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rac-(*Z*)-2-(1-Naphthylmethylene)-1-azabicyclo[2.2.2]octan-3-ol

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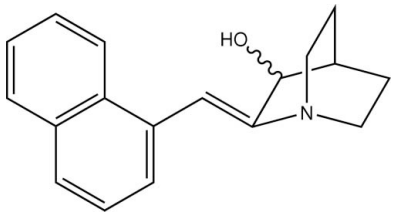
Key indicators: single-crystal X-ray study; T = 90 K; mean σ(C–C) = 0.002 Å; disorder in main residue; R factor = 0.047; wR factor = 0.126; data-to-parameter ratio = 15.3.

The title compound, $C_{18}H_{19}NO$, in racemic form, was obtained by the reaction of naphthalene-1-carboxaldehyde with 1-azabicyclo[2.2.2]octan-3-one in the presence of methanolic potassium hydroxide and subsequent reduction of the product with sodium borohydride to the secondary alcohol. The double bond linking the 1-naphthyl and 1-azabicyclo[2.2.2]-octan-3-ol moieties has Z geometry. The C=C—CH=C torsion angle [42.4 (2)°] indicates a deviation of the 1-naphthyl ring from the plane of the double bond connected to the azabicyclic ring. Part of the 1-azabicyclo[2.2.2]octan-3-ol moiety is disordered, with the approximate ratio of occupancies being 63:37.

Related literature

For related literature, see: Sekhar *et al.* (2007); Sonar *et al.* (2004); Wilson (1992).



Experimental

Crystal data

$C_{18}H_{19}NO$
M_r = 265.34
Monoclinic, $P2_1/c$
a = 6.1892 (1) Å
b = 8.8706 (2) Å
c = 25.1693 (5) Å
β = 96.0631 (8)°
V = 1374.11 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 90.0 (2) K
0.25 × 0.20 × 0.15 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan *SCALEPACK* (Otwinowski & Minor, 1997)
T_{min} = 0.981, T_{max} = 0.988
5940 measured reflections
3132 independent reflections
2155 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.126
S = 1.02
3132 reflections
205 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL/PC* (Sheldrick, 1995); software used to prepare material for publication: *SHELXL97* and local procedures.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2484).

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supplementary materials

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rac-(*Z*)-2-(1-Naphthylmethylene)-1-azabicyclo[2.2.2]octan-3-ol

V. N. Sonar, S. Parkin and P. A. Crooks

Comment

Recently, we have reported (Sekhar *et al.*, 2007) on the radio- sensitizing activity of *N*-arylsubstituted rac-(*Z*)-2-(1*H*-indol-3-ylmethylene)-1-azabicyclo[2.2.2]octan-3-ols. In addition to these indole analogues, we also synthesized 1-azabicyclo[2.2.2]octan-3-ols linked to non-indolic systems, such 1-naphthyl systems, to compare their radio-sensitizing activities with those of the indole analogs.

The crystal structure of the title compound confirmed the molecular structure and atom connectivity as illustrated in Fig. 1. The title compound comprises a 1-azabicyclo[2.2.2]octan-3-ol moiety and a 1-naphthyl group linked *via* the C7=C8 bond that has the *Z* geometry. The bond angles around the C7 and C8 atoms deviate from the ideal value [120°]; the angles for N1—C8—C9, C7=C8—N1, and C7=C8—C1 [113.35 (18), 124.84 (13), and 129.11 (14)°, respectively] are distorted. These deviations contribute to the release of the intramolecular nonbonded interactions. The C2=C1—C7=C8 torsion angle [−42.4 (2)°]indicates a deviation of the 1-naphthyl ring from the plane of the double bond connected to the azabicyclic ring. Also, the C1—C7 bond length, in comparison with the standard value for a C_{ar}—C_{sp^2} single bond [1.470 (15) Å; Wilson, 1992], suggests absence of conjugation to the π electron system of the 1-naphthyl ring.

