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4,4-Dimethyl-2-phenyl-4,5-dihydropyrrolo[2,3,4-*kl*]acridin-1(2*H*)-one

Izarul Islam,[a] Pijush Kanti Roy,[b] Ennio Zangrando,[c] Pran Gopal Karmaker[d] and Harendra Nath Roy[a]*

[a]Department of Chemistry, University of Rajshahi, Rajshahi-6205, Bangladesh, [b]Department of Chemistry, Faculty of Science, Mawlana Bhashani Science and Technology University, Tangail-1902, Bangladesh, [c]Department of Chemical and Pharmaceutical Sciences, University of Trieste, Italy, and [d]Chemical Synthesis and Pollution Control Key Laboratory of Sichuan Province, College of Chemistry and Chemical Engineering, China West Normal University, Nanchong 637002, People's Republic of China. *Correspondence e-mail: hnroy19@ru.ac.bd

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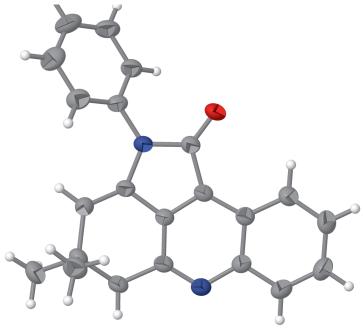
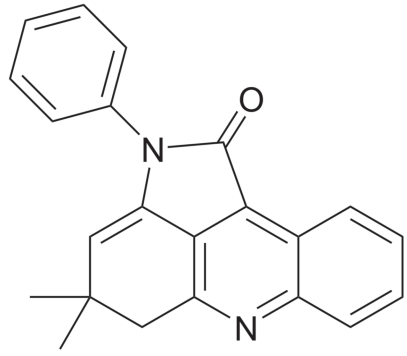
In the title compound, $C_{22}H_{18}N_2O$, the pendant phenyl ring is twisted by 43.85 (1)° with respect to the acridine moiety, which has almost coplanar atoms apart from the sp^3 carbon atoms. The extended structure features aromatic π–π stacking with a centroid-to-centroid distance of 3.489 (2) Å and weak C—H···O hydrogen bonds.

3D view



Chemical scheme



Structure description

Pyrroloacridines are a type of fused heterocyclic compounds that combine the structures of pyrrole and acridine. As a result of their appealing biological and therapeutic properties attributed to their ability to intercalate DNA (Belmont *et al.*, 2007), organic chemists are currently paying close attention to the synthesis of these compounds through multi-step procedures (Dandia *et al.* 2015; Hao *et al.* 2013; Jiang *et al.* 2012; Ray *et al.* 2014; Wang *et al.* 2012). As part of our work in this area, we now describe the synthesis and structure of the title compound, $C_{22}H_{18}N_2O$.

The molecular structure of the title molecule is shown in Fig. 1. The chemical structure consists of a central acridine core fused to a pyrrolidone ring, a combination of rings that contributes to its planarity with the exception of the sp^3 carbon atoms (C19, C20 displaced by 0.445 (2), and −0.157 (2) Å, respectively), and of the C1–C6 phenyl ring bound to the pyrrol N atom. The carbonyl C=O bond length is 1.2187 (15) Å, and all other bond distances are as expected. The phenyl ring forms a dihedral angle of 43.85 (1)° with the mean plane through the acridin moiety. This conformation is similar to that found in the structures having a 3-nitrophenyl or 4-methylphenyl ring replacing the phenyl ring, where the corresponding dihedral angles are 48.84 (5) and 44.72 (4)°, respectively (Hao *et al.* 2013). The 9-fluoro derivative (Dandia *et al.* 2015) has the phenyl

