Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

10,11-Dihydrocarbamazepine–acetic acid (1/1)

Andrea Johnston,[a] Alastair J. Florence,[a]* Philippe Fernandes,[a] Norman Shankland[a] and Alan R. Kennedy[b]

[a]Solid-State Research Group, Strathclyde Institute of Pharmacy and Biomedical Sciences, University of Strathclyde, 27 Taylor Street, Glasgow G4 0NR, Scotland, and [b]WestCHEM, Department of Pure and Applied Chemistry, University of Strathclyde, 295 Cathedral Street, Glasgow G1 1XL, Scotland

Correspondence e-mail: alastair.florence@strath.ac.uk

Key indicators

Single-crystal X-ray study
T = 123 K
Mean σ(C–C) = 0.005 Å
R factor = 0.076
wR factor = 0.147
Data-to-parameter ratio = 12.5

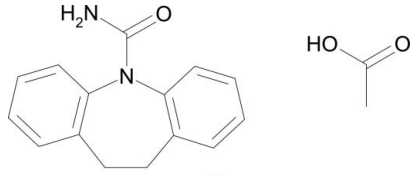
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 12 October 2006
Accepted 24 October 2006

In the title compound [systematic name: 10,11-dihydro-5*H*-dibenz[*b*,*f*]azepine-5-carboxamide–ethanoic acid (1/1)], $C_{15}H_{14}N_2O\cdot C_2H_4O_2$, the dihydrocarbamazepine and acetic acid molecules are hydrogen bonded to form an $R_2^2(8)$ motif, which is further connected into a centrosymmetric double motif arrangement.

Comment

10,11-Dihydrocarbamazepine (DHC) is a recognized impurity in carbamazepine (CBZ), a dibenzazepine drug used to control seizures (Cyr *et al.*, 1987). DHC is known to crystallize in three polymorphic forms: monoclinic form I (Bandoli *et al.*, 1992), orthorhombic form II (Harrison *et al.*, 2006) and triclinic form III (Leech *et al.*, 2006). The title compound, (I), was produced during an automated parallel crystallization study (Florence, Johnston, Fernandes *et al.*, 2006) of DHC as part of a wider study into the predicted and experimental structures of CBZ (Florence, Johnston, Price *et al.*, 2006; Florence, Leech *et al.*, 2006). The sample was identified as a new form using multi-sample foil transmission X-ray powder diffraction analysis (Florence *et al.*, 2003). Subsequent manual recrystallization from a saturated acetic acid solution by slow evaporation at 298 K yielded single crystals of (I) suitable for X-ray diffraction.



(I)

The crystal structure of (I) is essentially isostructural with that of CBZ–acetic acid (1/1) (Fleischman *et al.*, 2003). Accordingly, it displays the same space group with very similar unit-cell parameters and packing arrangements. Specifically, the DHC and acetic acid molecules are connected *via* O2—H1···O1 and N2—H2N···O3 hydrogen bonds (Table 1) to form an $R_2^2(8)$ (Etter, 1990) dimer motif (Fig. 1). A third hydrogen bond, N2—H1N···O3^{i} [symmetry code (i) $1-x$, $1-y$, $-z$], joins adjacent dimers to form a centrosymmetric double motif arrangement (Fig. 2).

Experimental

Crystals of (I) were grown from a saturated acetic acid solution of 10,11-dihydrocarbamazepine by isothermal solvent evaporation at 298 K.

Crystal data

$C_{15}H_{14}N_2O\cdot C_2H_4O_2$
M_r = 298.33
Monoclinic, $P2_1/c$
a = 5.3104 (4) Å
b = 15.4246 (17) Å
c = 18.732 (2) Å
β = 95.106 (7)°
V = 1528.3 (3) Å^3
Z = 4
D_x = 1.297 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 123 (2) K
Needle, colourless
0.35 × 0.08 × 0.04 mm

Data collection

Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: none
10078 measured reflections
2652 independent reflections
1605 reflections with $I > 2\sigma(I)$
R_{int} = 0.103
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.147
S = 1.13
2652 reflections
212 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0421P)^2 + 0.9028P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H1···O1	1.03 (4)	1.53 (4)	2.547 (3)	167 (4)
N2—H1N···O3^{i}	0.88 (4)	2.20 (3)	2.894 (4)	136 (3)
N2—H2N···O3	0.95 (4)	2.04 (4)	2.970 (4)	164 (4)

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

H atoms bonded to N and O were located in difference maps and refined isotropically (distances are given in Table 1). All other H atoms were positioned geometrically and treated as riding with C—H = 0.95–0.99 Å, and with U_{iso}(H) = 1.2U_{eq}(C), or U_{iso}(H) = 1.5U_{eq}(C) for the methyl group.