Experimental

The title compound was prepared according to the previously reported procedure of Sonar *et al.* (2004). Crystallization from ethyl acetate afforded colorless crystals. ^{1}H NMR ($CDCl_3$, p.p.m.): δ 1.45–2.13 (m, 3H), 1.94–2.04 (m, 2H), 2.12 (p, 1H), 2.79–3.05 (m, 4H), 4.47 (s, 1H), 6.99 (s, 1H), 7.44–7.53 (m, 3H), 7.75 (d, 1H), 7.84 (dd, 2H), 8.07 (dd, 1H). ^{13}C NMR ($CDCl_3$, p.p.m.): δ 19.22, 25.37, 31.21, 47.85, 48.88, 71.51, 120.17, 124.22, 125.53, 125.72, 125.83, 127.45, 128.67, 131.80, 132.16, 133.62, 153.52.

Refinement

All H atoms were found in difference Fourier maps and subsequently placed in idealized positions with constrained distances of 0.99 Å (R_2CH_2), 1.00 Å (R_3CH), 0.95 Å ($C_{Ar}H$) and 0.84 Å (OH). U_{iso}(H) values were set to either 1.5U_{eq} (OH only) or 1.2U_{eq} of the attached atom. The crystal structure is centrosymmetric and therefore it is a racemic mixture of isomers. The two enantiomers have very nearly the same shape and the position of the hydroxyl group for each is very similar. This inevitably leads to a form of disorder in which one enantiomer substitutes for the other. In this case the occupancy factor ratio is 63:37. A single restraint equation was required in the least-squares refinement to ensure similarity of the C—O bond lengths of the two enantiomers (SADI in *SHELXL97*; Sheldrick, 1997).

Figures

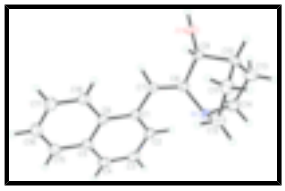

Fig. 1. A view of the title molecule, with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. The azabicyclic ring is disordered and only the ring with the major occupancy is shown.

rac-(*Z*)-2-(1-Naphthylmethylene)-1-azabicyclo[2.2.2]octan-3-ol

Crystal data

$C_{18}H_{19}NO$	F_{000} = 568
M_r = 265.34	D_x = 1.283 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3326 reflections
a = 6.1892 (1) Å	θ = 1.0–27.5º
b = 8.8706 (2) Å	μ = 0.08 mm^{-1}
c = 25.1693 (5) Å	T = 90.0 (2) K
β = 96.0631 (8)º	Block, colourless
V = 1374.11 (5) Å^3	0.25 × 0.20 × 0.15 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	3132 independent reflections
Radiation source: fine-focus sealed tube	2155 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.035
Detector resolution: 18 pixels mm^{-1}	θ_{max} = 27.5º
T = 90.0(2) K	θ_{min} = 1.6º
ω scans at fixed χ = 55°	h = −8→8
Absorption correction: multi-scan Scalepack (Otwinowski & Minor, 1997)	k = −11→11
T_{min} = 0.981, T_{max} = 0.988	l = −32→32
5940 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H-atom parameters constrained
$wR(F^2)$ = 0.126	$w = 1/[\sigma^2(F_o^2) + (0.0611P)^2 + 0.3438P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.005

3132 reflections	$\Delta\rho_{max}$ = 0.27 e Å^{-3}
205 parameters	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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.

