2)	0.0428 (12)
C10	0.9162 (4)	0.8107 (4)	0.2313 (2)	0.0509 (14)
H10A	0.9143	0.7404	0.2014	0.061*
H10B	0.9878	0.8496	0.2352	0.061*
C11	0.8254 (4)	0.8998 (4)	0.1980 (2)	0.0488 (13)
C12	0.8287 (4)	1.0068 (4)	0.2482 (2)	0.0493 (13)
H12A	0.8943	1.0552	0.2478	0.059*
H12B	0.7645	1.0580	0.2323	0.059*
C13	0.8302 (4)	0.9670 (4)	0.3218 (2)	0.0366 (11)
C14	0.7585 (4)	1.1721 (4)	0.3375 (2)	0.0451 (13)
C15	0.6474 (4)	1.1843 (5)	0.3061 (3)	0.0553 (14)
H15	0.5985	1.1196	0.3053	0.066*
C16	0.6102 (5)	1.2960 (6)	0.2757 (3)	0.0606 (15)
H16	0.5364	1.3049	0.2535	0.073*
C17	0.6813 (5)	1.3918 (5)	0.2784 (2)	0.0482 (13)
C18	0.7907 (5)	1.3809 (4)	0.3102 (3)	0.0512 (14)
H18	0.8386	1.4467	0.3120	0.061*
C19	0.8288 (4)	1.2708 (4)	0.3395 (2)	0.0485 (13)
H19	0.9031	1.2628	0.3609	0.058*
C20	0.7766 (4)	1.2110 (5)	0.5983 (2)	0.0627 (16)
H20A	0.7244	1.2707	0.5759	0.094*
H20B	0.8498	1.2452	0.6076	0.094*
H20C	0.7577	1.1866	0.6411	0.094*
C21	0.6601 (4)	1.0405 (5)	0.5397 (3)	0.0646 (16)
H21A	0.6584	0.9707	0.5103	0.097*
H21B	0.6047	1.0977	0.5182	0.097*
H21C	0.6453	1.0156	0.5835	0.097*
C22	0.7141 (5)	0.8362 (5)	0.1861 (3)	0.0776 (18)
H22A	0.6560	0.8949	0.1725	0.116*
H22B	0.7055	0.7970	0.2281	0.116*
H22C	0.7102	0.7765	0.1502	0.116*
C23	0.8478 (5)	0.9489 (5)	0.1293 (3)	0.0778 (19)
H23A	0.9185	0.9890	0.1376	0.117*
H23B	0.7908	1.0058	0.1097	0.117*
H23C	0.8481	0.8826	0.0977	0.117*
C24	0.7569 (4)	0.7316 (4)	0.4168 (2)	0.0367 (11)
C25	0.7729 (4)	0.6100 (4)	0.4390 (2)	0.0412 (12)
H25	0.8435	0.5783	0.4548	0.049*
C26	0.6803 (5)	0.5407 (4)	0.4362 (2)	0.0456 (13)
C27	0.5756 (4)	0.5854 (5)	0.4145 (2)	0.0469 (13)
C28	0.5562 (4)	0.7023 (5)	0.3925 (2)	0.0526 (14)
H28	0.4849	0.7325	0.3772	0.063*
C29	0.6500 (4)	0.7736 (4)	0.3946 (2)	0.0494 (13)