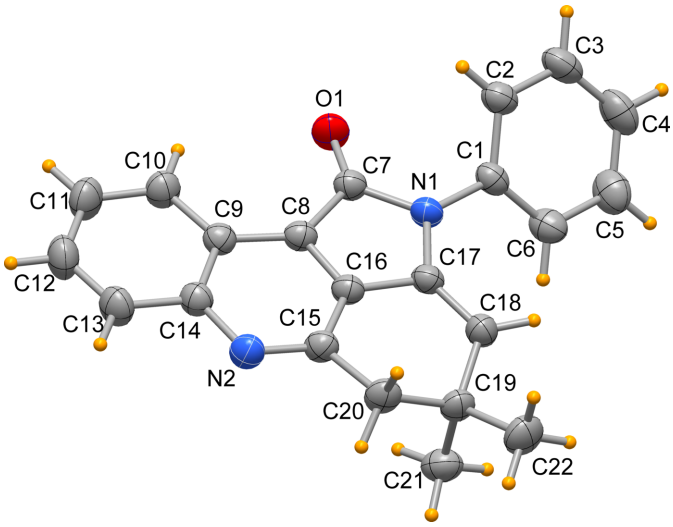


Figure 1
The molecular structure of the title molecule (displacement ellipsoids at the 50% probability level).

ring tilted by 49.32 (1)° with respect to the acridin fragment. Thus all the cited analogous derivatives exhibit similar conformations.

The crystal packing evidences π–π-stacked dimers with a centroid-to-centroid distance of 3.489 (2) Å (Fig. 2). In addition, a weak C3—H3···O1($2-x, 2-y, 1-z$) hydrogen bond is observed with H···O = 2.53 Å, C···O = 3.438 (2) Å and C—H···O = 165°.

Synthesis and crystallization

Dimedone (1.00 mmol), aniline (1.00 mmol) and nicotinic acid (5–10 mol %) were mixed in 5.0 ml of toluene and the reaction mixture was heated over an oil-bath at reflux conditions with an efficient $CaCl_2$ guard-tube for 6–8 h. Isatin (1.00 mmol) was added sequentially to the reaction mixture and it was heated to reflux till the completion of the reaction that was monitored by TLC with UV detector at 365 nm. Then, the solvent was evaporated and the residue purified by column chromatography (acetone/petroleum ether, 1:6). Single crystals suitable for X-ray analysis were obtained from slow evaporation of an ethanolic solution of the product containing few drops of acetone: colour: light brown, yield: 80%, melting point: 191–193°C

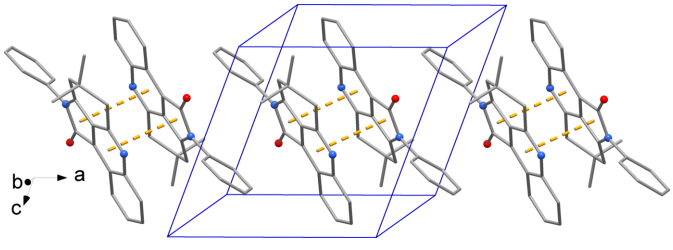


Figure 2
Detail of the crystal packing showing the π-stacking interactions as dashed lines (H atoms not indicated for the sake of clarity).

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{18}N_2O$
M_r	326.38
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	297
a, b, c (Å)	9.430 (3), 9.997 (4), 10.203 (4)
α, β, γ (°)	99.833 (14), 107.559 (14), 106.866 (14)
V (Å^3)	841.8 (6)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.30 × 0.30 × 0.28
Data collection	
Diffractometer	Bruker APEXII CCD
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22780, 3806, 3047
R_{int}	0.041
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.053, 0.138, 1.12
No. of reflections	3806
No. of parameters	228
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.37, −0.49

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2019/2* (Sheldrick, 2015*b*) and *DIAMOND* (Brandenburg & Putz, 1999).

^{1}H NMR (400 MHz, $CDCl_3$): δ_H (p.p.m.)= 8.73 (*dd*, J = 8, 8 Hz, 1H, Ar—H), 8.16 (*d*, J = 8 Hz, 1H, Ar—H), 7.83 (*m*, 1H, Ar—H), 7.75 (*m*, 1H, Ar—H), 7.68–7.54 (*m*, 4H, Ar—H), 7.53–7.41 (1*H*, Ar—H), 5.63 (*s*, 1H, ali-H), 3.22 (*s*, 2H, ali-H), 1.33 (*s*, 6H, ali-H).

^{13}C NMR (100 MHz, $CDCl_3$): δ_C (p.p.m.), 166.75, 154.60, 149.73, 134.78, 133.37, 129.55, 129.46, 129.39, 127.80, 127.48, 126.46, 126.40, 124.99, 124.25, 122.63, 118.36, 44.21, 37.11, 30.89.