Some disorder caused by this being a mixture of isomers. The model is a compromise but the fit is quite good.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
N1	0.79527 (18)	0.14764 (14)	0.08644 (5)	0.0224 (3)	
C1	0.7826 (2)	−0.17785 (16)	0.12963 (6)	0.0191 (3)	
C2	0.9384 (2)	−0.19584 (17)	0.09501 (6)	0.0222 (3)	
H2	0.9302	−0.1371	0.0633	0.027*	
C3	1.1100 (2)	−0.29966 (18)	0.10563 (6)	0.0250 (4)	
H3	1.2152	−0.3105	0.0810	0.030*	
C4	1.1258 (2)	−0.38435 (18)	0.15093 (6)	0.0255 (4)	
H4	1.2445	−0.4518	0.1581	0.031*	
C5	0.9682 (2)	−0.37340 (17)	0.18746 (6)	0.0219 (3)	
C6	0.7926 (2)	−0.26997 (16)	0.17679 (6)	0.0189 (3)	
C7	0.6004 (2)	−0.07164 (18)	0.11800 (6)	0.0235 (3)	
H7	0.4624	−0.1077	0.1255	0.028*	
C8	0.6021 (2)	0.06755 (19)	0.09843 (6)	0.0266 (4)	
C9	0.3949 (6)	0.1687 (4)	0.09465 (13)	0.0179 (7)	0.630 (3)
H9	0.3507	0.1890	0.1311	0.021*	0.630 (3)
O1	0.2307 (2)	0.0842 (2)	0.06349 (7)	0.0257 (5)	0.630 (3)
H1O	0.1103	0.0985	0.0752	0.038*	0.630 (3)
C9'	0.3883 (12)	0.1425 (9)	0.0770 (2)	0.0179 (7)	0.370 (3)
H9'	0.3260	0.0949	0.0427	0.021*	0.370 (3)
O1'	0.2545 (4)	0.1171 (4)	0.11801 (11)	0.0263 (9)	0.370 (3)
H1O'	0.1238	0.1153	0.1050	0.039*	0.370 (3)
C10	0.4502 (2)	0.31263 (17)	0.06831 (6)	0.0217 (3)	
H10	0.3214	0.3810	0.0625	0.026*	
C11	0.601 (2)	0.3579 (11)	0.1187 (5)	0.032 (2)	0.370 (3)
H11A	0.6208	0.4687	0.1192	0.038*	0.370 (3)
H11B	0.5325	0.3290	0.1510	0.038*	0.370 (3)

C11'	0.6166 (12)	0.3993 (6)	0.1062 (3)	0.0263 (11)	0.630 (3)
H11C	0.5526	0.4295	0.1390	0.032*	0.630 (3)
H11D	0.6662	0.4909	0.0886	0.032*	0.630 (3)
C12	0.8142 (2)	0.28499 (19)	0.12014 (6)	0.0286 (4)	
H12A	0.8672	0.2576	0.1574	0.034*	
H12B	0.9200	0.3554	0.1067	0.034*	
C13	0.5584 (3)	0.2930 (2)	0.01790 (7)	0.0416 (5)	
H13A	0.5985	0.3927	0.0043	0.050*	
H13B	0.4565	0.2440	−0.0098	0.050*	
C14	0.7627 (2)	0.19550 (19)	0.02959 (6)	0.0264 (4)	
H14A	0.7498	0.1051	0.0064	0.032*	
H14B	0.8911	0.2534	0.0209	0.032*	
C15	0.9787 (3)	−0.46434 (19)	0.23397 (6)	0.0285 (4)	
H15	1.0977	−0.5314	0.2416	0.034*	
C16	0.8215 (3)	−0.4573 (2)	0.26784 (6)	0.0321 (4)	
H16	0.8300	−0.5201	0.2986	0.039*	
C17	0.6457 (3)	−0.35661 (19)	0.25718 (6)	0.0283 (4)	
H17	0.5352	−0.3527	0.2806	0.034*	
C18	0.6331 (2)	−0.26472 (18)	0.21344 (6)	0.0228 (3)	
H18	0.5155	−0.1959	0.2074	0.027*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0157 (6)	0.0194 (7)	0.0326 (7)	0.0002 (5)	0.0044 (5)	0.0048 (6)
C1	0.0175 (7)	0.0144 (7)	0.0248 (7)	−0.0022 (6)	−0.0011 (6)	−0.0019 (6)
C2	0.0232 (7)	0.0188 (8)	0.0244 (7)	−0.0046 (6)	0.0021 (6)	0.0006 (6)
C3	0.0206 (7)	0.0221 (8)	0.0332 (8)	−0.0027 (6)	0.0070 (6)	−0.0052 (7)
C4	0.0188 (7)	0.0193 (8)	0.0378 (9)	0.0022 (6)	−0.0001 (6)	−0.0036 (7)
C5	0.0203 (7)	0.0171 (8)	0.0270 (8)	−0.0016 (6)	−0.0045 (6)	−0.0015 (6)
C6	0.0193 (7)	0.0151 (7)	0.0214 (7)	−0.0028 (6)	−0.0016 (5)	−0.0011 (6)
C7	0.0156 (7)	0.0249 (8)	0.0300 (8)	−0.0014 (6)	0.0023 (6)	0.0055 (7)
C8	0.0147 (7)	0.0260 (9)	0.0394 (9)	0.0007 (6)	0.0039 (6)	0.0096 (7)
C9	0.0169 (8)	0.0195 (17)	0.017 (2)	0.0000 (10)	0.0003 (15)	−0.0030 (15)
O1	0.0133 (8)	0.0252 (10)	0.0382 (11)	−0.0003 (7)	0.0011 (7)	−0.0080 (8)
C9'	0.0169 (8)	0.0195 (17)	0.017 (2)	0.0000 (10)	0.0003 (15)	−0.0030 (15)
O1'	0.0130 (14)	0.040 (2)	0.0262 (17)	0.0033 (13)	0.0056 (11)	0.0075 (13)
C10	0.0165 (7)	0.0187 (8)	0.0298 (8)	0.0048 (6)	0.0027 (6)	0.0012 (6)
C11	0.035 (4)	0.017 (5)	0.042 (6)	−0.001 (4)	−0.002 (3)	−0.006 (3)
C11'	0.0203 (17)	0.017 (3)	0.042 (3)	0.007 (2)	0.0035 (18)	−0.0090 (19)
C12	0.0215 (8)	0.0330 (10)	0.0305 (8)	0.0004 (7)	−0.0010 (6)	−0.0049 (7)
C13	0.0270 (9)	0.0675 (14)	0.0314 (9)	0.0121 (9)	0.0084 (7)	0.0178 (9)
C14	0.0253 (8)	0.0268 (9)	0.0287 (8)	0.0017 (7)	0.0098 (6)	−0.0004 (7)
C15	0.0269 (8)	0.0241 (9)	0.0324 (9)	0.0015 (7)	−0.0069 (7)	0.0044 (7)
C16	0.0388 (9)	0.0305 (10)	0.0252 (8)	−0.0046 (8)	−0.0051 (7)	0.0067 (7)
C17	0.0299 (8)	0.0324 (10)	0.0225 (8)	−0.0059 (7)	0.0029 (6)	−0.0011 (7)
C18	0.0220 (7)	0.0217 (8)	0.0243 (8)	−0.0005 (6)	0.0005 (6)	−0.0028 (6)

