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8-Methoxy-2-methylquinoline

Yi-Zhen Wang

Chemistry Department, Nanchang University, Nanchang 330031, People's Republic of China
Correspondence e-mail: wangtingyang_0@126.com

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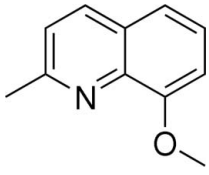
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.132; data-to-parameter ratio = 14.3.

In the title crystal structure, $C_{11}H_{11}NO$, there are two independent molecules in the asymmetric unit. In one of the molecules, the dihedral angle between the two six-membered rings of the quinoline system is 1.43 (9)° and in the other molecule the angle is 0.74 (1)°. In both molecules, the methoxy group in essentially coplanar with the quinoline group, with C—O—C—C torsion angles of 3.3 (3) and 3.1 (3)°.

Related literature

The title compound was synthesized by literature methods (Leir, 1977; Kitamura *et al.*, 2000). Quinoline derivatives have been shown to have anti-cancer and anti-malarial properties (Lee *et al.*, 1991; Nicolaou *et al.*, 1991). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{11}H_{11}NO$
M_r = 173.21
Monoclinic, $C2/c$
a = 12.3699 (15) Å
b = 13.3799 (16) Å
c = 22.502 (3) Å
β = 95.685 (2)°
V = 3706.0 (8) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 291 (2) K
0.44 × 0.33 × 0.29 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.966, T_{max} = 0.977
11508 measured reflections
3434 independent reflections
2459 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.132
S = 1.02
3434 reflections
240 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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, 1998); 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: LH2411).

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supplementary materials

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8-Methoxy-2-methylquinoline

Y.-Z. Wang

Comment

Complexes containing the quinoline moiety can have pharmacological activity. Quinoline derivatives with additional substituents have good in anti-cancer and anti-malarial properties (Lee *et al.*, 1991; Nicolaou *et al.*, 1991) and this has aroused our inerest. Herein we describe the synthesis of the title compound and have determined its crystal structure.

The asymmetric unit (Fig. 1) of the crystal structure contains two independent molecules. The bond lengths and angles are normal (Allen *et al.*, 1987). The dihedral angle of between the N1/C1/C2/C3/C4/C9 plane and the C4—C9 plane is 1.43 (9)° and the dihedral angle of between the N2/C20/C12/C13/C14/C15 plane and the C15—C20 plane is 0.74 (1)°. The C11—O1—C8—C7 torsion angle is 3.3 (3)° and the C22—O2—C19—C18 torsion angle is −3.1 (3)°.

Experimental

The title compound was synthesized by the reaction of 2-methylquinolin-8-ol with iodomethane and potassium carbonate in acetone at rt for 12 h, according to a literature method (Leir, 1977; Kitamura *et al.*, 2000). After filtration, the resulting solution was evaporated. Short column chromatogaphy on silica gel with chloroform and recrystallization from hexane gave a white solid. Single crystals suitable for X-ray diffraction were obtained by recrystallization of the title compound from absolute acetionitrile and ethyl ether.

Refinement

H atoms were located in a difference map but were placed in calculated positions and refined in a riding-model approximation with C—H = 0.93–0.96Å and U_{iso}(H)=1.2U_{eq}(C) or 1.5U_{eq}(methyl C)

Figures

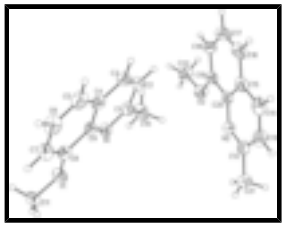


Fig. 1. The asymmetric unit of the title compound showing 30% probability displacement ellipsoids and the atomic numbering.

8-Methoxy-2-methylquinoline

Crystal data

$C_{11}H_{11}NO$ F_{000} = 1472

M_r = 173.21	D_x = 1.242 Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 2679 reflections
a = 12.3699 (15) Å	θ = 2.4–23.8º
b = 13.3799 (16) Å	μ = 0.08 mm^{-1}
c = 22.502 (3) Å	T = 291 (2) K
β = 95.685 (2)º	Block, colourless
V = 3706.0 (8) Å^3	0.44 × 0.33 × 0.29 mm
Z = 16	

Data collection

Bruker APEXII diffractometer	3434 independent reflections
Radiation source: fine-focus sealed tube	2459 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.028
T = 291(2) K	θ_{max} = 25.5º
φ and ω scans	θ_{min} = 2.4º
Absorption correction: multi-scan (SADABS; Bruker, 2005)	h = −14→14
T_{min} = 0.966, T_{max} = 0.977	k = −16→16
11508 measured reflections	l = −27→26