HRMS(ESI): m/z $[M + H]^+$ calculated for $C_{22}H_{19}N_2O$: 327.399, found 327.1491.

Refinement

Crystal data, data collection and structure refinement are summarized in Table 1.

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full crystallographic data

IUCrData (2025). **10**, x250361 [https://doi.org/10.1107/S241431462500361X]

4,4-Dimethyl-2-phenyl-4,5-dihydropyrrolo[2,3,4-*kl*]acridin-1(2*H*)-one

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11,11-Dimethyl-14-phenyl-8,14-diazatetracyclo[7.6.1.0^{2,7}.0^{13,16}]hexadeca-1(16),2(7),3,5,8,12-hexaen-15-one

Crystal data

$C_{22}H_{18}N_2O$
M_r = 326.38
Triclinic, $P\overline{1}$
a = 9.430 (3) Å
b = 9.997 (4) Å
c = 10.203 (4) Å
α = 99.833 (14)°
β = 107.559 (14)°
γ = 106.866 (14)°
V = 841.8 (6) Å^3
Z = 2
$F(000)$ = 344
D_x = 1.288 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9587 reflections
θ = 2.2–26.7°
μ = 0.08 mm^{-1}
T = 297 K
Block, brown
0.30 × 0.30 × 0.28 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
φ and ω scans
22780 measured reflections
3806 independent reflections
3047 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 27.5°, θ_{min} = 2.2°
h = −12→12
k = −12→12
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.138
S = 1.12
3806 reflections
228 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0778P)^2 + 0.0906P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.
Refinement. H atoms were located at geometrical positions and refined as riding atoms.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.77493 (12)	0.67107 (10)	0.34393 (10)	0.0482 (3)
N1	0.85067 (12)	0.60933 (10)	0.55938 (10)	0.0351 (3)
N2	0.39760 (12)	0.19595 (11)	0.39073 (12)	0.0404 (3)
C1	0.99874 (14)	0.72885 (12)	0.63425 (12)	0.0346 (3)
C2	1.00582 (16)	0.86935 (13)	0.62965 (14)	0.0409 (3)
H2	0.914571	0.884859	0.579572	0.049*
C3	1.14935 (18)	0.98514 (14)	0.70003 (15)	0.0502 (4)
H3	1.155281	1.078553	0.695182	0.060*
C4	1.28445 (18)	0.96283 (16)	0.77777 (17)	0.0560 (4)
H4	1.380240	1.041467	0.826627	0.067*
C5	1.27703 (17)	0.82358 (17)	0.78282 (17)	0.0538 (4)
H5	1.367944	0.809007	0.835261	0.065*
C6	1.13471 (16)	0.70562 (14)	0.71007 (15)	0.0442 (3)
H6	1.130304	0.611866	0.712011	0.053*
C7	0.74945 (15)	0.59113 (12)	0.41867 (13)	0.0347 (3)
C8	0.61124 (14)	0.45417 (12)	0.38158 (12)	0.0328 (3)
C9	0.46972 (14)	0.37668 (13)	0.25861 (12)	0.0344 (3)
C10	0.42702 (17)	0.41674 (15)	0.12990 (14)	0.0429 (3)
H10	0.493807	0.501397	0.121915	0.052*
C11	0.28797 (18)	0.33172 (17)	0.01693 (14)	0.0515 (4)
H11	0.261021	0.358521	−0.067512	0.062*
C12	0.18646 (18)	0.20460 (17)	0.02846 (15)	0.0526 (4)
H12	0.092101	0.147652	−0.048569	0.063*
C13	0.22420 (16)	0.16301 (15)	0.15150 (15)	0.0475 (3)
