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9-(1,3-Benzodioxol-5-yl)-3,3,6,6-tetramethyl-10-*p*-tolyl-3,4,6,7-tetrahydroacridine-1,8(2*H*,5*H*,9*H*,10*H*)-dione

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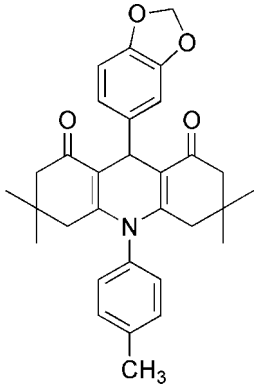
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.051; wR factor = 0.163; data-to-parameter ratio = 14.3.

The title compound, $C_{31}H_{33}NO_4$, was synthesized by the reaction of dimedone with 1,3-benzodioxole-5-carbaldehyde and *p*-toluidine in water. The dihydropyridine and both of the cyclohexenone rings are not planar and have flattened boat conformations, while the remaining rings are planar. The dihedral angle between the planar rings of the 1,3-benzodioxole system is 1.30 (2)°, so they are nearly coplanar; the angle between the benzene and benzodioxole rings is 9.7 (1)°.

Related literature

For general background, see: Wysocka-Skrzela & Ledochowski (1976); Nasim & Brychey (1979); Thull & Testa (1994); Reil *et al.* (1994); Mandi *et al.* (1994); Tu *et al.* (2004); Cremer & Pople (1975). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{31}H_{33}NO_4$
M_r = 483.58
Monoclinic, $P2_1/c$
a = 12.344 (3) Å
b = 11.074 (2) Å
c = 19.772 (3) Å
β = 102.286 (3)°
V = 2640.8 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
0.45 × 0.43 × 0.41 mm

Data collection

Bruker CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.965, T_{max} = 0.968
13410 measured reflections
4650 independent reflections
2042 reflections with $I > 2\sigma(I)$
R_{int} = 0.065

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.163
S = 1.00
4650 reflections
325 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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: HK2306).

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supplementary materials

Acta Cryst. (2007). E**63**, o3811 [**doi:10.1107/S1600536807038998**]

9-(1,3-Benzodioxol-5-yl)-3,3,6,6-tetramethyl-10-*p*-tolyl-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, (I).

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

Rings A (O3/O4/C27/C28/C31), B (C25—C30) and C (C14—C19) are, of course, planar and the dihedral angle between rings A and B is A/B = 1.30 (2)°, so they are also nearly co-planar. Rings D (C1—C6), E (N1/C1/C6—C8/C13) and F (C8—C13) are not planar, having total puckering amplitudes, Q_T, of 0.475 (3), 0.222 (2) and 0.476 (3) Å, respectively, and flattened boat conformations [φ = 131.26 (3)°, θ = 54.78 (3)°; φ = 122.70 (2)°, θ = 73.60 (3)° and φ = 1.73 (3)°, θ = 121.14 (3)°, respectively] (Cremer & Pople, 1975).

As can be seen from the packing diagram (Fig. 2), the molecules of (I) are elongated along the *c* axis. Dipole-dipole and van der Waals interactions may be effective in the molecular packing.

Experimental

The title compound was prepared by the reaction of dimedone (0.28 g, 2 mmol) with benzo[*d*][1,3]dioxole-5-carbaldehyde (0.15 g, 1 mmol) and *p*-toluidine (0.17 g, 1 mmol) at 403 K under microwave irradiation (maximum power 150 W, initial power 100 W) for 6 min (yield; 0.43 g, 89%, m.p. 536–537 K). Single crystals suitable for X-ray analysis were obtained from an ethanol solution (95%) by slow evaporation.

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, 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

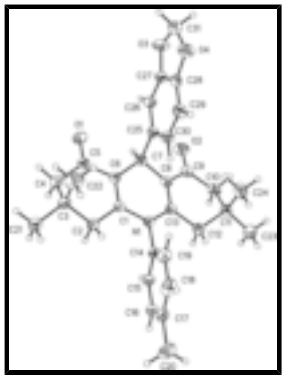

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Fig. 2. A packing diagram of (I).