H29	0.6401	0.8541	0.3802	0.059*
C30	0.5615 (5)	0.3901 (5)	0.4419 (3)	0.0703 (17)
H30A	0.5416	0.3617	0.4842	0.084*
H30B	0.5459	0.3254	0.4079	0.084*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1397 (16)	0.0704 (11)	0.0800 (12)	0.0544 (11)	0.0247 (11)	0.0268 (9)
N1	0.054 (3)	0.026 (2)	0.036 (2)	0.0083 (19)	0.0150 (19)	0.0030 (17)
O1	0.073 (3)	0.052 (2)	0.057 (2)	0.006 (2)	0.006 (2)	0.0148 (18)
O2	0.074 (3)	0.046 (2)	0.074 (3)	0.025 (2)	0.019 (2)	0.0100 (19)
O3	0.082 (3)	0.035 (2)	0.097 (3)	−0.012 (2)	0.026 (2)	0.015 (2)
O4	0.065 (3)	0.062 (3)	0.081 (3)	−0.024 (2)	0.017 (2)	−0.003 (2)
C1	0.033 (3)	0.035 (3)	0.045 (3)	−0.002 (2)	0.009 (2)	0.005 (2)
C2	0.059 (3)	0.036 (3)	0.048 (3)	−0.001 (2)	0.020 (3)	−0.001 (2)
C3	0.054 (3)	0.042 (3)	0.042 (3)	−0.001 (3)	0.019 (3)	−0.003 (2)
C4	0.066 (4)	0.051 (3)	0.048 (3)	−0.010 (3)	0.016 (3)	0.002 (3)
C5	0.034 (3)	0.040 (3)	0.050 (3)	−0.005 (2)	0.004 (2)	0.011 (2)
C6	0.037 (3)	0.036 (3)	0.037 (3)	−0.002 (2)	0.008 (2)	0.003 (2)
C7	0.041 (3)	0.030 (3)	0.050 (3)	0.003 (2)	0.016 (2)	0.007 (2)
C8	0.035 (3)	0.030 (3)	0.042 (3)	−0.001 (2)	0.012 (2)	−0.002 (2)
C9	0.038 (3)	0.039 (3)	0.053 (3)	0.003 (2)	0.014 (2)	−0.001 (2)
C10	0.068 (4)	0.041 (3)	0.050 (3)	0.009 (3)	0.024 (3)	−0.002 (2)
C11	0.072 (4)	0.030 (3)	0.046 (3)	0.005 (3)	0.018 (3)	−0.003 (2)
C12	0.073 (4)	0.035 (3)	0.045 (3)	−0.003 (3)	0.025 (3)	0.000 (2)
C13	0.040 (3)	0.027 (3)	0.047 (3)	−0.002 (2)	0.017 (2)	0.001 (2)
C14	0.054 (4)	0.032 (3)	0.053 (3)	0.002 (3)	0.020 (3)	−0.002 (2)
C15	0.047 (4)	0.050 (3)	0.070 (4)	0.000 (3)	0.014 (3)	−0.007 (3)
C16	0.058 (4)	0.073 (4)	0.047 (3)	0.028 (3)	0.003 (3)	−0.001 (3)
C17	0.063 (4)	0.040 (3)	0.044 (3)	0.021 (3)	0.017 (3)	0.005 (2)