Geometric parameters (Å, °)

N1—C8	1.4495 (19)	O1'—H1O'	0.8400
N1—C12	1.482 (2)	C10—C13	1.506 (2)
N1—C14	1.4858 (19)	C10—C11'	1.534 (8)
C1—C2	1.376 (2)	C10—C11	1.548 (15)
C1—C6	1.437 (2)	C10—H10	1.0000
C1—C7	1.475 (2)	C11—C12	1.464 (14)
C2—C3	1.410 (2)	C11—H11A	0.9900
C2—H2	0.9500	C11—H11B	0.9900
C3—C4	1.360 (2)	C11'—C12	1.599 (7)
C3—H3	0.9500	C11'—H11C	0.9900
C4—C5	1.413 (2)	C11'—H11D	0.9900
C4—H4	0.9500	C12—H12A	0.9900
C5—C15	1.418 (2)	C12—H12B	0.9900
C5—C6	1.426 (2)	C13—C14	1.535 (2)
C6—C18	1.421 (2)	C13—H13A	0.9900
C7—C8	1.330 (2)	C13—H13B	0.9900
C7—H7	0.9500	C14—H14A	0.9900
C8—C9'	1.528 (8)	C14—H14B	0.9900
C8—C9	1.560 (4)	C15—C16	1.361 (2)
C9—O1	1.429 (3)	C15—H15	0.9500
C9—C10	1.495 (4)	C16—C17	1.412 (2)
C9—H9	1.0000	C16—H16	0.9500
O1—H1O	0.8400	C17—C18	1.365 (2)
C9'—O1'	1.408 (6)	C17—H17	0.9500
C9'—C10	1.578 (8)	C18—H18	0.9500
C9'—H9'	1.0000		
C8—N1—C12	107.51 (12)	C9—C10—H10	111.5
C8—N1—C14	108.03 (12)	C13—C10—H10	111.5
C12—N1—C14	108.10 (12)	C11'—C10—H10	105.0
C2—C1—C6	119.03 (13)	C11—C10—H10	111.5
C2—C1—C7	121.38 (13)	C9'—C10—H10	113.5
C6—C1—C7	119.51 (13)	C12—C11—C10	111.7 (8)
C1—C2—C3	121.35 (14)	C12—C11—H11A	109.3
C1—C2—H2	119.3	C10—C11—H11A	109.3
C3—C2—H2	119.3	C12—C11—H11B	109.3
C4—C3—C2	120.37 (14)	C10—C11—H11B	109.3
C4—C3—H3	119.8	H11A—C11—H11B	107.9
C2—C3—H3	119.8	C10—C11'—C12	105.4 (4)
C3—C4—C5	120.93 (14)	C10—C11'—H11C	110.7
C3—C4—H4	119.5	C12—C11'—H11C	110.7
C5—C4—H4	119.5	C10—C11'—H11D	110.7
C4—C5—C15	121.57 (14)	C12—C11'—H11D	110.7
C4—C5—C6	119.13 (13)	H11C—C11'—H11D	108.8
C15—C5—C6	119.30 (14)	C11—C12—N1	109.4 (5)
C18—C6—C5	117.81 (13)	N1—C12—C11'	112.5 (3)
C18—C6—C1	123.05 (13)	C11—C12—H12A	109.8