9-(1,3-Benzodioxol-5-yl)-3,3,6,6-tetramethyl-10-*p*-tolyl-3,4,6,7- tetrahydroacridine-1,8(2*H*,5H,9*H*,10H)-dione

Crystal data

$C_{31}H_{33}NO_4$	F_{000} = 1032
M_r = 483.58	D_x = 1.216 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 536-537 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 12.344 (3) Å	Cell parameters from 1625 reflections
b = 11.074 (2) Å	θ = 2.4–20.0º
c = 19.772 (3) Å	μ = 0.08 mm^{-1}
β = 102.286 (3)º	T = 298 (2) K
V = 2640.8 (9) Å^3	Block, yellow
Z = 4	0.45 × 0.43 × 0.41 mm

Data collection

Bruker CCD area-detector diffractometer	4650 independent reflections
Radiation source: fine-focus sealed tube	2042 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.065
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −14→14
T_{min} = 0.965, T_{max} = 0.968	k = −13→10
13410 measured reflections	l = −21→23

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.051$	H-atom parameters constrained
$wR(F^2) = 0.163$	$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 1.2257P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
4650 reflections	$\Delta\rho_{max} = 0.24$ e Å^{-3}
325 parameters	$\Delta\rho_{min} = -0.18$ 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 $F^2 > 2$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	0.7022 (2)	0.4428 (2)	0.13499 (13)	0.0414 (7)
O1	0.5690 (2)	0.8299 (2)	0.17756 (13)	0.0668 (8)
O2	0.5793 (2)	0.6872 (2)	−0.06130 (12)	0.0637 (8)
O3	0.8218 (2)	1.0740 (2)	0.04178 (14)	0.0713 (8)
O4	0.9999 (2)	1.0020 (3)	0.08198 (13)	0.0699 (8)
C1	0.6706 (3)	0.5297 (3)	0.17899 (16)	0.0384 (8)
C2	0.6709 (3)	0.4912 (3)	0.25162 (16)	0.0503 (10)
H2A	0.7352	0.4406	0.2682	0.060*
H2B	0.6053	0.4430	0.2516	0.060*
C3	0.6732 (3)	0.5971 (3)	0.30138 (17)	0.0488 (9)
C4	0.5838 (3)	0.6862 (3)	0.26838 (17)	0.0539 (10)
H4A	0.5117	0.6487	0.2643	0.065*
H4B	0.5867	0.7561	0.2983	0.065*
C5	0.5963 (3)	0.7270 (3)	0.19842 (18)	0.0452 (9)
C6	0.6389 (3)	0.6409 (3)	0.15455 (16)	0.0383 (8)
C7	0.6459 (3)	0.6822 (3)	0.08302 (16)	0.0413 (9)
H7	0.5780	0.7271	0.0635	0.050*
C8	0.6505 (3)	0.5736 (3)	0.03775 (16)	0.0390 (8)