C18	0.063 (4)	0.036 (3)	0.060 (3)	0.007 (3)	0.025 (3)	0.009 (3)
C19	0.049 (3)	0.041 (3)	0.056 (3)	0.002 (3)	0.013 (3)	0.004 (3)
C20	0.083 (4)	0.056 (4)	0.053 (3)	0.002 (3)	0.021 (3)	−0.007 (3)
C21	0.056 (4)	0.079 (4)	0.065 (4)	−0.001 (3)	0.026 (3)	−0.002 (3)
C22	0.082 (5)	0.063 (4)	0.076 (4)	0.003 (4)	−0.012 (4)	0.007 (3)
C23	0.148 (6)	0.047 (3)	0.045 (3)	0.004 (4)	0.035 (4)	−0.006 (3)
C24	0.040 (3)	0.033 (3)	0.038 (3)	0.002 (2)	0.009 (2)	0.008 (2)
C25	0.041 (3)	0.034 (3)	0.047 (3)	0.001 (2)	0.007 (2)	0.003 (2)
C26	0.065 (4)	0.030 (3)	0.045 (3)	−0.001 (3)	0.020 (3)	0.003 (2)
C27	0.053 (4)	0.041 (3)	0.050 (3)	−0.014 (3)	0.019 (3)	−0.006 (2)
C28	0.040 (3)	0.057 (4)	0.061 (3)	0.002 (3)	0.011 (3)	0.010 (3)
C29	0.051 (3)	0.042 (3)	0.055 (3)	0.005 (3)	0.011 (3)	0.017 (2)
C30	0.089 (5)	0.046 (4)	0.088 (4)	−0.016 (4)	0.047 (4)	−0.006 (3)

Geometric parameters (Å, °)

Cl1—C17	1.725 (5)	C12—H12A	0.9700
N1—C13	1.397 (5)	C12—H12B	0.9700
N1—C1	1.399 (5)	C14—C19	1.385 (6)
N1—C14	1.455 (5)	C14—C15	1.388 (6)
O1—C5	1.231 (5)	C15—C16	1.400 (7)
O2—C9	1.231 (5)	C15—H15	0.9300

O3—C26	1.387 (5)	C16—C17	1.364 (7)
O3—C30	1.410 (6)	C16—H16	0.9300
O4—C27	1.386 (5)	C17—C18	1.369 (7)
O4—C30	1.424 (6)	C18—C19	1.380 (6)
C1—C6	1.339 (6)	C18—H18	0.9300
C1—C2	1.504 (6)	C19—H19	0.9300
C2—C3	1.543 (6)	C20—H20A	0.9600
C2—H2A	0.9700	C20—H20B	0.9600
C2—H2B	0.9700	C20—H20C	0.9600
C3—C21	1.513 (6)	C21—H21A	0.9600
C3—C4	1.518 (6)	C21—H21B	0.9600
C3—C20	1.538 (6)	C21—H21C	0.9600
C4—C5	1.502 (6)	C22—H22A	0.9600
C4—H4A	0.9700	C22—H22B	0.9600
C4—H4B	0.9700	C22—H22C	0.9600
C5—C6	1.477 (6)	C23—H23A	0.9600
C6—C7	1.499 (6)	C23—H23B	0.9600
C7—C24	1.508 (6)	C23—H23C	0.9600
C7—C8	1.518 (6)	C24—C29	1.379 (6)
