organic compounds

1-[2-(1-Hydroxycyclohexyl)-2-(4-methoxyphenyl)ethyl]dimethylammonium chloride (venlafaxine hydrochloride)

Daniel Vega,[a]***** **Daniel Fernández**[b] **and Gustavo Echeverría**[c]

[a]Departamento de Física, Comisión Nacional de Energía Atómica, Buenos Aires, Argentina, [b]Escuela de Ciencia y Tecnología, Universidad Nacional de General San Martín, Buenos Aires, Argentina, and [c]LANADI, Departamento de Física, Universidad Nacional de La Plata, La Plata, Argentina
Correspondence e-mail: vega@cnea.gov.ar

The crystal structure of racemic venlafaxine hydrochloride, $C_{17}H_{28}NO_2^+ \cdot Cl^-$, consists of two types of parallel chains formed by translated venlafaxine$^+$ cations, hydrogen bonded by Cl^- anions, and characterized by the opposite chirality of their constituent molecules. These chains organize in two different types of broad layers of opposite handedness, related by a glide plane.

Comment

The title compound, (I), is a representative of a novel group of antidepressants and is characterized by its ability to inhibit selectively the presynaptic reuptake of both serotonin and noradrenaline, with no affinity for the histaminergic, adrenergic and cholinergic receptors responsible for the toxicity associated with traditional antidepressant treatment (Briley, 1998; Burnett & Dinan, 1998). These novel pharmacological properties of venlafaxine may enhance its efficacy as well as its safety/tolerability profile, especially in the treatment of severely depressed patients (Holliday & Benfield, 1995; Dinan & Burnett, 1997; Leonard, 1999).

(I)
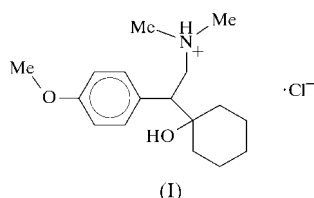
The clinical administration and the antidepressant activity determinations were mainly performed on the racemic venlafaxine hydrochloride derivative. However, the only known structural study was performed on an *S* enantiomorph of a hydrobromide derivative (hereafter VHBr), which crystallizes in space group $P2_1$ [this structure is in the Cambridge Structural Database (Allen *et al.*, 1983) with refcode

KIDGUZ; it was deposited as supplementary material for a paper by Yardley *et al.* (1990), but in the final publication this structure is not actually described].

Two different crystalline forms of the racemic venlafaxine hydrochloride derivative could be identified by X-ray powder methods, while single crystals of only one of them could be obtained (hereafter VHCl). Its X-ray structure determination was carried out in order to study its molecular conformation and to compare it with VHBr.

The asymmetric unit of the title compound (Fig. 1) consists of a $C_{17}H_{28}NO_2^+$ cation and a Cl^- anion. The dimethylammonium N atom, N1, shows quaternary character due to proton transfer from HCl and consequently bears the positive charge in the molecular cation. The N1 bond angles range from 107 to 114° (see Table 1) confirming the tetrahedral bond configuration. The hexanolic ring adopts a chair conformation, with C8, C10, C11 and C13 defining a plane (mean deviation 0.004 Å), and C9 and C12 being 0.645 (5) and -0.661 (5) Å out of the plane, respectively.

The comparison of both the VHCl and VHBr structures shows no significant differences between the relevant geometric parameters except for a torsion angle at the methoxy substituent and differences expected due to the unequal size of the halogen anion. A least-squares fit, using the facilities provided by *XP* in the *SHELXTL/PC* package (Sheldrick, 1991), gave an r.m.s. deviation of 0.05 Å. The maximum deviations occur at the halogen (0.11 Å) and C17 (0.14 Å) locations. C17 is the C atom of the methoxy substituent of the benzene and the location difference is evidence of the dissimilarity between the C3—C4—O1—C17 torsion angle in VHCl [-10.9 (7)°] and the corresponding one in VHBr (-0.5°).