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.046	$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2 + 2.2555P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.132	$(\Delta/\sigma)_{max} < 0.001$
S = 1.02	$\Delta\rho_{max}$ = 0.38 e Å^{-3}
3434 reflections	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
240 parameters	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0015 (2)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	0.74271 (11)	0.15865 (9)	0.58693 (6)	0.0568 (4)
O2	0.13317 (12)	0.16984 (9)	0.70878 (6)	0.0594 (4)
N1	0.57238 (12)	0.23122 (11)	0.63623 (6)	0.0464 (4)
N2	0.11457 (12)	0.21770 (12)	0.59369 (7)	0.0533 (4)
C1	0.48732 (15)	0.26629 (15)	0.66019 (8)	0.0521 (5)
C2	0.47217 (17)	0.36938 (16)	0.66988 (9)	0.0614 (6)
H2	0.4105	0.3917	0.6863	0.074*
C3	0.54767 (18)	0.43539 (15)	0.65518 (9)	0.0593 (5)
H3	0.5382	0.5033	0.6618	0.071*
C4	0.64109 (15)	0.40149 (13)	0.62969 (8)	0.0494 (5)
C5	0.72433 (18)	0.46566 (15)	0.61435 (10)	0.0633 (6)
H5	0.7192	0.5342	0.6204	0.076*
C6	0.81189 (19)	0.42698 (16)	0.59080 (10)	0.0686 (6)
H6	0.8669	0.4696	0.5812	0.082*
C7	0.82133 (17)	0.32373 (16)	0.58059 (9)	0.0594 (5)
H7	0.8820	0.2990	0.5641	0.071*
C8	0.74178 (15)	0.25964 (13)	0.59475 (8)	0.0461 (4)
C9	0.64900 (14)	0.29722 (12)	0.62055 (7)	0.0419 (4)
C10	0.40475 (18)	0.19176 (18)	0.67682 (12)	0.0774 (7)
H10A	0.3412	0.1956	0.6488	0.116*
H10B	0.3854	0.2063	0.7162	0.116*
H10C	0.4349	0.1257	0.6762	0.116*
C11	0.83617 (17)	0.11558 (17)	0.56500 (10)	0.0682 (6)
H11A	0.8431	0.1401	0.5255	0.102*
H11B	0.8288	0.0442	0.5639	0.102*
H11C	0.8997	0.1334	0.5908	0.102*
C12	0.10418 (16)	0.23993 (18)	0.53695 (9)	0.0614 (6)
C13	0.09775 (19)	0.34002 (19)	0.51669 (10)	0.0703 (6)
H13	0.0884	0.3530	0.4759	0.084*
C14	0.10492 (18)	0.41715 (18)	0.55569 (10)	0.0687 (6)
H14	0.1016	0.4828	0.5421	0.082*
C15	0.11774 (15)	0.39576 (14)	0.61825 (10)	0.0557 (5)
C16	0.12603 (18)	0.47028 (16)	0.66199 (12)	0.0712 (6)
H16	0.1237	0.5375	0.6513	0.085*
C17	0.13752 (19)	0.44278 (17)	0.72031 (11)	0.0704 (6)
H17	0.1433	0.4926	0.7492	0.085*
C18	0.14103 (17)	0.34306 (15)	0.73898 (9)	0.0583 (5)
H18	0.1492	0.3273	0.7794	0.070*
C19	0.13227 (15)	0.26878 (13)	0.69660 (9)	0.0498 (5)
C20	0.12074 (13)	0.29363 (13)	0.63434 (8)	0.0421 (4)