C9	0.6207 (3)	0.5911 (3)	−0.03669 (18)	0.0480 (9)
C10	0.6382 (3)	0.4893 (3)	−0.08332 (17)	0.0555 (10)
H10A	0.6586	0.5231	−0.1241	0.067*
H10B	0.5685	0.4469	−0.0984	0.067*
C11	0.7264 (3)	0.3986 (3)	−0.05075 (17)	0.0488 (9)
C12	0.7002 (3)	0.3592 (3)	0.01839 (16)	0.0490 (10)
H12A	0.6336	0.3102	0.0093	0.059*
H12B	0.7605	0.3095	0.0431	0.059*
C13	0.6836 (3)	0.4639 (3)	0.06375 (17)	0.0402 (8)
C14	0.7402 (3)	0.3254 (3)	0.16314 (16)	0.0392 (8)
C15	0.6674 (3)	0.2303 (3)	0.15984 (17)	0.0451 (9)
H15	0.5932	0.2403	0.1386	0.054*
C16	0.7049 (3)	0.1200 (3)	0.18810 (18)	0.0536 (10)
H16	0.6552	0.0561	0.1852	0.064*
C17	0.8131 (4)	0.1026 (4)	0.22012 (18)	0.0551 (11)
C18	0.8859 (3)	0.1980 (4)	0.22254 (19)	0.0655 (12)
H18	0.9601	0.1874	0.2437	0.079*
C19	0.8505 (3)	0.3091 (4)	0.19402 (18)	0.0542 (10)
H19	0.9006	0.3723	0.1957	0.065*
C20	0.8529 (4)	−0.0184 (4)	0.2516 (2)	0.0914 (16)
H20A	0.8080	−0.0425	0.2834	0.137*
H20B	0.9288	−0.0117	0.2757	0.137*
H20C	0.8470	−0.0776	0.2155	0.137*
C21	0.6505 (4)	0.5493 (3)	0.36970 (18)	0.0774 (14)
H21A	0.7069	0.4922	0.3895	0.116*
H21B	0.5793	0.5104	0.3612	0.116*
H21C	0.6509	0.6153	0.4012	0.116*
C22	0.7864 (3)	0.6590 (4)	0.3155 (2)	0.0779 (13)
H22A	0.7863	0.7252	0.3468	0.117*
H22B	0.8014	0.6886	0.2728	0.117*
H22C	0.8426	0.6020	0.3357	0.117*
C23	0.7232 (3)	0.2880 (4)	−0.09762 (18)	0.0687 (12)
H23A	0.7775	0.2303	−0.0757	0.103*
H23B	0.7392	0.3123	−0.1411	0.103*
H23C	0.6508	0.2520	−0.1055	0.103*
C24	0.8414 (3)	0.4561 (4)	−0.0385 (2)	0.0699 (12)
H24A	0.8433	0.5258	−0.0093	0.105*
H24B	0.8574	0.4800	−0.0820	0.105*
H24C	0.8959	0.3987	−0.0163	0.105*
C25	0.7441 (3)	0.7655 (3)	0.08364 (16)	0.0401 (9)
C26	0.7270 (3)	0.8843 (3)	0.06044 (16)	0.0443 (9)
H26	0.6558	0.9144	0.0445	0.053*
C27	0.8177 (3)	0.9550 (3)	0.06181 (17)	0.0474 (9)
C28	0.9232 (3)	0.9124 (4)	0.08529 (18)	0.0486 (10)
C29	0.9437 (3)	0.7974 (4)	0.10848 (18)	0.0541 (10)
H29	1.0154	0.7691	0.1246	0.065*
C30	0.8513 (3)	0.7243 (3)	0.10683 (18)	0.0503 (10)
H30	0.8622	0.6447	0.1219	0.060*
C31	0.9356 (4)	1.1062 (4)	0.0568 (2)	0.0729 (13)