A pair of [010] translated molecular cations of venlafaxine are linked by two hydrogen bonds to the chloride anion (Table 2). A search of hydrogen bonds to Cl atoms in the Cambridge Structural Database (Allen *et al.*, 1983; version of October 1999, *ca* 200 000 entries), restricted to bond distances H···Cl < 2.8 Å and to angles O—H···Cl and N—H···Cl > 130°, shows that the second (N1—H1A···Cl1) is a very strong one; only 8% of those hydrogen bonds found (661 over 7988)
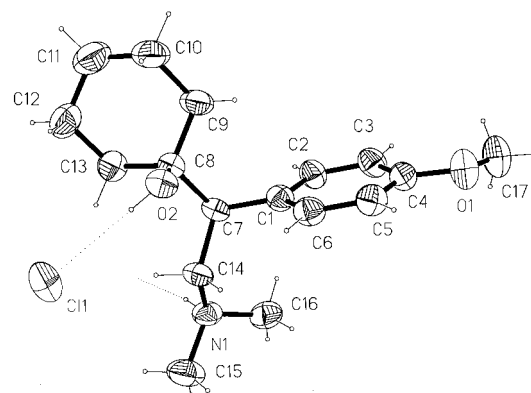

Figure 1
View of the molecular cation and the chloride anion showing the numbering scheme used, with displacement ellipsoids drawn at the 50% probability level. The Cl hydrogen bonds are depicted by dotted lines.

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were shorter than the one present in this structure [mean value H$\cdots$Cl 2.403 (2) Å over 7988 hits, this work 2.141 (9) Å]; meanwhile, the first one falls within a normal hydrogen-bond range [mean value H$\cdots$Cl 2.310 (3) Å, over 3288 hits, this work 2.331 (9) Å]. Thus, the main structural cohesion is provided by the two hydrogen bonds determining a chain running along the crystallographic b axis [b = 5.8810 (12) Å]. A similar chain is responsible for the structural cohesion in VHBr, where two [100] translated molecular cations are linked through a bromide anion by a pair of hydrogen bonds (N1$\cdots$Br1 3.164 and O2$\cdots$Br1 3.333 Å), the chain running along the crystallographic a axis [a = 5.905 (2) Å].

The twofold screw axis, along [001] in VHCl [c = 11.448 (2) Å] and along [010] in VHBr [b = 11.625 (3) Å], packs chains of molecular cations of the same chirality determining a broad layer parallel to (100) and (001), respectively. In VHCl, another layer, which contains chains of molecular cations of opposite handedness, is generated by the presence of the c glide plane as a consequence of the racemic condition of VHCl, determining a stacking of sheets of opposite chirality. In VHBr, instead, due to its non-racemic constitution, layers containing molecular cations of the same handedness are stacked. The interlayer spacing is almost the same in both structures, equal to $0.5d_{100}$ for VHCl [13.1153 (5) Å] and to d_{001} for VHBr [13.430 (4) Å].

Experimental

The title compound was obtained from Laboratorios Gador. Crystals suitable for X-ray diffraction were obtained by slow evaporation from a water solution.

Crystal data

$C_{17}H_{28}NO_2^+\cdot Cl^-$	Mo $K\alpha$ radiation
$M_r = 313.85$	Cell parameters from 25
Orthorhombic, $Pca2_1$	reflections
$a = 26.230$ (5) Å	$\theta = 10–20°$
$b = 5.8810$ (12) Å	$\mu = 0.221$ mm^{-1}
$c = 11.448$ (2) Å	$T = 293$ (2) K
$V = 1766.0$ (6) Å^3	Prism, colorless
$Z = 4$	$0.44 \times 0.32 \times 0.28$ mm
$D_x = 1.180$ Mg m^{-3}	

Data collection

CAD-4 diffractometer	$R_{int} = 0.087$
ω–2θ scans	$\theta_{max} = 29.99°$
Absorption correction: numerical	$h = 0 \rightarrow 30$
integration (Sheldrick, 1976)	$k = -1 \rightarrow 8$
$T_{min} = 0.92$, $T_{max} = 0.93$	$l = 0 \rightarrow 16$
2879 measured reflections	2 standard reflections
2094 independent reflections (plus	every 98 reflections
380 Friedel-related reflections)	intensity decay: <1%
1629 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0652P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.043$	$+ 0.7255P]$
$wR(F^2) = 0.149$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.046$	$(\Delta/\sigma)_{max} = 0.005$
2474 reflections	$\Delta\rho_{max} = 0.23$ e Å^{-3}
190 parameters	$\Delta\rho_{min} = -0.27$ e Å^{-3}
H atoms treated by a mixture of	Absolute structure: Flack (1983)
independent and constrained	Flack parameter: 0.14 (13)
refinement	

Table 1
Selected geometric parameters (Å, °).