C5—C6—C1	119.13 (13)	N1—C12—H12A	109.8
C8—C7—C1	129.11 (14)	C11'—C12—H12A	122.2
C8—C7—H7	115.4	C11—C12—H12B	109.8
C1—C7—H7	115.4	N1—C12—H12B	109.8
C7—C8—N1	124.84 (13)	C11'—C12—H12B	92.5
C7—C8—C9'	119.6 (3)	H12A—C12—H12B	108.2
N1—C8—C9'	114.6 (3)	C10—C13—C14	109.53 (13)
C7—C8—C9	121.19 (18)	C10—C13—H13A	109.8
N1—C8—C9	113.35 (18)	C14—C13—H13A	109.8
O1—C9—C10	112.8 (3)	C10—C13—H13B	109.8
O1—C9—C8	105.3 (2)	C14—C13—H13B	109.8
C10—C9—C8	107.0 (2)	H13A—C13—H13B	108.2
O1—C9—H9	110.5	N1—C14—C13	111.77 (12)
C10—C9—H9	110.5	N1—C14—H14A	109.3
C8—C9—H9	110.5	C13—C14—H14A	109.3
O1'—C9'—C8	103.1 (5)	N1—C14—H14B	109.3
O1'—C9'—C10	115.1 (4)	C13—C14—H14B	109.3
C8—C9'—C10	104.5 (4)	H14A—C14—H14B	107.9
O1'—C9'—H9'	111.2	C16—C15—C5	121.16 (14)
C8—C9'—H9'	111.2	C16—C15—H15	119.4
C10—C9'—H9'	111.2	C5—C15—H15	119.4
C9'—O1'—H1O'	109.5	C15—C16—C17	119.84 (14)
C9—C10—C13	114.70 (18)	C15—C16—H16	120.1
C9—C10—C11'	108.8 (2)	C17—C16—H16	120.1
C13—C10—C11'	104.7 (3)	C18—C17—C16	120.54 (15)
C9—C10—C11	90.3 (3)	C18—C17—H17	119.7
C13—C10—C11	115.9 (5)	C16—C17—H17	119.7
C13—C10—C9'	98.2 (2)	C17—C18—C6	121.31 (14)
C11'—C10—C9'	123.4 (3)	C17—C18—H18	119.3
C11—C10—C9'	105.6 (4)	C6—C18—H18	119.3
C6—C1—C2—C3	−1.7 (2)	C8—C9—C10—C11	−70.2 (5)
C7—C1—C2—C3	−178.68 (13)	O1—C9—C10—C9'	−38.9 (11)
C1—C2—C3—C4	−0.4 (2)	C8—C9—C10—C9'	76.5 (12)
C2—C3—C4—C5	1.8 (2)	O1'—C9'—C10—C9	33.5 (8)
C3—C4—C5—C15	177.98 (14)	C8—C9'—C10—C9	−78.8 (12)
C3—C4—C5—C6	−1.0 (2)	O1'—C9'—C10—C13	−171.8 (4)
C4—C5—C6—C18	178.17 (13)	C8—C9'—C10—C13	75.9 (3)
C15—C5—C6—C18	−0.9 (2)	O1'—C9'—C10—C11'	74.6 (6)
C4—C5—C6—C1	−1.0 (2)	C8—C9'—C10—C11'	−37.7 (5)
C15—C5—C6—C1	179.93 (13)	O1'—C9'—C10—C11	68.3 (7)
C2—C1—C6—C18	−176.80 (13)	C8—C9'—C10—C11	−44.0 (6)
C7—C1—C6—C18	0.2 (2)	C9—C10—C11—C12	81.2 (5)
C2—C1—C6—C5	2.4 (2)	C13—C10—C11—C12	−36.6 (6)
C7—C1—C6—C5	179.41 (13)	C11'—C10—C11—C12	−93 (2)
C2—C1—C7—C8	−42.4 (2)	C9'—C10—C11—C12	70.8 (6)
C6—C1—C7—C8	140.60 (17)	C9—C10—C11'—C12	55.3 (4)
C1—C7—C8—N1	−3.0 (3)	C13—C10—C11'—C12	−67.7 (3)
C1—C7—C8—C9'	165.1 (2)	C11—C10—C11'—C12	62 (2)
C1—C7—C8—C9	−173.36 (17)	C9'—C10—C11'—C12	42.7 (5)

