The crystal structure of racemic venlafaxine hydrochloride, C₁₇H₂₈NO₂ 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).

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 VHB Br), which crystallizes in space group P2₁ [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 VHB Br.

The asymmetric unit of the title compound (Fig. 1) consists of a C₁₇H₂₈NO₂⁺ 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 VHB Br 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 VHB Br [−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)
were shorter than the one present in this structure [mean value H···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···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 \([b = 5.8810 (12) \text{ Å}]\). 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 \((\text{N1} \cdots \text{Br1} 3.164 \text{ Å} \text{ and O2} \cdots \text{Br1} 3.333 \text{ Å})\), the chain running along the crystallographic a axis \([a = 5.905 (2) \text{ Å}]\).

The twofold screw axis, along [001] in VHCl \([c = 11.448 (2) \text{ Å}]\) and along [010] in VHBr \([b = 11.625 (3) \text{ Å}]\), 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 condition of VHCl, determining a stacking of sheets containing molecular cations of the same chirality, layers containing molecular cations of opposite handedness are stacked. The interlayer spacing is almost the same in both structures, equal to 0.5d\(_{100}\) for VHCl \([13.1153 (5) \text{ Å}]\) and to d\(_{001}\) for VHBr \([13.430 (4) \text{ Å}]\).

### 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**

\[
\begin{align*}
\text{C}_{17}\text{H}_{28}\text{NO}_{2}\text{Cl}^{-} & \\
M & = 313.85 \\
\text{Orthorhombic, Pca2}_{1} & \\
a & = 26.230 (5) \text{ Å} \\
b & = 5.8810 (12) \text{ Å} \\
c & = 11.448 (2) \text{ Å} \\
\text{V} & = 1766.0 (6) \text{ Å}^3 \\
Z & = 4 \\
D_{\text{c}} & = 1.180 \text{ Mg m}^{-3} \\
\hline
\text{Mo K\textalpha radiation} & \\
\text{Cell parameters from 25} & \\
\theta & = 10-20^\circ \\
\mu & = 0.221 \text{ mm}^{-1} \\
T & = 293 (2) \text{ K} \\
\text{Prism, colorless} & \\
0.44 & \times 0.32 & \times 0.28 \text{ mm} \\
\hline
\text{Data collection} & \\
\text{CAD-4 diffractometer} & \\
\text{ω-20 scans} & \\
\text{Absorption correction: numerical} & \\
\text{integration} (Sheldrick, 1976) & \\
T_{\text{min}} & = 0.92, T_{\text{max}} & = 0.93 \\
2879 & \text{measured reflections} & \\
2094 & \text{independent reflections (plus} & \\
380 & \text{Friedel-related reflections} \\
1629 & \text{reflections with } I > 2\sigma(I) \\
\hline
\text{Refinement} & \\
\text{Reefinement on } F^2 & \\
R[F^2 > 2\sigma(F^2)] & = 0.043 \\
wR(F^2) & = 0.149 \\
S & = 1.046 \\
2474 & \text{reflections} & \\
190 & \text{parameters} \\
H \text{ atoms treated by a mixture of independent and constrained} & \\
\text{reduction} & \\
\text{w} & = 1/[\sigma(F^2) + (0.0652P)^2 + 0.7255P] & \\
\text{where } P & = (F^2 + 2F'_C)/3 \\
\text{C} & = 0.055 \\
\Delta F_{\text{Max}} & = 0.23 \text{ e Å}^{-3} \\
\Delta F_{\text{Min}} & = -0.27 \text{ e Å}^{-3} \\
\text{Absolute structure: Flack} (1983) & \\
\text{Flack parameter: 0.14 (13)}
\end{align*}
\]

### 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···A | D─H | H···A | D─A | D─H···A |
|---------|------|-------|-----|--------|
| O2─H2B···Cl1 | 0.85 | 2.33 | 3.181 (9) | 180 |
| N1─H1A···Cl1 | 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 Δψ synthesis and were subsequently refined with restrained O─H distances and individual isotropic displacement parameters. Data collection was performed at the Laboratorio Nacional de Difracción (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: SHELXL97 (Sheldrick, 1997); molecular graphics: XP in SHELXL97; software used to prepare material for publication: PARST (Nardelli, 1983) and CSD (Allen et al., 1983).

The authors would like to thank Dr Dora Tombari for suggesting the problem as well as for helpful discussions. This work has been funded through a project of the Universidad Nacional de General San Martin.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: NA1473). Services for accessing these data are described at the back of the journal.

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

Daniel Vega, Daniel Fernández and Gustavo Echeverría

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: P**ARST** (Nardelli, 1983) and CSD (Allen et al., 1983).