C4—O1	1.367 (5)	C15—N1	1.501 (6)
C8—O2	1.432 (4)	C16—N1	1.482 (6)
C14—N1	1.504 (5)	C17—O1	1.401 (6)
C16—N1—C15	110.7 (4)	C15—N1—C14	108.9 (3)
C16—N1—C14	114.2 (3)	C4—O1—C17	118.8 (4)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O2—H2$B\cdots$Cl1	0.85	2.33	3.181 (9)	180
N1—H1$A\cdots$Cl1^i	0.91	2.14	3.046 (9)	173

Symmetry code: (i) $x, 1 + y, z$.

H atoms attached to carbon were placed at idealized positions and allowed to ride with isotropic displacement parameters 1.2 times larger than those of their hosts. Those bonded to oxygen were located in a ΔF synthesis and were subsequently refined with restrained O—H distances and individual isotropic displacement parameters. Data collection was performed at the Laboratorio Nacional de Difraccion (LANADI).

Data collection: *CAD*-4/*PC* (Enraf–Nonius, 1993); cell refinement: *CAD*-4/*PC*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *XS* in *SHELXTL/PC* (Sheldrick, 1991); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL/PC*; software used to prepare material for publication: *PARST* (Nardelli, 1983) and *CSD* (Allen *et al.*, 1983).

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supporting information

1-[2-(1-Hydroxycyclohexyl)-2-(4-methoxyphenyl)ethyl]dimethylammonium chloride (venlafaxine hydrochloride)

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Computing details

Data collection: *CAD-4-PC* (Enraf Nonius, 1993); cell refinement: *CAD-4-PC*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: XS in *SHELXTL/PC* (Sheldrick, 1991); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL/PC*; software used to prepare material for publication: *PARST* (Nardelli, 1983) and CSD (Allen *et al.*, 1983).

1-[2-(dimethylamino)-1-(4-methoxyphenyl)ethyl]cyclohexanol hydrochloride (Venlafaxine Hydrochloride)

Crystal data

$C_{17}H_{28}NO_2{}^+ \cdot Cl^-$	$F(000) = 680$
$M_r = 313.85$	$D_x = 1.180$ Mg m^{-3}
Orthorhombic, $Pca2_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2c -2ac	Cell parameters from 25 reflections
$a = 26.230$ (5) Å	$\theta = 10–20°$
$b = 5.8810$ (12) Å	$\mu = 0.22$ mm^{-1}
$c = 11.448$ (2) Å	$T = 293$ K
$V = 1766.0$ (6) Å^3	Prism, colorless
$Z = 4$	$0.44 \times 0.32 \times 0.28$ mm

Data collection

CAD4 diffractometer	2474 independent reflections
Radiation source: rotating anode	1629 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{int} = 0.087$
$\omega–2\theta$ scans	$\theta_{max} = 30.0°$, $\theta_{min} = 1.6°$
Absorption correction: numerical Integration *SHELX76* (Sheldrick, 1976)	$h = 0 \rightarrow 30$
	$k = -1 \rightarrow 8$
	$l = 0 \rightarrow 16$
$T_{min} = 0.92$, $T_{max} = 0.93$	2 standard reflections every 98 reflections
2879 measured reflections	intensity decay: <1%

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.043$	Secondary atom site location: difference Fourier map
$wR(F^2) = 0.149$	
$S = 1.05$	Hydrogen site location: inferred from neighbouring sites
2474 reflections	
190 parameters	H atoms treated by a mixture of independent and constrained refinement
1 restraint	

Calculated $w = 1/[\sigma^2(F_o^2) + (0.0652P)^2 + 0.7255P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.005$

$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}
Absolute structure: Flack (1983)
Absolute structure parameter: 0.14 (13)