Data collection: *COLLECT* (Hooft, 1988) and *DENZO* (Otwinowski & Minor, 1997); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

The authors thank the Basic Technology Programme of the UK Research Councils for funding this work under the project Control and Prediction of the Organic Solid State (http://www.cposs.org.uk).

References

Bandoli, G., Nicolini, M., Ongaro, A., Volpe, G. & Rubello, A. (1992). *J. Chem. Crystallogr.* **22**, 177–183.
Cyr, T. D., Matsui, F., Sears, R. W., Curran, N. M. & Lovering, E. G. (1987). *J. Assoc. Off. Anal. Chem.* **70**, 836–840.
Etter, M. C. (1990). *Acc. Chem. Res.* **23**, 120–126.
Fleischman, S. G., Kuduva, S. S., McMahon, J. A., Moulton, B., Walsh, R. D. B., Rodriguez-Hornedo, N. & Zaworotko, M. J. (2003). *Cryst. Growth Des.* **3**, 909–919.

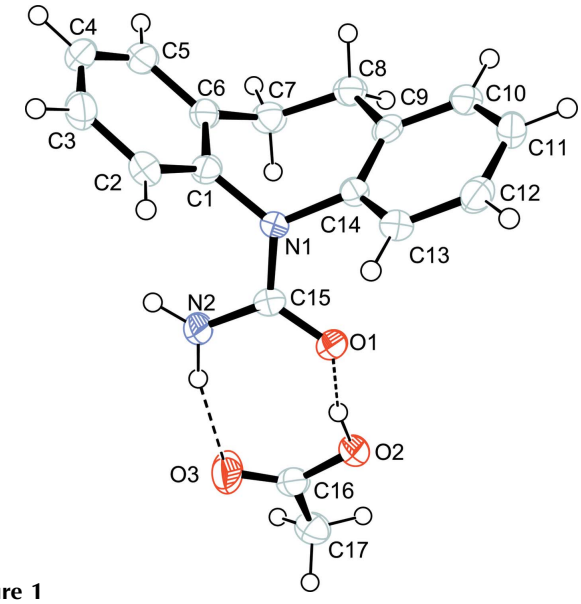


Figure 1
The asymmetric unit of (I), showing 50% probability displacement ellipsoids. Hydrogen bonds are shown as dashed lines.

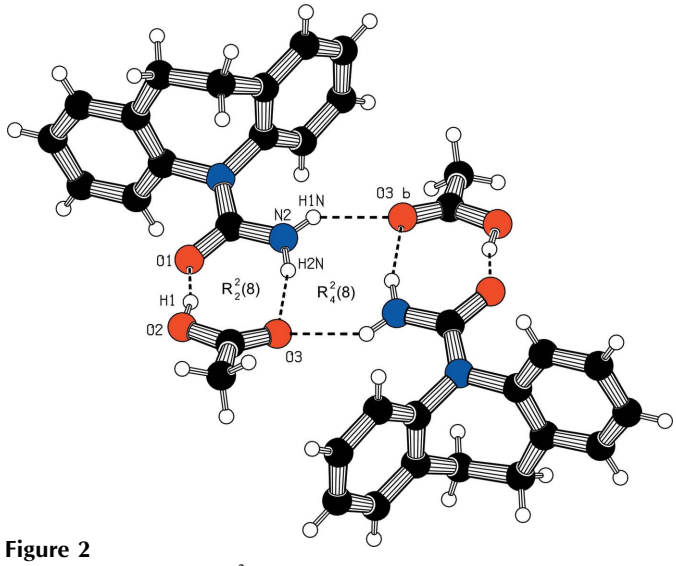


Figure 2
The hydrogen bonded $R_2^2(8)$ motifs of (I) joined in a centrosymmetric arrangement *via* an $R_4^2(8)$ motif. Hydrogen bonds are shown as dashed lines. [Symmetry code: (*b*) $1-x, 1-y, -z$.]