H31A	0.9488	1.1696	0.0914	0.087*
H31B	0.9566	1.1361	0.0153	0.087*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0571 (19)	0.0329 (18)	0.0359 (17)	0.0049 (14)	0.0135 (14)	0.0042 (13)
O1	0.085 (2)	0.0431 (18)	0.0772 (19)	0.0212 (15)	0.0280 (16)	0.0116 (14)
O2	0.0771 (19)	0.0545 (18)	0.0542 (17)	0.0051 (15)	0.0020 (14)	0.0155 (14)
O3	0.081 (2)	0.0406 (17)	0.093 (2)	−0.0135 (15)	0.0198 (17)	0.0097 (15)
O4	0.0692 (19)	0.061 (2)	0.080 (2)	−0.0239 (17)	0.0171 (15)	−0.0025 (15)
C1	0.045 (2)	0.032 (2)	0.040 (2)	−0.0010 (17)	0.0122 (17)	0.0021 (16)
C2	0.073 (3)	0.039 (2)	0.042 (2)	0.0074 (19)	0.021 (2)	0.0046 (17)
C3	0.068 (3)	0.036 (2)	0.043 (2)	0.004 (2)	0.0111 (19)	−0.0001 (17)
C4	0.066 (3)	0.051 (3)	0.049 (2)	0.008 (2)	0.022 (2)	−0.0032 (19)
C5	0.043 (2)	0.041 (2)	0.053 (2)	0.0018 (18)	0.0128 (18)	0.0017 (19)
C6	0.040 (2)	0.035 (2)	0.042 (2)	0.0031 (16)	0.0123 (16)	0.0015 (16)
C7	0.041 (2)	0.039 (2)	0.043 (2)	0.0034 (17)	0.0088 (17)	0.0061 (17)
C8	0.042 (2)	0.037 (2)	0.038 (2)	−0.0010 (17)	0.0075 (16)	0.0043 (16)
C9	0.049 (2)	0.047 (2)	0.047 (2)	−0.0054 (19)	0.0072 (18)	0.0058 (19)
C10	0.064 (3)	0.059 (3)	0.043 (2)	−0.005 (2)	0.0090 (19)	0.0058 (19)
C11	0.056 (2)	0.052 (2)	0.040 (2)	−0.003 (2)	0.0127 (18)	−0.0005 (18)
C12	0.063 (3)	0.044 (2)	0.041 (2)	−0.0014 (19)	0.0144 (19)	0.0001 (17)
C13	0.044 (2)	0.040 (2)	0.038 (2)	−0.0028 (17)	0.0110 (17)	0.0015 (17)
C14	0.047 (2)	0.034 (2)	0.037 (2)	0.0069 (18)	0.0098 (18)	0.0021 (16)
C15	0.049 (2)	0.039 (2)	0.048 (2)	−0.0010 (18)	0.0118 (18)	0.0054 (17)
C16	0.068 (3)	0.041 (2)	0.055 (2)	0.004 (2)	0.019 (2)	0.0076 (19)
C17	0.077 (3)	0.048 (3)	0.042 (2)	0.022 (2)	0.016 (2)	0.0038 (19)
C18	0.060 (3)	0.080 (3)	0.050 (3)	0.030 (3)	−0.005 (2)	0.000 (2)
C19	0.051 (3)	0.055 (3)	0.055 (2)	0.001 (2)	0.008 (2)	−0.003 (2)
C20	0.137 (4)	0.068 (3)	0.067 (3)	0.055 (3)	0.018 (3)	0.017 (2)
C21	0.141 (4)	0.051 (3)	0.044 (2)	0.007 (3)	0.029 (3)	−0.003 (2)
C22	0.082 (3)	0.061 (3)	0.077 (3)	0.002 (2)	−0.012 (3)	0.005 (2)
C23	0.095 (3)	0.065 (3)	0.048 (2)	−0.001 (3)	0.019 (2)	−0.002 (2)
C24	0.061 (3)	0.082 (3)	0.071 (3)	−0.010 (2)	0.025 (2)	−0.009 (2)
C25	0.046 (2)	0.036 (2)	0.038 (2)	−0.0022 (17)	0.0087 (17)	0.0043 (16)
C26	0.048 (2)	0.038 (2)	0.045 (2)	−0.0003 (18)	0.0069 (18)	0.0083 (17)
C27	0.062 (3)	0.035 (2)	0.047 (2)	−0.004 (2)	0.017 (2)	0.0045 (17)
C28	0.056 (3)	0.048 (3)	0.045 (2)	−0.013 (2)	0.0188 (19)	−0.0056 (18)
C29	0.044 (2)	0.060 (3)	0.058 (2)	−0.002 (2)	0.0090 (19)	0.005 (2)
C30	0.050 (2)	0.042 (2)	0.059 (2)	0.003 (2)	0.013 (2)	0.0099 (18)
C31	0.098 (4)	0.052 (3)	0.080 (3)	−0.021 (3)	0.044 (3)	−0.010 (2)

Geometric parameters (Å, °)

N1—C13	1.398 (4)	C14—C15	1.376 (4)
N1—C1	1.407 (4)	C14—C19	1.381 (4)
N1—C14	1.453 (4)	C15—C16	1.382 (4)
O1—C5	1.233 (4)	C15—H15	0.9300