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. The complete reflection sphere up to a θ angle of 25° was measured and some extra reflections were collected up to a maximun θ angle of 30°. This increase both the number of reflections as well as the resolution at the expense of having a lower completeness parameter (91.8%).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.47903 (5)	0.33859 (19)	0.10142 (10)	0.0590 (3)
C1	0.37670 (15)	0.9127 (6)	0.4310 (3)	0.0394 (8)
C2	0.34982 (17)	1.1020 (7)	0.4664 (4)	0.0438 (9)
H2A	0.3455	1.2247	0.4120	0.080*
C3	0.32937 (17)	1.1220 (7)	0.5796 (4)	0.0470 (10)
H3A	0.3097	1.2530	0.6010	0.080*
C4	0.33739 (17)	0.9482 (7)	0.6590 (4)	0.0449 (9)
C5	0.36319 (17)	0.7541 (7)	0.6232 (4)	0.0469 (10)
H5A	0.3678	0.6307	0.6771	0.080*
C6	0.38266 (16)	0.7372 (7)	0.5123 (4)	0.0440 (9)
H6A	0.4015	0.6033	0.4914	0.080*
C7	0.39775 (14)	0.8977 (6)	0.3085 (3)	0.0353 (7)
H7A	0.3946	1.0462	0.2744	0.080*
C8	0.36839 (15)	0.7271 (6)	0.2283 (3)	0.0365 (8)
C9	0.31125 (16)	0.7343 (8)	0.2521 (4)	0.0508 (10)
H9A	0.2998	0.8879	0.2413	0.080*
H9B	0.3039	0.6921	0.3313	0.080*
C10	0.28122 (19)	0.5832 (9)	0.1685 (5)	0.0618 (13)
H10A	0.2455	0.5953	0.1854	0.080*
H10B	0.2913	0.4281	0.1812	0.080*
C11	0.2923 (2)	0.6423 (11)	0.0410 (5)	0.0713 (16)
H11A	0.2800	0.7932	0.0254	0.080*
H11B	0.2747	0.5393	−0.0101	0.080*
C12	0.3489 (2)	0.6303 (9)	0.0156 (4)	0.0616 (13)
H12A	0.3605	0.4761	0.0226	0.080*
H12B	0.3555	0.6806	−0.0627	0.080*
C13	0.37860 (17)	0.7823 (7)	0.0994 (4)	0.0470 (9)
H15A	0.4144	0.7612	0.0855	0.080*
H15B	0.3707	0.9391	0.0849	0.080*

C14	0.45509 (14)	0.8337 (6)	0.3085 (4)	0.0406 (8)
H14A	0.4621	0.7534	0.2373	0.080*
H14B	0.4619	0.7317	0.3721	0.080*
C15	0.54460 (18)	0.9497 (9)	0.3079 (5)	0.0661 (13)
H15C	0.5675	1.0771	0.3100	0.080*
H15D	0.5519	0.8499	0.3721	0.080*
H15E	0.5489	0.8689	0.2357	0.080*
C16	0.48347 (19)	1.1784 (7)	0.4197 (5)	0.0547 (11)
H16B	0.5076	1.3011	0.4193	0.080*
H16C	0.4495	1.2390	0.4200	0.080*
H16D	0.4885	1.0873	0.4883	0.080*
C17	0.3028 (2)	1.1515 (9)	0.8207 (5)	0.0702 (15)
H17A	0.2937	1.1284	0.9010	0.080*
H17B	0.3286	1.2670	0.8156	0.080*
H17C	0.2733	1.1986	0.7774	0.080*
N1	0.49066 (13)	1.0339 (6)	0.3150 (3)	0.0447 (8)
H1A	0.4843	1.1224	0.2515	0.080*
O1	0.32147 (14)	0.9488 (5)	0.7727 (3)	0.0619 (9)
O2	0.38455 (10)	0.5002 (4)	0.2546 (3)	0.0416 (6)
H2B	0.4098	0.4569	0.2136	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0681 (7)	0.0567 (5)	0.0522 (5)	0.0171 (5)	0.0173 (6)	0.0082 (6)
C1	0.037 (2)	0.0394 (17)	0.0417 (19)	−0.0046 (15)	0.0010 (17)	0.0015 (16)
C2	0.045 (3)	0.0421 (19)	0.0438 (19)	0.0057 (17)	0.0059 (17)	0.0023 (16)
C3	0.046 (3)	0.0435 (19)	0.052 (3)	0.0076 (17)	0.0072 (19)	0.0016 (18)
C4	0.042 (3)	0.051 (2)	0.0421 (19)	−0.0039 (18)	0.0028 (18)	−0.0042 (18)
C5	0.049 (3)	0.0432 (19)	0.048 (2)	0.0014 (18)	−0.0011 (18)	0.0061 (17)
C6	0.042 (2)	0.0400 (18)	0.050 (2)	0.0070 (17)	−0.0023 (18)	0.0004 (17)
C7	0.0265 (19)	0.0340 (15)	0.0455 (19)	0.0003 (13)	0.0039 (16)	0.0025 (15)
C8	0.034 (2)	0.0363 (16)	0.0390 (18)	0.0006 (15)	0.0012 (15)	0.0010 (15)
C9	0.032 (2)	0.057 (2)	0.064 (3)	0.0007 (19)	−0.001 (2)	−0.005 (2)
C10	0.039 (3)	0.065 (3)	0.081 (4)	−0.006 (2)	−0.003 (3)	−0.010 (3)
C11	0.061 (4)	0.081 (4)	0.071 (4)	0.002 (3)	−0.023 (3)	−0.008 (3)
C12	0.067 (3)	0.074 (3)	0.044 (2)	0.003 (3)	−0.012 (2)	−0.002 (2)
C13	0.051 (3)	0.048 (2)	0.0422 (19)	0.0013 (17)	0.000 (2)	0.010 (2)
C14	0.028 (2)	0.0411 (17)	0.053 (2)	0.0022 (15)	0.0010 (17)	−0.0025 (18)
C15	0.039 (3)	0.083 (3)	0.076 (3)	0.000 (2)	0.001 (3)	0.012 (3)
C16	0.048 (3)	0.053 (2)	0.063 (3)	−0.012 (2)	−0.008 (2)	−0.005 (2)
C17	0.091 (4)	0.068 (3)	0.051 (3)	0.007 (3)	0.017 (3)	−0.008 (2)
N1	0.034 (2)	0.0521 (19)	0.0480 (18)	−0.0096 (14)	−0.0017 (15)	0.0061 (16)
O1	0.081 (3)	0.0593 (18)	0.0458 (17)	0.0014 (17)	0.0130 (16)	−0.0014 (15)
O2	0.0390 (15)	0.0365 (11)	0.0494 (15)	−0.0012 (11)	0.0012 (12)	0.0044 (12)