C12—N1—C8—C7	−119.28 (17)	C10—C11—C12—N1	−22.5 (6)
C14—N1—C8—C7	124.27 (17)	C10—C11—C12—C11'	81 (3)
C12—N1—C8—C9'	72.0 (3)	C8—N1—C12—C11	−44.8 (4)
C14—N1—C8—C9'	−44.4 (3)	C14—N1—C12—C11	71.6 (4)
C12—N1—C8—C9	51.73 (19)	C8—N1—C12—C11'	−63.9 (3)
C14—N1—C8—C9	−64.72 (19)	C14—N1—C12—C11'	52.5 (3)
C7—C8—C9—O1	−56.6 (3)	C10—C11'—C12—C11	−74 (2)
N1—C8—C9—O1	132.0 (2)	C10—C11'—C12—N1	9.9 (4)
C9'—C8—C9—O1	34.1 (10)	C9—C10—C13—C14	−55.7 (2)
C7—C8—C9—C10	−176.91 (17)	C11'—C10—C13—C14	63.5 (3)
N1—C8—C9—C10	11.7 (2)	C11—C10—C13—C14	47.6 (4)
C9'—C8—C9—C10	−86.2 (12)	C9'—C10—C13—C14	−64.2 (3)
C7—C8—C9'—O1'	48.6 (5)	C8—N1—C14—C13	57.09 (18)
N1—C8—C9'—O1'	−142.1 (3)	C12—N1—C14—C13	−58.97 (17)
C9—C8—C9'—O1'	−51.6 (9)	C10—C13—C14—N1	0.4 (2)
C7—C8—C9'—C10	169.3 (2)	C4—C5—C15—C16	−177.35 (15)
N1—C8—C9'—C10	−21.4 (3)	C6—C5—C15—C16	1.7 (2)
C9—C8—C9'—C10	69.1 (11)	C5—C15—C16—C17	−0.9 (2)
O1—C9—C10—C13	−66.7 (3)	C15—C16—C17—C18	−0.8 (2)
C8—C9—C10—C13	48.7 (2)	C16—C17—C18—C6	1.6 (2)
O1—C9—C10—C11'	176.5 (3)	C5—C6—C18—C17	−0.7 (2)
C8—C9—C10—C11'	−68.1 (3)	C1—C6—C18—C17	178.45 (14)
O1—C9—C10—C11	174.5 (5)		

Fig. 1