O2—C9	1.234 (4)	C16—C17	1.364 (5)
O3—C27	1.380 (4)	C16—H16	0.9300
O3—C31	1.417 (5)	C17—C18	1.381 (5)
O4—C28	1.382 (4)	C17—C20	1.514 (5)
O4—C31	1.429 (5)	C18—C19	1.385 (5)
C1—C6	1.350 (4)	C18—H18	0.9300
C1—C2	1.497 (4)	C19—H19	0.9300
C2—C3	1.527 (4)	C20—H20A	0.9600
C2—H2A	0.9700	C20—H20B	0.9600
C2—H2B	0.9700	C20—H20C	0.9600
C3—C4	1.520 (5)	C21—H21A	0.9600
C3—C22	1.528 (5)	C21—H21B	0.9600
C3—C21	1.531 (5)	C21—H21C	0.9600
C4—C5	1.494 (4)	C22—H22A	0.9600
C4—H4A	0.9700	C22—H22B	0.9600
C4—H4B	0.9700	C22—H22C	0.9600
C5—C6	1.460 (4)	C23—H23A	0.9600
C6—C7	1.506 (4)	C23—H23B	0.9600
C7—C8	1.508 (4)	C23—H23C	0.9600
C7—C25	1.521 (4)	C24—H24A	0.9600
C7—H7	0.9800	C24—H24B	0.9600
C8—C13	1.348 (4)	C24—H24C	0.9600
C8—C9	1.452 (4)	C25—C30	1.384 (4)
C9—C10	1.501 (5)	C25—C26	1.394 (4)
C10—C11	1.521 (5)	C26—C27	1.362 (4)
C10—H10A	0.9700	C26—H26	0.9300
C10—H10B	0.9700	C27—C28	1.370 (5)
C11—C24	1.527 (5)	C28—C29	1.359 (5)
C11—C23	1.531 (5)	C29—C30	1.393 (4)
C11—C12	1.533 (4)	C29—H29	0.9300
C12—C13	1.506 (4)	C30—H30	0.9300
C12—H12A	0.9700	C31—H31A	0.9700
C12—H12B	0.9700	C31—H31B	0.9700
C13—N1—C1	120.1 (3)	C14—C15—H15	120.0
C13—N1—C14	120.4 (3)	C16—C15—H15	120.0
C1—N1—C14	119.0 (3)	C17—C16—C15	121.5 (4)
C27—O3—C31	106.0 (3)	C17—C16—H16	119.2
C28—O4—C31	105.1 (3)	C15—C16—H16	119.2
C6—C1—N1	120.0 (3)	C16—C17—C18	118.3 (4)
C6—C1—C2	123.0 (3)	C16—C17—C20	121.0 (4)
N1—C1—C2	117.0 (3)	C18—C17—C20	120.7 (4)
C1—C2—C3	113.3 (3)	C17—C18—C19	121.2 (4)
C1—C2—H2A	108.9	C17—C18—H18	119.4
C3—C2—H2A	108.9	C19—C18—H18	119.4
C1—C2—H2B	108.9	C14—C19—C18	119.5 (4)
C3—C2—H2B	108.9	C14—C19—H19	120.3
H2A—C2—H2B	107.7	C18—C19—H19	120.3
C4—C3—C2	108.1 (3)	C17—C20—H20A	109.5
C4—C3—C22	109.8 (3)	C17—C20—H20B	109.5