C7—H7	0.9800	C24—C25	1.407 (6)
C8—C13	1.343 (6)	C25—C26	1.365 (6)
C8—C9	1.455 (6)	C25—H25	0.9300
C9—C10	1.498 (6)	C26—C27	1.365 (6)
C10—C11	1.530 (6)	C27—C28	1.362 (6)
C10—H10A	0.9700	C28—C29	1.392 (6)
C10—H10B	0.9700	C28—H28	0.9300
C11—C22	1.514 (7)	C29—H29	0.9300
C11—C12	1.534 (6)	C30—H30A	0.9700
C11—C23	1.539 (6)	C30—H30B	0.9700
C12—C13	1.514 (6)		
C13—N1—C1	120.1 (4)	C19—C14—N1	121.8 (5)
C13—N1—C14	119.7 (4)	C15—C14—N1	118.7 (4)
C1—N1—C14	119.8 (4)	C14—C15—C16	118.7 (5)
C26—O3—C30	105.7 (4)	C14—C15—H15	120.7
C27—O4—C30	105.1 (4)	C16—C15—H15	120.7
C6—C1—N1	119.5 (4)	C17—C16—C15	120.6 (5)
C6—C1—C2	123.5 (4)	C17—C16—H16	119.7
N1—C1—C2	117.0 (4)	C15—C16—H16	119.7
C1—C2—C3	112.6 (4)	C16—C17—C18	121.0 (5)
C1—C2—H2A	109.1	C16—C17—Cl1	119.1 (5)
C3—C2—H2A	109.1	C18—C17—Cl1	119.9 (4)
C1—C2—H2B	109.1	C17—C18—C19	119.1 (5)
C3—C2—H2B	109.1	C17—C18—H18	120.5
H2A—C2—H2B	107.8	C19—C18—H18	120.5
C21—C3—C4	110.5 (4)	C18—C19—C14	121.2 (5)
C21—C3—C20	109.7 (4)	C18—C19—H19	119.4
C4—C3—C20	109.5 (4)	C14—C19—H19	119.4
C21—C3—C2	111.1 (4)	C3—C20—H20A	109.5
C4—C3—C2	106.8 (4)	C3—C20—H20B	109.5

C20—C3—C2	109.2 (4)	H20A—C20—H20B	109.5
C5—C4—C3	115.6 (4)	C3—C20—H20C	109.5
C5—C4—H4A	108.4	H20A—C20—H20C	109.5
C3—C4—H4A	108.4	H20B—C20—H20C	109.5
C5—C4—H4B	108.4	C3—C21—H21A	109.5
C3—C4—H4B	108.4	C3—C21—H21B	109.5
H4A—C4—H4B	107.4	H21A—C21—H21B	109.5
O1—C5—C6	120.4 (4)	C3—C21—H21C	109.5
O1—C5—C4	121.3 (4)	H21A—C21—H21C	109.5
C6—C5—C4	118.2 (4)	H21B—C21—H21C	109.5
C1—C6—C5	119.0 (4)	C11—C22—H22A	109.5
C1—C6—C7	123.9 (4)	C11—C22—H22B	109.5
C5—C6—C7	117.1 (4)	H22A—C22—H22B	109.5
C6—C7—C24	111.4 (4)	C11—C22—H22C	109.5
C6—C7—C8	108.8 (3)	H22A—C22—H22C	109.5
C24—C7—C8	111.7 (4)	H22B—C22—H22C	109.5
C6—C7—H7	108.3	C11—C23—H23A	109.5