C21	0.0976 (2)	0.15372 (19)	0.49351 (10)	0.0782 (7)
H21A	0.1038	0.0919	0.5152	0.117*
H21B	0.1557	0.1587	0.4684	0.117*
H21C	0.0292	0.1557	0.4693	0.117*
C22	0.14963 (19)	0.14123 (16)	0.77003 (9)	0.0656 (6)
H22A	0.2182	0.1667	0.7874	0.098*
H22B	0.1495	0.0697	0.7730	0.098*
H22C	0.0923	0.1681	0.7910	0.098*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0583 (8)	0.0426 (7)	0.0716 (9)	0.0057 (6)	0.0180 (7)	−0.0039 (6)
O2	0.0761 (10)	0.0469 (8)	0.0541 (8)	−0.0032 (7)	0.0014 (7)	0.0026 (6)
N1	0.0460 (9)	0.0412 (8)	0.0520 (9)	0.0012 (7)	0.0056 (7)	0.0019 (7)
N2	0.0501 (9)	0.0555 (10)	0.0535 (10)	0.0042 (7)	0.0004 (7)	−0.0022 (8)
C1	0.0487 (11)	0.0561 (12)	0.0513 (11)	0.0053 (9)	0.0042 (9)	−0.0007 (9)
C2	0.0579 (12)	0.0648 (14)	0.0615 (13)	0.0159 (11)	0.0062 (10)	−0.0135 (10)
C3	0.0707 (14)	0.0439 (11)	0.0604 (12)	0.0164 (10)	−0.0077 (10)	−0.0119 (9)
C4	0.0575 (12)	0.0394 (10)	0.0482 (10)	0.0008 (9)	−0.0092 (9)	0.0002 (8)
C5	0.0745 (15)	0.0373 (10)	0.0746 (14)	−0.0064 (10)	−0.0105 (11)	0.0067 (10)
C6	0.0669 (14)	0.0552 (14)	0.0828 (16)	−0.0143 (11)	0.0035 (12)	0.0170 (11)
C7	0.0542 (12)	0.0593 (13)	0.0654 (13)	−0.0018 (10)	0.0094 (10)	0.0115 (10)
C8	0.0508 (11)	0.0415 (10)	0.0456 (10)	0.0015 (8)	0.0019 (8)	0.0040 (8)
C9	0.0458 (10)	0.0366 (9)	0.0417 (9)	0.0021 (8)	−0.0031 (7)	0.0020 (7)
C10	0.0572 (13)	0.0820 (16)	0.0961 (18)	−0.0022 (12)	0.0238 (12)	0.0037 (14)
C11	0.0636 (13)	0.0661 (14)	0.0767 (15)	0.0162 (11)	0.0161 (11)	−0.0117 (11)
C12	0.0510 (12)	0.0786 (15)	0.0539 (13)	0.0065 (10)	0.0011 (9)	0.0012 (11)
C13	0.0709 (15)	0.0822 (17)	0.0576 (13)	0.0059 (12)	0.0045 (11)	0.0189 (13)
C14	0.0637 (14)	0.0650 (14)	0.0776 (16)	0.0030 (11)	0.0076 (11)	0.0263 (13)
C15	0.0448 (11)	0.0440 (11)	0.0785 (14)	−0.0002 (8)	0.0060 (9)	0.0024 (10)
C16	0.0699 (15)	0.0409 (12)	0.1033 (19)	−0.0010 (10)	0.0119 (13)	−0.0010 (12)
C17	0.0768 (15)	0.0548 (14)	0.0808 (16)	−0.0026 (11)	0.0133 (12)	−0.0164 (12)
C18	0.0627 (13)	0.0539 (12)	0.0588 (12)	−0.0026 (10)	0.0080 (10)	−0.0150 (10)
C19	0.0464 (10)	0.0414 (10)	0.0617 (12)	0.0014 (8)	0.0058 (9)	−0.0001 (9)
C20	0.0365 (9)	0.0393 (10)	0.0503 (10)	0.0011 (7)	0.0031 (7)	−0.0004 (8)
C21	0.0836 (17)	0.0966 (19)	0.0523 (13)	0.0148 (14)	−0.0028 (11)	−0.0174 (12)
C22	0.0803 (15)	0.0649 (14)	0.0503 (12)	−0.0001 (11)	−0.0009 (10)	0.0121 (10)