C2—C3—C22	110.6 (3)	H20A—C20—H20B	109.5
C4—C3—C21	110.5 (3)	C17—C20—H20C	109.5
C2—C3—C21	108.7 (3)	H20A—C20—H20C	109.5
C22—C3—C21	109.1 (3)	H20B—C20—H20C	109.5
C5—C4—C3	112.7 (3)	C3—C21—H21A	109.5
C5—C4—H4A	109.1	C3—C21—H21B	109.5
C3—C4—H4A	109.1	H21A—C21—H21B	109.5
C5—C4—H4B	109.1	C3—C21—H21C	109.5
C3—C4—H4B	109.1	H21A—C21—H21C	109.5
H4A—C4—H4B	107.8	H21B—C21—H21C	109.5
O1—C5—C6	120.8 (3)	C3—C22—H22A	109.5
O1—C5—C4	120.9 (3)	C3—C22—H22B	109.5
C6—C5—C4	118.3 (3)	H22A—C22—H22B	109.5
C1—C6—C5	119.8 (3)	C3—C22—H22C	109.5
C1—C6—C7	122.9 (3)	H22A—C22—H22C	109.5
C5—C6—C7	117.3 (3)	H22B—C22—H22C	109.5
C6—C7—C8	109.4 (3)	C11—C23—H23A	109.5
C6—C7—C25	112.4 (3)	C11—C23—H23B	109.5
C8—C7—C25	111.0 (3)	H23A—C23—H23B	109.5
C6—C7—H7	108.0	C11—C23—H23C	109.5
C8—C7—H7	108.0	H23A—C23—H23C	109.5
C25—C7—H7	108.0	H23B—C23—H23C	109.5
C13—C8—C9	119.8 (3)	C11—C24—H24A	109.5
C13—C8—C7	122.6 (3)	C11—C24—H24B	109.5
C9—C8—C7	117.5 (3)	H24A—C24—H24B	109.5
O2—C9—C8	120.6 (3)	C11—C24—H24C	109.5
O2—C9—C10	120.4 (3)	H24A—C24—H24C	109.5
C8—C9—C10	118.9 (3)	H24B—C24—H24C	109.5
C9—C10—C11	114.8 (3)	C30—C25—C26	119.2 (3)
C9—C10—H10A	108.6	C30—C25—C7	120.5 (3)
C11—C10—H10A	108.6	C26—C25—C7	120.3 (3)
C9—C10—H10B	108.6	C27—C26—C25	118.0 (3)
C11—C10—H10B	108.6	C27—C26—H26	121.0
H10A—C10—H10B	107.5	C25—C26—H26	121.0
C10—C11—C24	110.4 (3)	C26—C27—C28	121.8 (3)
C10—C11—C23	110.4 (3)	C26—C27—O3	128.5 (4)
C24—C11—C23	109.5 (3)	C28—C27—O3	109.6 (3)
C10—C11—C12	107.3 (3)	C29—C28—C27	122.1 (3)
C24—C11—C12	110.0 (3)	C29—C28—O4	127.5 (4)
C23—C11—C12	109.2 (3)	C27—C28—O4	110.4 (3)
C13—C12—C11	113.2 (3)	C28—C29—C30	116.4 (3)
C13—C12—H12A	108.9	C28—C29—H29	121.8
C11—C12—H12A	108.9	C30—C29—H29	121.8
C13—C12—H12B	108.9	C25—C30—C29	122.4 (3)
C11—C12—H12B	108.9	C25—C30—H30	118.8
H12A—C12—H12B	107.8	C29—C30—H30	118.8
C8—C13—N1	120.4 (3)	O3—C31—O4	108.8 (3)
C8—C13—C12	122.4 (3)	O3—C31—H31A	109.9
N1—C13—C12	117.2 (3)	O4—C31—H31A	109.9