H13	0.154790	0.078417	0.157119	0.057*
C14	0.36693 (15)	0.24652 (13)	0.27015 (13)	0.0368 (3)
C15	0.53139 (14)	0.27159 (13)	0.50142 (13)	0.0357 (3)
C16	0.63918 (14)	0.39923 (12)	0.49598 (12)	0.0325 (3)
C17	0.78949 (14)	0.48942 (12)	0.60979 (12)	0.0326 (3)
C18	0.84327 (16)	0.44642 (13)	0.72607 (13)	0.0387 (3)
H18	0.933264	0.509730	0.804289	0.046*
C19	0.75654 (16)	0.29286 (13)	0.73030 (13)	0.0389 (3)
C20	0.57421 (16)	0.23479 (15)	0.64175 (14)	0.0420 (3)
H20A	0.532291	0.129698	0.622742	0.050*
H20B	0.522641	0.274877	0.698854	0.050*
C21	0.83069 (18)	0.19303 (15)	0.66618 (16)	0.0499 (4)
H21A	0.786913	0.097045	0.675034	0.075*
H21B	0.944299	0.231561	0.716766	0.075*
H21C	0.807088	0.188238	0.566775	0.075*
C22	0.7832 (2)	0.29030 (18)	0.88549 (15)	0.0551 (4)
H22A	0.737958	0.353005	0.926232	0.083*
H22B	0.895682	0.323682	0.940287	0.083*
H22C	0.732800	0.192598	0.887174	0.083*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0543 (6)	0.0394 (5)	0.0430 (5)	0.0031 (4)	0.0157 (4)	0.0210 (4)
N1	0.0367 (6)	0.0278 (5)	0.0364 (5)	0.0061 (4)	0.0118 (4)	0.0115 (4)
N2	0.0362 (6)	0.0375 (6)	0.0434 (6)	0.0065 (5)	0.0132 (5)	0.0163 (5)
C1	0.0364 (7)	0.0288 (6)	0.0358 (6)	0.0063 (5)	0.0163 (5)	0.0064 (5)
C2	0.0475 (7)	0.0315 (6)	0.0423 (7)	0.0109 (5)	0.0183 (6)	0.0105 (5)
C3	0.0618 (9)	0.0289 (6)	0.0526 (8)	0.0053 (6)	0.0244 (7)	0.0073 (6)
C4	0.0456 (8)	0.0440 (8)	0.0585 (9)	−0.0038 (6)	0.0194 (7)	0.0011 (7)
C5	0.0364 (7)	0.0560 (9)	0.0589 (9)	0.0108 (6)	0.0147 (6)	0.0080 (7)
C6	0.0412 (7)	0.0369 (7)	0.0532 (8)	0.0133 (6)	0.0184 (6)	0.0099 (6)
C7	0.0382 (6)	0.0302 (6)	0.0351 (6)	0.0100 (5)	0.0138 (5)	0.0111 (5)
C8	0.0351 (6)	0.0305 (6)	0.0350 (6)	0.0108 (5)	0.0155 (5)	0.0120 (5)
C9	0.0352 (6)	0.0335 (6)	0.0347 (6)	0.0116 (5)	0.0141 (5)	0.0100 (5)
C10	0.0452 (7)	0.0439 (7)	0.0367 (6)	0.0101 (6)	0.0148 (6)	0.0153 (5)
C11	0.0532 (9)	0.0582 (9)	0.0341 (7)	0.0136 (7)	0.0096 (6)	0.0150 (6)
C12	0.0437 (8)	0.0550 (8)	0.0388 (7)	0.0057 (6)	0.0038 (6)	0.0062 (6)
C13	0.0395 (7)	0.0429 (7)	0.0461 (7)	0.0023 (6)	0.0104 (6)	0.0106 (6)
C14	0.0338 (6)	0.0351 (6)	0.0380 (6)	0.0085 (5)	0.0129 (5)	0.0104 (5)
C15	0.0331 (6)	0.0339 (6)	0.0405 (6)	0.0093 (5)	0.0145 (5)	0.0152 (5)
C16	0.0336 (6)	0.0295 (6)	0.0348 (6)	0.0098 (5)	0.0136 (5)	0.0113 (5)
C17	0.0359 (6)	0.0267 (5)	0.0350 (6)	0.0094 (5)	0.0143 (5)	0.0098 (5)
C18	0.0401 (7)	0.0334 (6)	0.0348 (6)	0.0078 (5)	0.0088 (5)	0.0096 (5)
C19	0.0434 (7)	0.0366 (6)	0.0366 (6)	0.0115 (5)	0.0132 (5)	0.0184 (5)
C20	0.0414 (7)	0.0405 (7)	0.0438 (7)	0.0084 (6)	0.0165 (6)	0.0216 (6)
C21	0.0546 (8)	0.0415 (7)	0.0583 (8)	0.0198 (6)	0.0212 (7)	0.0214 (6)
C22	0.0647 (10)	0.0584 (9)	0.0421 (7)	0.0191 (8)	0.0166 (7)	0.0259 (7)