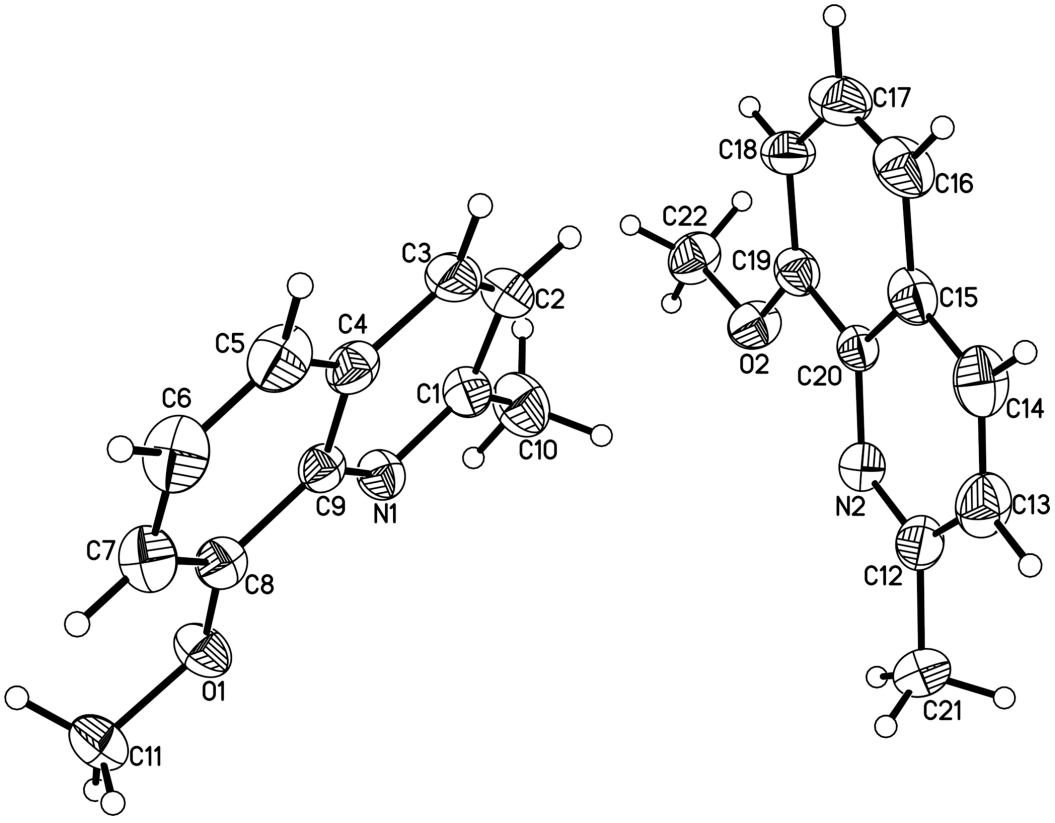
Geometric parameters (Å, °)

O1—C8	1.363 (2)	C10—H10C	0.9600
O1—C11	1.423 (2)	C11—H11A	0.9600
O2—C19	1.352 (2)	C11—H11B	0.9600
O2—C22	1.426 (2)	C11—H11C	0.9600
N1—C1	1.315 (2)	C12—C13	1.414 (3)
N1—C9	1.367 (2)	C12—C21	1.509 (3)
N2—C12	1.305 (2)	C13—C14	1.352 (3)
N2—C20	1.364 (2)	C13—H13	0.9300

C1—C2	1.412 (3)	C14—C15	1.430 (3)
C1—C10	1.501 (3)	C14—H14	0.9300
C2—C3	1.350 (3)	C15—C16	1.398 (3)
C2—H2	0.9300	C15—C20	1.413 (3)
C3—C4	1.415 (3)	C16—C17	1.357 (3)
C3—H3	0.9300	C16—H16	0.9300
C4—C5	1.410 (3)	C17—C18	1.398 (3)
C4—C9	1.415 (2)	C17—H17	0.9300
C5—C6	1.355 (3)	C18—C19	1.374 (3)
C5—H5	0.9300	C18—H18	0.9300
C6—C7	1.407 (3)	C19—C20	1.433 (2)
C6—H6	0.9300	C21—H21A	0.9600
C7—C8	1.366 (3)	C21—H21B	0.9600
C7—H7	0.9300	C21—H21C	0.9600
C8—C9	1.428 (2)	C22—H22A	0.9600
C10—H10A	0.9600	C22—H22B	0.9600
C10—H10B	0.9600	C22—H22C	0.9600
C8—O1—C11	117.64 (15)	H11A—C11—H11C	109.5
C19—O2—C22	117.16 (16)	H11B—C11—H11C	109.5
C1—N1—C9	118.59 (16)	N2—C12—C13	121.9 (2)
C12—N2—C20	118.68 (17)	N2—C12—C21	117.0 (2)
N1—C1—C2	122.38 (19)	C13—C12—C21	121.2 (2)
N1—C1—C10	117.18 (18)	C14—C13—C12	121.0 (2)
C2—C1—C10	120.44 (18)	C14—C13—H13	119.5
C3—C2—C1	119.72 (19)	C12—C13—H13	119.5
C3—C2—H2	120.1	C13—C14—C15	118.7 (2)
C1—C2—H2	120.1	C13—C14—H14	120.7
C2—C3—C4	120.14 (18)	C15—C14—H14	120.7
C2—C3—H3	119.9	C16—C15—C20	120.8 (2)
C4—C3—H3	119.9	C16—C15—C14	122.9 (2)
C5—C4—C3	123.36 (19)	C20—C15—C14	116.31 (19)
C5—C4—C9	120.15 (18)	C17—C16—C15	118.7 (2)
C3—C4—C9	116.49 (18)	C17—C16—H16	120.6
C6—C5—C4	119.66 (19)	C15—C16—H16	120.6
C6—C5—H5	120.2	C16—C17—C18	123.1 (2)
C4—C5—H5	120.2	C16—C17—H17	118.4
C5—C6—C7	121.4 (2)	C18—C17—H17	118.4
C5—C6—H6	119.3	C19—C18—C17	118.9 (2)
C7—C6—H6	119.3	C19—C18—H18	120.5
C8—C7—C6	120.3 (2)	C17—C18—H18	120.5
C8—C7—H7	119.8	O2—C19—C18	124.69 (18)
C6—C7—H7	119.8	O2—C19—C20	115.04 (16)
O1—C8—C7	125.21 (18)	C18—C19—C20	120.26 (17)
O1—C8—C9	114.78 (15)	N2—C20—C15	123.38 (17)
C7—C8—C9	120.01 (17)	N2—C20—C19	118.44 (16)
N1—C9—C4	122.67 (16)	C15—C20—C19	118.18 (17)
N1—C9—C8	118.89 (15)	C12—C21—H21A	109.5
C4—C9—C8	118.44 (16)	C12—C21—H21B	109.5
C1—C10—H10A	109.5	H21A—C21—H21B	109.5