C15—C14—C19	119.6 (3)	O3—C31—H31B	109.9
C15—C14—N1	120.8 (3)	O4—C31—H31B	109.9
C19—C14—N1	119.6 (3)	H31A—C31—H31B	108.3
C14—C15—C16	119.9 (3)		
C13—N1—C1—C6	−10.5 (5)	C7—C8—C13—C12	−173.0 (3)
C14—N1—C1—C6	177.6 (3)	C1—N1—C13—C8	9.5 (5)
C13—N1—C1—C2	167.6 (3)	C14—N1—C13—C8	−178.7 (3)
C14—N1—C1—C2	−4.3 (4)	C1—N1—C13—C12	−169.3 (3)
C6—C1—C2—C3	−20.7 (5)	C14—N1—C13—C12	2.4 (4)
N1—C1—C2—C3	161.2 (3)	C11—C12—C13—C8	25.4 (5)
C1—C2—C3—C4	49.0 (4)	C11—C12—C13—N1	−155.8 (3)
C1—C2—C3—C22	−71.2 (4)	C13—N1—C14—C15	−78.8 (4)
C1—C2—C3—C21	169.0 (3)	C1—N1—C14—C15	93.1 (4)
C2—C3—C4—C5	−55.9 (4)	C13—N1—C14—C19	101.7 (4)
C22—C3—C4—C5	64.9 (4)	C1—N1—C14—C19	−86.5 (4)
C21—C3—C4—C5	−174.7 (3)	C19—C14—C15—C16	0.8 (5)
C3—C4—C5—O1	−147.4 (3)	N1—C14—C15—C16	−178.8 (3)
C3—C4—C5—C6	34.3 (4)	C14—C15—C16—C17	0.6 (5)
N1—C1—C6—C5	174.2 (3)	C15—C16—C17—C18	−1.4 (5)
C2—C1—C6—C5	−3.8 (5)	C15—C16—C17—C20	179.3 (3)
N1—C1—C6—C7	−6.2 (5)	C16—C17—C18—C19	0.7 (6)
C2—C1—C6—C7	175.8 (3)	C20—C17—C18—C19	−179.9 (3)
O1—C5—C6—C1	178.5 (3)	C15—C14—C19—C18	−1.3 (5)
C4—C5—C6—C1	−3.1 (5)	N1—C14—C19—C18	178.2 (3)
O1—C5—C6—C7	−1.1 (5)	C17—C18—C19—C14	0.6 (6)
C4—C5—C6—C7	177.3 (3)	C6—C7—C25—C30	62.9 (4)
C1—C6—C7—C8	20.9 (4)	C8—C7—C25—C30	−60.0 (4)
C5—C6—C7—C8	−159.5 (3)	C6—C7—C25—C26	−117.5 (3)
C1—C6—C7—C25	−102.9 (4)	C8—C7—C25—C26	119.7 (3)
C5—C6—C7—C25	76.7 (4)	C30—C25—C26—C27	−0.1 (5)
C6—C7—C8—C13	−21.9 (4)	C7—C25—C26—C27	−179.7 (3)
C25—C7—C8—C13	102.7 (4)	C25—C26—C27—C28	−0.2 (5)
C6—C7—C8—C9	160.0 (3)	C25—C26—C27—O3	−180.0 (3)
C25—C7—C8—C9	−75.4 (4)	C31—O3—C27—C26	177.2 (4)
C13—C8—C9—O2	172.4 (3)	C31—O3—C27—C28	−2.6 (4)
C7—C8—C9—O2	−9.5 (5)	C26—C27—C28—C29	0.1 (5)
C13—C8—C9—C10	−5.9 (5)	O3—C27—C28—C29	179.9 (3)
C7—C8—C9—C10	172.2 (3)	C26—C27—C28—O4	−179.4 (3)
O2—C9—C10—C11	157.5 (3)	O3—C27—C28—O4	0.4 (4)
C8—C9—C10—C11	−24.2 (5)	C31—O4—C28—C29	−177.6 (4)
C9—C10—C11—C24	−68.8 (4)	C31—O4—C28—C27	1.9 (4)
C9—C10—C11—C23	170.0 (3)	C27—C28—C29—C30	0.3 (5)
C9—C10—C11—C12	51.1 (4)	O4—C28—C29—C30	179.7 (3)
C10—C11—C12—C13	−51.2 (4)	C26—C25—C30—C29	0.5 (5)
C24—C11—C12—C13	68.9 (4)	C7—C25—C30—C29	−179.8 (3)
C23—C11—C12—C13	−170.9 (3)	C28—C29—C30—C25	−0.6 (5)
C9—C8—C13—N1	−173.8 (3)	C27—O3—C31—O4	3.7 (4)
C7—C8—C13—N1	8.2 (5)	C28—O4—C31—O3	−3.5 (4)
C9—C8—C13—C12	5.0 (5)		