Geometric parameters (Å, º)

C1—C2	1.378 (5)	C11—H11A	0.9600
C1—C6	1.398 (6)	C11—H11B	0.9600
C1—C7	1.510 (5)	C12—C13	1.525 (7)
C2—C3	1.407 (6)	C12—H12A	0.9600
C2—H2A	0.9600	C12—H12B	0.9600
C3—C4	1.384 (6)	C13—H15A	0.9599
C3—H3A	0.9600	C13—H15B	0.9600
C4—O1	1.367 (5)	C14—N1	1.504 (5)
C4—C5	1.389 (6)	C14—H14A	0.9600
C5—C6	1.372 (6)	C14—H14B	0.9600
C5—H5A	0.9600	C15—N1	1.501 (6)
C6—H6A	0.9597	C15—H15C	0.9599
C7—C14	1.550 (5)	C15—H15D	0.9600
C7—C8	1.563 (5)	C15—H15E	0.9600
C7—H7A	0.9600	C16—N1	1.482 (6)
C8—O2	1.432 (4)	C16—H16B	0.9599
C8—C9	1.524 (6)	C16—H16C	0.9604
C8—C13	1.535 (6)	C16—H16D	0.9600
C9—C10	1.525 (7)	C17—O1	1.401 (6)
C9—H9A	0.9600	C17—H17A	0.9601
C9—H9B	0.9600	C17—H17B	0.9599
C10—C11	1.528 (8)	C17—H17C	0.9601
C10—H10A	0.9601	N1—H1A	0.9100
C10—H10B	0.9599	O2—H2B	0.8502
C11—C12	1.515 (8)		
C2—C1—C6	117.2 (4)	C10—C11—H11B	110.3
C2—C1—C7	120.5 (3)	H11A—C11—H11B	108.1
C6—C1—C7	122.3 (4)	C11—C12—C13	110.6 (4)
C1—C2—C3	122.2 (4)	C11—C12—H12A	109.8
C1—C2—H2A	118.4	C13—C12—H12A	109.8
C3—C2—H2A	119.3	C11—C12—H12B	110.0
C4—C3—C2	119.0 (4)	C13—C12—H12B	108.3
C4—C3—H3A	120.4	H12A—C12—H12B	108.1
C2—C3—H3A	120.5	C12—C13—C8	113.1 (4)
O1—C4—C3	125.3 (4)	C12—C13—H15A	108.6
O1—C4—C5	115.6 (4)	C8—C13—H15A	107.6
C3—C4—C5	119.2 (4)	C12—C13—H15B	110.1
C6—C5—C4	120.9 (4)	C8—C13—H15B	109.4
C6—C5—H5A	119.6	H15A—C13—H15B	107.9
C4—C5—H5A	119.5	N1—C14—C7	114.3 (3)
C5—C6—C1	121.4 (4)	N1—C14—H14A	107.9
C5—C6—H6A	118.7	C7—C14—H14A	107.8
C1—C6—H6A	119.8	N1—C14—H14B	109.6
C1—C7—C14	111.6 (3)	C7—C14—H14B	109.5
C1—C7—C8	113.7 (3)	H14A—C14—H14B	107.5