Geometric parameters (Å, º)

O1—C7	1.2187 (15)	C11—C12	1.399 (2)
N1—C7	1.4102 (17)	C11—H11	0.9300
N1—C17	1.4222 (15)	C12—C13	1.368 (2)
N1—C1	1.4275 (16)	C12—H12	0.9300
N2—C15	1.3169 (17)	C13—C14	1.4120 (18)
N2—C14	1.3912 (17)	C13—H13	0.9300
C1—C6	1.3900 (19)	C15—C16	1.4037 (17)
C1—C2	1.3962 (18)	C15—C20	1.5052 (18)
C2—C3	1.381 (2)	C16—C17	1.4416 (17)
C2—H2	0.9300	C17—C18	1.3369 (17)
C3—C4	1.385 (2)	C18—C19	1.5307 (18)
C3—H3	0.9300	C18—H18	0.9300
C4—C5	1.384 (2)	C19—C22	1.5325 (19)
C4—H4	0.9300	C19—C21	1.540 (2)
C5—C6	1.387 (2)	C19—C20	1.5538 (19)
C5—H5	0.9300	C20—H20A	0.9700
C6—H6	0.9300	C20—H20B	0.9700

C7—C8	1.4855 (17)	C21—H21A	0.9600
C8—C16	1.3605 (17)	C21—H21B	0.9600
C8—C9	1.4189 (17)	C21—H21C	0.9600
C9—C10	1.4147 (18)	C22—H22A	0.9600
C9—C14	1.4269 (18)	C22—H22B	0.9600
C10—C11	1.370 (2)	C22—H22C	0.9600
C10—H10	0.9300		

C7—N1—C17	110.79 (10)	C12—C13—H13	119.5
C7—N1—C1	123.16 (10)	C14—C13—H13	119.5
C17—N1—C1	125.95 (10)	N2—C14—C13	117.52 (11)
C15—N2—C14	118.19 (11)	N2—C14—C9	124.43 (11)
C6—C1—C2	120.32 (12)	C13—C14—C9	118.04 (12)
C6—C1—N1	120.42 (11)	N2—C15—C16	120.22 (11)
C2—C1—N1	119.26 (11)	N2—C15—C20	123.64 (11)
C3—C2—C1	119.52 (13)	C16—C15—C20	116.03 (11)
C3—C2—H2	120.2	C8—C16—C15	123.23 (12)
C1—C2—H2	120.2	C8—C16—C17	111.80 (11)
C2—C3—C4	120.34 (13)	C15—C16—C17	124.96 (11)
C2—C3—H3	119.8	C18—C17—N1	135.06 (11)
C4—C3—H3	119.8	C18—C17—C16	120.24 (11)
C5—C4—C3	120.05 (13)	N1—C17—C16	104.60 (10)
C5—C4—H4	120.0	C17—C18—C19	119.91 (11)
C3—C4—H4	120.0	C17—C18—H18	120.0
C4—C5—C6	120.36 (14)	C19—C18—H18	120.0
C4—C5—H5	119.8	C18—C19—C22	110.21 (11)
C6—C5—H5	119.8	C18—C19—C21	106.57 (11)
C5—C6—C1	119.39 (13)	C22—C19—C21	109.13 (11)
C5—C6—H6	120.3	C18—C19—C20	112.81 (10)
C1—C6—H6	120.3	C22—C19—C20	109.02 (11)
O1—C7—N1	126.03 (11)	C21—C19—C20	109.02 (11)
O1—C7—C8	128.23 (12)	C15—C20—C19	114.02 (10)
N1—C7—C8	105.72 (10)	C15—C20—H20A	108.7
C16—C8—C9	119.06 (11)	C19—C20—H20A	108.7
C16—C8—C7	106.99 (11)	C15—C20—H20B	108.7
C9—C8—C7	133.94 (11)	C19—C20—H20B	108.7
C10—C9—C8	125.67 (12)	H20A—C20—H20B	107.6
C10—C9—C14	119.51 (12)	C19—C21—H21A	109.5
C8—C9—C14	114.81 (11)	C19—C21—H21B	109.5
C11—C10—C9	120.48 (13)	H21A—C21—H21B	109.5
C11—C10—H10	119.8	C19—C21—H21C	109.5
C9—C10—H10	119.8	H21A—C21—H21C	109.5
C10—C11—C12	120.07 (13)	H21B—C21—H21C	109.5
C10—C11—H11	120.0	C19—C22—H22A	109.5
C12—C11—H11	120.0	C19—C22—H22B	109.5
C13—C12—C11	120.87 (13)	H22A—C22—H22B	109.5
C13—C12—H12	119.6	C19—C22—H22C	109.5
C11—C12—H12	119.6	H22A—C22—H22C	109.5