C24—C7—H7	108.3	C11—C23—H23B	109.5
C8—C7—H7	108.3	H23A—C23—H23B	109.5
C13—C8—C9	120.3 (4)	C11—C23—H23C	109.5
C13—C8—C7	122.2 (4)	H23A—C23—H23C	109.5
C9—C8—C7	117.5 (4)	H23B—C23—H23C	109.5
O2—C9—C8	121.3 (4)	C29—C24—C25	118.7 (4)
O2—C9—C10	120.8 (4)	C29—C24—C7	121.0 (4)
C8—C9—C10	117.9 (4)	C25—C24—C7	120.3 (4)
C9—C10—C11	113.0 (4)	C26—C25—C24	117.1 (4)
C9—C10—H10A	109.0	C26—C25—H25	121.4
C11—C10—H10A	109.0	C24—C25—H25	121.4
C9—C10—H10B	109.0	C25—C26—C27	122.7 (4)
C11—C10—H10B	109.0	C25—C26—O3	127.6 (5)
H10A—C10—H10B	107.8	C27—C26—O3	109.7 (5)
C22—C11—C10	109.3 (4)	C28—C27—C26	122.2 (5)
C22—C11—C12	110.8 (4)	C28—C27—O4	127.6 (5)
C10—C11—C12	107.1 (4)	C26—C27—O4	110.2 (4)
C22—C11—C23	110.4 (5)	C27—C28—C29	115.6 (5)
C10—C11—C23	110.7 (4)	C27—C28—H28	122.2
C12—C11—C23	108.4 (4)	C29—C28—H28	122.2
C13—C12—C11	113.1 (4)	C24—C29—C28	123.7 (5)
C13—C12—H12A	109.0	C24—C29—H29	118.2
C11—C12—H12A	109.0	C28—C29—H29	118.2
C13—C12—H12B	109.0	O3—C30—O4	109.3 (4)
C11—C12—H12B	109.0	O3—C30—H30A	109.8
H12A—C12—H12B	107.8	O4—C30—H30A	109.8
C8—C13—N1	120.8 (4)	O3—C30—H30B	109.8
C8—C13—C12	122.8 (4)	O4—C30—H30B	109.8
N1—C13—C12	116.4 (4)	H30A—C30—H30B	108.3
C19—C14—C15	119.5 (5)		
C13—N1—C1—C6	−10.8 (6)	C7—C8—C13—C12	−175.6 (4)
C14—N1—C1—C6	177.3 (4)	C1—N1—C13—C8	11.7 (6)

C13—N1—C1—C2	169.5 (4)	C14—N1—C13—C8	−176.4 (4)
C14—N1—C1—C2	−2.4 (6)	C1—N1—C13—C12	−167.2 (4)
C6—C1—C2—C3	−25.2 (6)	C14—N1—C13—C12	4.7 (6)
N1—C1—C2—C3	154.4 (4)	C11—C12—C13—C8	20.6 (7)
C1—C2—C3—C21	−68.6 (5)	C11—C12—C13—N1	−160.5 (4)
C1—C2—C3—C4	51.9 (5)	C13—N1—C14—C19	−93.0 (5)
C1—C2—C3—C20	170.2 (4)	C1—N1—C14—C19	78.9 (5)
C21—C3—C4—C5	69.5 (5)	C13—N1—C14—C15	84.7 (5)
C20—C3—C4—C5	−169.5 (4)	C1—N1—C14—C15	−103.3 (5)