C14—C7—C8	108.8 (3)	N1—C15—H15C	109.3
C1—C7—H7A	107.1	N1—C15—H15D	110.4
C14—C7—H7A	107.7	H15C—C15—H15D	109.5
C8—C7—H7A	107.6	N1—C15—H15E	108.7
O2—C8—C9	106.2 (3)	H15C—C15—H15E	109.5
O2—C8—C13	110.3 (3)	H15D—C15—H15E	109.5
C9—C8—C13	109.7 (3)	N1—C16—H16B	110.0
O2—C8—C7	109.2 (3)	N1—C16—H16C	109.5
C9—C8—C7	111.2 (3)	H16B—C16—H16C	109.5
C13—C8—C7	110.1 (3)	N1—C16—H16D	108.9
C8—C9—C10	112.3 (4)	H16B—C16—H16D	109.5
C8—C9—H9A	108.1	H16C—C16—H16D	109.5
C10—C9—H9A	107.9	O1—C17—H17A	110.0
C8—C9—H9B	111.1	O1—C17—H17B	109.4
C10—C9—H9B	109.7	H17A—C17—H17B	109.5
H9A—C9—H9B	107.5	O1—C17—H17C	109.0
C9—C10—C11	111.6 (4)	H17A—C17—H17C	109.5
C9—C10—H10A	109.6	H17B—C17—H17C	109.5
C11—C10—H10A	111.1	C16—N1—C15	110.7 (4)
C9—C10—H10B	108.5	C16—N1—C14	114.2 (3)
C11—C10—H10B	108.0	C15—N1—C14	108.9 (3)
H10A—C10—H10B	107.9	C16—N1—H1A	107.2
C12—C11—C10	111.0 (4)	C15—N1—H1A	108.6
C12—C11—H11A	109.6	C14—N1—H1A	107.1
C10—C11—H11A	108.9	C4—O1—C17	118.8 (4)
C12—C11—H11B	108.9	C8—O2—H2B	113.2
C6—C1—C2—C3	0.6 (6)	C1—C7—C8—C13	159.8 (3)
C7—C1—C2—C3	179.7 (4)	C14—C7—C8—C13	−75.1 (4)
C1—C2—C3—C4	1.4 (7)	O2—C8—C9—C10	−65.7 (5)
C2—C3—C4—O1	177.4 (4)	C13—C8—C9—C10	53.5 (5)
C2—C3—C4—C5	−3.1 (6)	C7—C8—C9—C10	175.5 (4)
O1—C4—C5—C6	−177.6 (4)	C8—C9—C10—C11	−55.2 (6)
C3—C4—C5—C6	2.9 (7)	C9—C10—C11—C12	55.6 (6)
C4—C5—C6—C1	−0.9 (7)	C10—C11—C12—C13	−55.3 (6)
C2—C1—C6—C5	−0.9 (6)	C11—C12—C13—C8	55.8 (5)
C7—C1—C6—C5	−179.9 (4)	O2—C8—C13—C12	62.4 (5)
C2—C1—C7—C14	129.1 (4)	C9—C8—C13—C12	−54.2 (5)
C6—C1—C7—C14	−51.9 (5)	C7—C8—C13—C12	−176.9 (4)
C2—C1—C7—C8	−107.3 (4)	C1—C7—C14—N1	−88.9 (4)
C6—C1—C7—C8	71.7 (5)	C8—C7—C14—N1	144.7 (3)
C1—C7—C8—O2	−79.0 (4)	C7—C14—N1—C16	58.8 (5)
C14—C7—C8—O2	46.1 (4)	C7—C14—N1—C15	−177.0 (4)
C1—C7—C8—C9	37.9 (4)	C3—C4—O1—C17	−10.9 (7)
C14—C7—C8—C9	163.0 (3)	C5—C4—O1—C17	169.6 (5)