Fig. 1

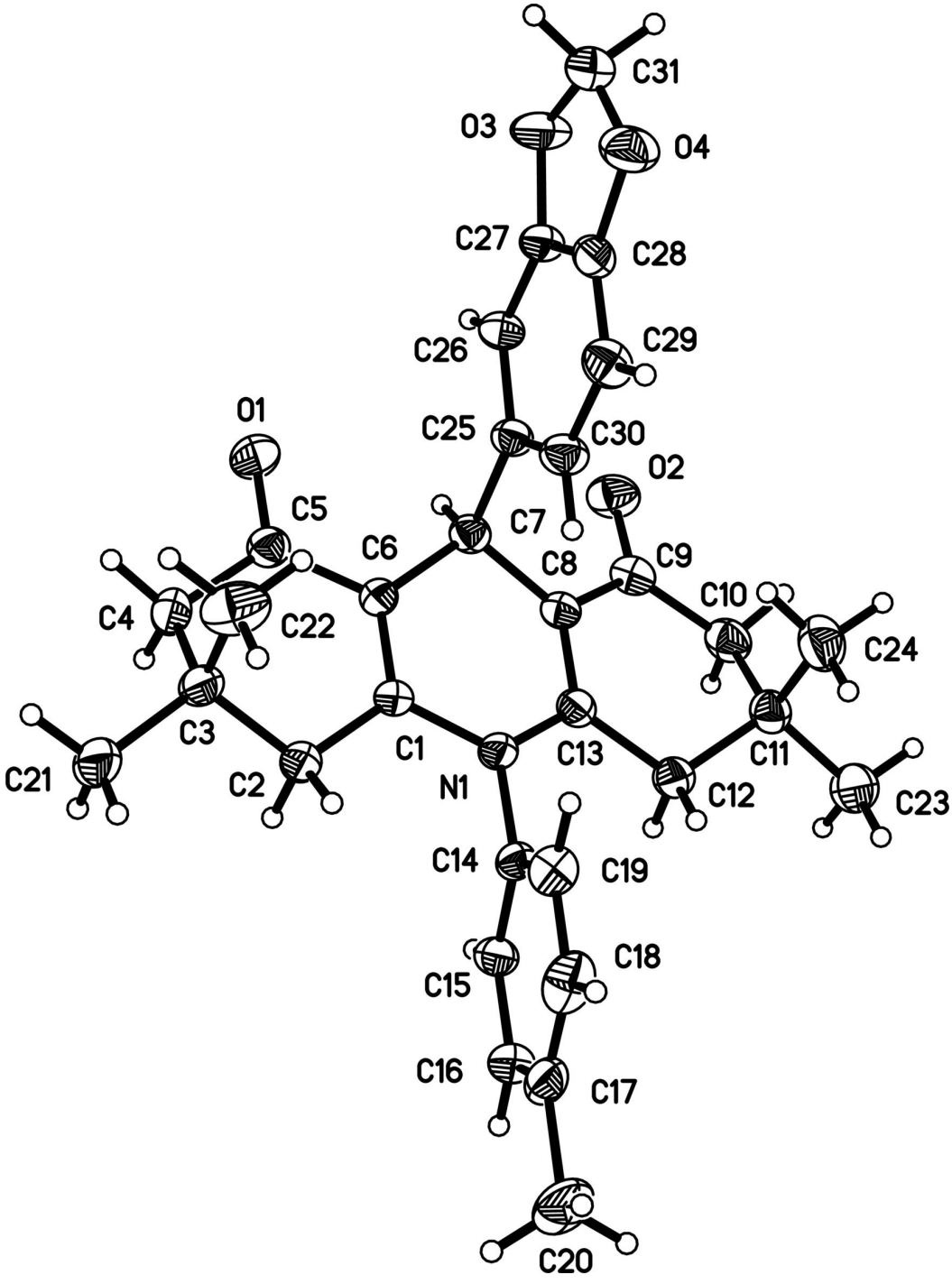
C31
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Fig. 2