C1—C10—H10B	109.5	C12—C21—H21C	109.5
H10A—C10—H10B	109.5	H21A—C21—H21C	109.5
C1—C10—H10C	109.5	H21B—C21—H21C	109.5
H10A—C10—H10C	109.5	O2—C22—H22A	109.5
H10B—C10—H10C	109.5	O2—C22—H22B	109.5
O1—C11—H11A	109.5	H22A—C22—H22B	109.5
O1—C11—H11B	109.5	O2—C22—H22C	109.5
H11A—C11—H11B	109.5	H22A—C22—H22C	109.5
O1—C11—H11C	109.5	H22B—C22—H22C	109.5
C9—N1—C1—C2	0.4 (3)	C20—N2—C12—C13	−0.9 (3)
C9—N1—C1—C10	179.95 (17)	C20—N2—C12—C21	180.00 (18)
N1—C1—C2—C3	−1.1 (3)	N2—C12—C13—C14	1.7 (3)
C10—C1—C2—C3	179.4 (2)	C21—C12—C13—C14	−179.2 (2)
C1—C2—C3—C4	0.6 (3)	C12—C13—C14—C15	−0.8 (3)
C2—C3—C4—C5	−178.65 (19)	C13—C14—C15—C16	179.9 (2)
C2—C3—C4—C9	0.5 (3)	C13—C14—C15—C20	−0.7 (3)
C3—C4—C5—C6	179.16 (19)	C20—C15—C16—C17	0.3 (3)
C9—C4—C5—C6	0.0 (3)	C14—C15—C16—C17	179.7 (2)
C4—C5—C6—C7	0.7 (3)	C15—C16—C17—C18	−0.3 (4)
C5—C6—C7—C8	−0.4 (3)	C16—C17—C18—C19	−0.1 (3)
C11—O1—C8—C7	3.3 (3)	C22—O2—C19—C18	−3.1 (3)
C11—O1—C8—C9	−176.03 (16)	C22—O2—C19—C20	177.11 (16)
C6—C7—C8—O1	−179.83 (18)	C17—C18—C19—O2	−179.17 (19)
C6—C7—C8—C9	−0.6 (3)	C17—C18—C19—C20	0.6 (3)
C1—N1—C9—C4	0.7 (3)	C12—N2—C20—C15	−0.8 (3)
C1—N1—C9—C8	179.74 (15)	C12—N2—C20—C19	−179.93 (17)
C5—C4—C9—N1	177.99 (17)	C16—C15—C20—N2	−179.05 (18)
C3—C4—C9—N1	−1.2 (3)	C14—C15—C20—N2	1.5 (3)
C5—C4—C9—C8	−1.0 (2)	C16—C15—C20—C19	0.1 (3)
C3—C4—C9—C8	179.81 (16)	C14—C15—C20—C19	−179.32 (17)
O1—C8—C9—N1	1.6 (2)	O2—C19—C20—N2	−1.6 (2)
C7—C8—C9—N1	−177.76 (17)	C18—C19—C20—N2	178.66 (17)
O1—C8—C9—C4	−179.40 (15)	O2—C19—C20—C15	179.20 (16)
C7—C8—C9—C4	1.3 (3)	C18—C19—C20—C15	−0.6 (3)

Fig. 1


C17
C18
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C22
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C9
N1
N2
C13
C7
C8
C12
O1
C21
C11