C2—C3—C4—C5	−51.4 (5)	C19—C14—C15—C16	1.5 (7)
C3—C4—C5—O1	−158.2 (4)	N1—C14—C15—C16	−176.3 (4)
C3—C4—C5—C6	22.8 (6)	C14—C15—C16—C17	−1.6 (7)
N1—C1—C6—C5	173.5 (4)	C15—C16—C17—C18	0.7 (8)
C2—C1—C6—C5	−6.8 (7)	C15—C16—C17—Cl1	179.6 (4)
N1—C1—C6—C7	−7.6 (7)	C16—C17—C18—C19	0.3 (7)
C2—C1—C6—C7	172.0 (4)	Cl1—C17—C18—C19	−178.6 (4)
O1—C5—C6—C1	−170.5 (4)	C17—C18—C19—C14	−0.3 (7)
C4—C5—C6—C1	8.5 (6)	C15—C14—C19—C18	−0.6 (7)
O1—C5—C6—C7	10.6 (6)	N1—C14—C19—C18	177.2 (4)
C4—C5—C6—C7	−170.4 (4)	C6—C7—C24—C29	58.3 (6)
C1—C6—C7—C24	−101.7 (5)	C8—C7—C24—C29	−63.6 (5)
C5—C6—C7—C24	77.2 (5)	C6—C7—C24—C25	−121.5 (4)
C1—C6—C7—C8	21.9 (6)	C8—C7—C24—C25	116.6 (4)
C5—C6—C7—C8	−159.2 (4)	C29—C24—C25—C26	0.7 (6)
C6—C7—C8—C13	−20.6 (6)	C7—C24—C25—C26	−179.5 (4)
C24—C7—C8—C13	102.7 (5)	C24—C25—C26—C27	−1.3 (7)
C6—C7—C8—C9	159.1 (4)	C24—C25—C26—O3	179.7 (4)
C24—C7—C8—C9	−77.5 (5)	C30—O3—C26—C25	−179.5 (5)
C13—C8—C9—O2	179.8 (5)	C30—O3—C26—C27	1.4 (5)
C7—C8—C9—O2	0.1 (7)	C25—C26—C27—C28	1.4 (8)
C13—C8—C9—C10	2.5 (7)	O3—C26—C27—C28	−179.5 (4)
C7—C8—C9—C10	−177.3 (4)	C25—C26—C27—O4	179.9 (4)
O2—C9—C10—C11	147.9 (5)	O3—C26—C27—O4	−0.9 (5)
C8—C9—C10—C11	−34.7 (6)	C30—O4—C27—C28	178.5 (5)
C9—C10—C11—C22	−63.5 (5)	C30—O4—C27—C26	0.0 (5)
C9—C10—C11—C12	56.6 (5)	C26—C27—C28—C29	−0.8 (7)
C9—C10—C11—C23	174.6 (4)	O4—C27—C28—C29	−179.1 (4)
C22—C11—C12—C13	69.9 (5)	C25—C24—C29—C28	−0.2 (7)
C10—C11—C12—C13	−49.2 (5)	C7—C24—C29—C28	180.0 (4)
C23—C11—C12—C13	−168.7 (4)	C27—C28—C29—C24	0.2 (7)
C9—C8—C13—N1	−174.2 (4)	C26—O3—C30—O4	−1.4 (6)
C7—C8—C13—N1	5.6 (7)	C27—O4—C30—O3	0.9 (5)
C9—C8—C13—C12	4.7 (7)		

Fig. 1

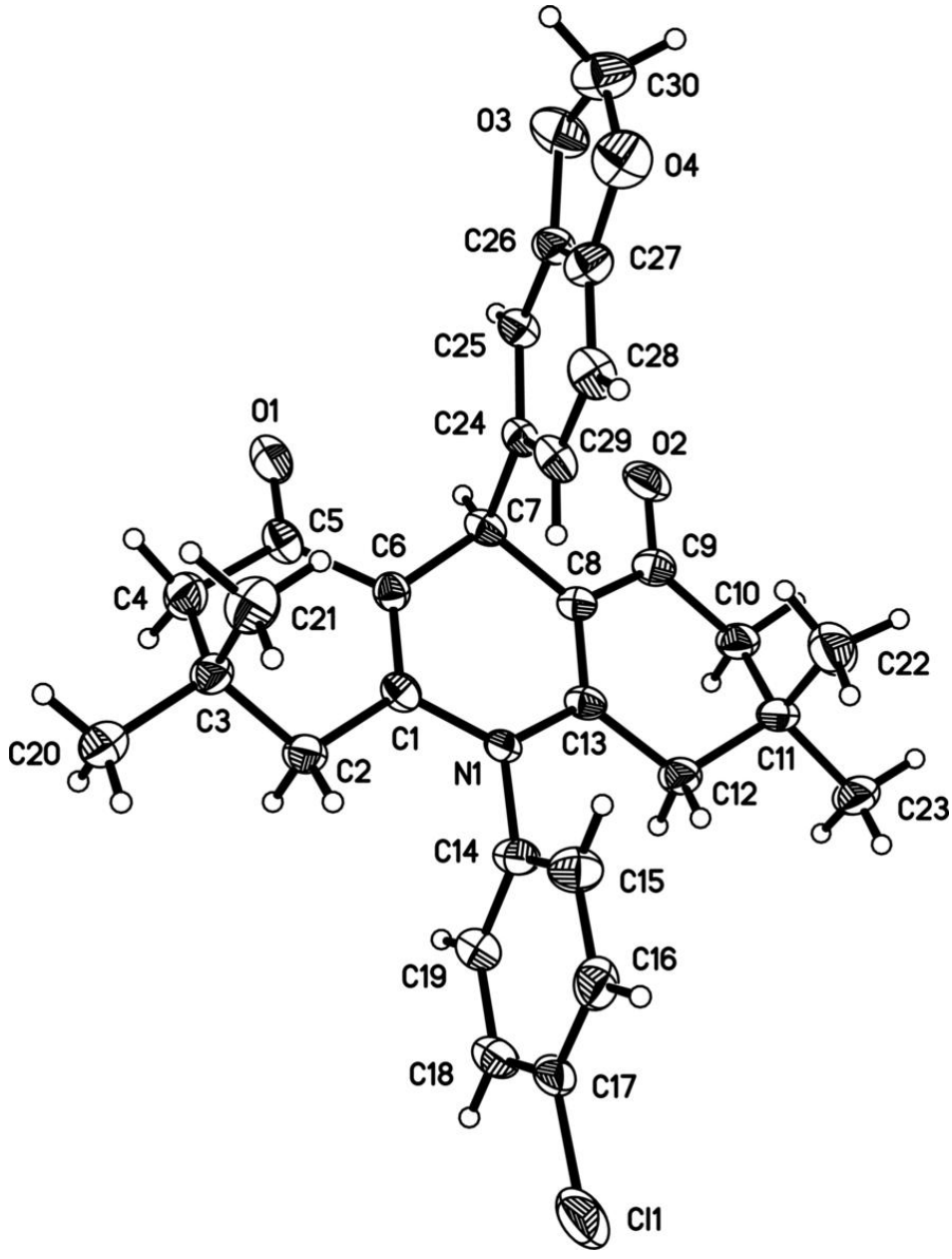
C30
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Fig. 2