Crystal data
\[\text{C}_{17}\text{H}_{28}\text{NO}_2^+\cdot\text{Cl}^-\]  
\[M_r = 313.85\]  
Orthorhombic, \(Pca_2_1\)  
Hall symbol: \(P 2c -2ac\)  
\(a = 26.230\ (5)\ \text{Å}\)  
\(b = 5.8810\ (12)\ \text{Å}\)  
\(c = 11.448\ (2)\ \text{Å}\)  
\(V = 1766.0\ (6)\ \text{Å}^3\)  
\(Z = 4\)

\[F(000) = 680\]  
\(D_\lambda = 1.180\ \text{Mg m}^{-3}\)  
Mo \(K\alpha\) radiation, \(\lambda = 0.71073\ \text{Å}\)  
Cell parameters from 25 reflections \(\theta = 10–20^\circ\)  
\(\mu = 0.22\ \text{mm}^{-1}\)  
\(T = 293\ \text{K}\)  
Prism, colorless  
\(0.44 \times 0.32 \times 0.28\ \text{mm}\)

Data collection
CAD4 diffractometer  
Radiation source: rotating anode  
Graphite monochromator  
\(\omega-2\theta\) scans  
Absorption correction: numerical Integration \(SHELX76\) (Sheldrick, 1976)  
\(\theta_{\text{min}} = 0.92, \theta_{\text{max}} = 0.93\)  
2879 measured reflections  
2474 independent reflections  
1629 reflections with \(I > 2\sigma(I)\)

Refinement
Refinement on \(F^2\)  
Least-squares matrix: full  
\(R[F^2 > 2\sigma(F^2)] = 0.043\)  
\(wR(F^2) = 0.149\)  
\(S = 1.05\)  
2474 reflections  
190 parameters  
1 restraint

Primary atom site location: structure-invariant direct methods  
Secondary atom site location: difference Fourier map  
Hydrogen site location: inferred from neighbouring sites  
H atoms treated by a mixture of independent and constrained refinement

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sup-1
Calculated \( w = 1/(\sigma^2(F_o^2) + (0.0652P)^2 + 0.7255P) \)
where \( P = (F_o^2 + 2F_c^2)/3 \)
\((\Delta/\sigma)_{\text{max}} = 0.005\)
\(\Delta \rho_{\text{max}} = 0.23 \text{ e Å}^{-3}\)
\(\Delta \rho_{\text{min}} = -0.27 \text{ e Å}^{-3}\)
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 \( \theta \) angle of 25° was measured and some extra reflections were collected up to a maximum \( \theta \) 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 (\( \text{Å}^2 \))

|     | \( x \)       | \( y \)       | \( z \)       | \( U_{eq}^*/U_{eq} \) |
|-----|---------------|---------------|---------------|-----------------------|
| C11 | 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*                |
|      | \(U^{11}\)   | \(U^{22}\)   | \(U^{33}\)   | \(U^{12}\)   | \(U^{13}\)   | \(U^{23}\)   |
|------|--------------|--------------|--------------|--------------|--------------|--------------|
| C11  | 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, °)

| Bond                  | Distance (Å) | Bond Angle (°) |
|-----------------------|--------------|----------------|
| C1—C2                 | 1.378 (5)    |                |
| C1—C6                 | 1.398 (6)    |                |
| C1—C7                 | 1.510 (5)    |                |
| C2—C3                 | 1.407 (6)    |                |
| C2—H2A                | 0.9600       |                |
| C3—C4                 | 1.384 (6)    |                |
| C3—H3A                | 0.9600       |                |
| C4—O1                 | 1.367 (5)    |                |
| C4—C5                 | 1.389 (6)    |                |
| C5—C6                 | 1.372 (6)    |                |
| C5—H5A                | 0.9600       |                |
| C6—H6A                | 0.9597       |                |
| C7—C14                | 1.550 (5)    |                |
| C7—C8                 | 1.563 (5)    |                |
| C7—H7A                | 0.9600       |                |
| C8—O2                 | 1.493 (4)    |                |
| C8—C9                 | 1.524 (6)    |                |
| C9—C10                | 1.525 (7)    |                |
| C9—H9A                | 0.9600       |                |
| C9—H9B                | 0.9600       |                |
| C10—C11               | 1.528 (8)    |                |
| C10—H10A              | 0.9601       |                |
| C10—H10B              | 0.9599       |                |
| C11—C12               | 1.515 (8)    |                |

| Bond                  | Distance (Å) | Bond Angle (°) |
|-----------------------|--------------|----------------|
| C2—C1                 | 117.2 (4)    |                |
| C2—C1                 | 120.5 (3)    |                |
| C6—C1                 | 122.3 (4)    |                |
| C1—C2                 | 122.2 (4)    |                |
| C1—C2                 | 118.4        |                |
| C3—C2                 | 119.3        |                |
| C4—C3                 | 119.0 (4)    |                |
| C4—C3                 | 120.4        |                |
| C2—C3                 | 120.5        |                |
| O1—C4                 | 125.3 (4)    |                |
| O1—C4                 | 115.6 (4)    |                |
| C3—C4                 | 119.2 (4)    |                |
| C6—C5                 | 120.9 (4)    |                |
| C6—C5                 | 119.6        |                |
| C4—C5                 | 119.5        |                |
| C5—C6                 | 121.4 (4)    |                |
| C5—C6                 | 118.7        |                |
| C1—C7                 | 119.8        |                |
| C1—C7                 | 111.6 (3)    |                |
| C1—C7                 | 113.7 (3)    |                |

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| Bond                | Angle (°) (°) | Bond                | Angle (°) (°) |
|---------------------|--------------|---------------------|--------------|
| 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        |
| C10—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)