C12—C13—C14	121.01 (13)	H22B—C22—H22C	109.5
C7—N1—C1—C6	−135.02 (13)	C10—C9—C14—N2	179.36 (11)
C17—N1—C1—C6	40.75 (17)	C8—C9—C14—N2	0.47 (18)
C7—N1—C1—C2	44.53 (16)	C10—C9—C14—C13	−0.68 (18)
C17—N1—C1—C2	−139.71 (12)	C8—C9—C14—C13	−179.57 (11)
C6—C1—C2—C3	0.56 (19)	C14—N2—C15—C16	−0.26 (18)
N1—C1—C2—C3	−178.99 (11)	C14—N2—C15—C20	175.80 (11)
C1—C2—C3—C4	−1.7 (2)	C9—C8—C16—C15	−2.69 (18)
C2—C3—C4—C5	1.4 (2)	C7—C8—C16—C15	178.19 (11)
C3—C4—C5—C6	0.1 (2)	C9—C8—C16—C17	178.58 (10)
C4—C5—C6—C1	−1.2 (2)	C7—C8—C16—C17	−0.54 (13)
C2—C1—C6—C5	0.9 (2)	N2—C15—C16—C8	2.16 (19)
N1—C1—C6—C5	−179.56 (11)	C20—C15—C16—C8	−174.19 (11)
C17—N1—C7—O1	−175.27 (12)	N2—C15—C16—C17	−179.28 (11)
C1—N1—C7—O1	1.07 (19)	C20—C15—C16—C17	4.37 (18)
C17—N1—C7—C8	3.10 (13)	C7—N1—C17—C18	172.77 (13)
C1—N1—C7—C8	179.43 (10)	C1—N1—C17—C18	−3.4 (2)
O1—C7—C8—C16	176.78 (12)	C7—N1—C17—C16	−3.37 (13)
N1—C7—C8—C16	−1.54 (13)	C1—N1—C17—C16	−179.58 (10)
O1—C7—C8—C9	−2.2 (2)	C8—C16—C17—C18	−174.48 (11)
N1—C7—C8—C9	179.53 (12)	C15—C16—C17—C18	6.82 (19)
C16—C8—C9—C10	−177.48 (11)	C8—C16—C17—N1	2.37 (13)
C7—C8—C9—C10	1.4 (2)	C15—C16—C17—N1	−176.33 (11)
C16—C8—C9—C14	1.34 (17)	N1—C17—C18—C19	−167.75 (12)
C7—C8—C9—C14	−179.83 (12)	C16—C17—C18—C19	7.93 (18)
C8—C9—C10—C11	178.88 (12)	C17—C18—C19—C22	−153.29 (12)
C14—C9—C10—C11	0.1 (2)	C17—C18—C19—C21	88.42 (15)
C9—C10—C11—C12	0.3 (2)	C17—C18—C19—C20	−31.17 (17)
C10—C11—C12—C13	−0.2 (2)	N2—C15—C20—C19	155.80 (12)
C11—C12—C13—C14	−0.4 (2)	C16—C15—C20—C19	−27.98 (16)
C15—N2—C14—C13	179.03 (12)	C18—C19—C20—C15	40.35 (16)
C15—N2—C14—C9	−1.02 (19)	C22—C19—C20—C15	163.13 (11)
C12—C13—C14—N2	−179.24 (12)	C21—C19—C20—C15	−77.82 (14)
C12—C13—C14—C9	0.8 (2)		