Florence, A. J., Baumgartner, B., Weston, C., Shankland, N., Kennedy, A. R., Shankland, K. & David, W. I. F. (2003). *J. Pharm. Sci.* **92**, 1930–1938.
Florence, A. J., Johnston, A., Fernandes, P., Shankland, N. & Shankland, K. (2006). *J. Appl. Cryst.* In the press.
Florence, A. J., Johnston, A., Price, S. L., Nowell, H., Shankland, N. & Kennedy, A. R. (2006). *J. Pharm. Sci.* **95**, 1918–1930.
Florence, A. J., Leech, C. K., Shankland, N., Shankland, K. & Johnston, A. (2006). *CrystEngComm*, **8**, 746–747.
Harrison, W. T. A., Yathirajan, H. S. & Anilkumar, H. G. (2006). *Acta Cryst.* C**62**, o240–o242.
Hooft, R. (1988). *COLLECT*. Nonius BV, Delft, The Netherlands.
Leech, C. K., Florence, A. J., Shankland, K., Shankland, N. & Johnston, A. (2006). *Acta Cryst.* E**62**. Submitted.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp 307–326. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supporting information

Acta Cryst. (2006). E**62**, o5361–o5362 [https://doi.org/10.1107/S1600536806044369]

10,11-Dihydrocarbamazepine–acetic acid (1/1)

Andrea Johnston, Alastair J. Florence, Philippe Fernandes, Norman Shankland and Alan R. Kennedy

10,11-dihydro-5*H*- dibenz[*b*,*f*]azepine-5-carboxamide–ethanoic acid (1/1)

Crystal data

$C_{15}H_{14}N_2O{\cdot}C_2H_4O_2$
$M_r = 298.33$
Monoclinic, $P2_1/c$
$a = 5.3104$ (4) Å
$b = 15.4246$ (17) Å
$c = 18.732$ (2) Å
$\beta = 95.106$ (7)°
$V = 1528.3$ (3) Å^3
$Z = 4$
$F(000) = 632$
$D_x = 1.297$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2544 reflections
$\theta = 1.0$–$25.0°$
$\mu = 0.09$ mm^{-1}
$T = 123$ K
Needle, colourless
0.35 × 0.08 × 0.04 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
10078 measured reflections
2652 independent reflections
1605 reflections with $I > 2\sigma(I)$
$R_{int} = 0.103$
$\theta_{max} = 25.0°$, $\theta_{min} = 3.4°$
$h = -6 \rightarrow 6$
$k = -18 \rightarrow 18$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.076$
$wR(F^2) = 0.147$
$S = 1.13$
2652 reflections
212 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0421P)^2 + 0.9028P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}

Special details

Experimental. Crystals desolvate on removal from solvent. Crystals shatter on contact with the cold-stream, data collected from shattered remains of a large needle.

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.8377 (4)	0.34174 (15)	0.13207 (12)	0.0352 (6)
N1	0.9605 (5)	0.27153 (17)	0.03492 (13)	0.0269 (7)
N2	0.7442 (6)	0.4022 (2)	0.02286 (18)	0.0389 (8)
C1	0.9582 (6)	0.2604 (2)	−0.04138 (17)	0.0283 (8)
C2	1.1325 (6)	0.3027 (2)	−0.07952 (18)	0.0338 (9)
H2	1.2500	0.3420	−0.0560	0.041*
C3	1.1349 (7)	0.2874 (2)	−0.15231 (19)	0.0396 (10)
H3	1.2547	0.3163	−0.1787	0.047*
C4	0.9643 (7)	0.2305 (2)	−0.18686 (19)	0.0401 (10)
H4	0.9675	0.2199	−0.2367	0.048*
C5	0.7880 (7)	0.1887 (2)	−0.14856 (18)	0.0381 (9)
H5	0.6695	0.1501	−0.1727	0.046*
C6	0.7827 (6)	0.2026 (2)	−0.07482 (17)	0.0300 (8)
C7	0.6026 (6)	0.1580 (2)	−0.02990 (18)	0.0359 (9)
H7A	0.4707	0.1288	−0.0620	0.043*
H7B	0.5179	0.2023	−0.0022	0.043*
C8	0.7257 (6)	0.0909 (2)	0.02226 (18)	0.0323 (9)
H8A	0.5933	0.0687	0.0515	0.039*
H8B	0.7807	0.0416	−0.0064	0.039*
C9	0.9487 (6)	0.1180 (2)	0.07306 (17)	0.0293 (8)
C10	1.0615 (7)	0.0537 (2)	0.11878 (18)	0.0339 (9)
H10	0.9928	−0.0032	0.1161	0.041*
C11	1.2663 (7)	0.0695 (2)	0.16708 (18)	0.0359 (9)
H11	1.3361	0.0243	0.1971	0.043*
C12	1.3711 (6)	0.1524 (2)	0.17175 (17)	0.0348 (9)
H12	1.5137	0.1642	0.2046	0.042*
C13	1.2646 (6)	0.2175 (2)	0.12785 (17)	0.0318 (9)
H13	1.3346	0.2742	0.1307	0.038*
C14	1.0568 (6)	0.2006 (2)	0.07973 (17)	0.0259 (8)
C15	0.8450 (6)	0.3395 (2)	0.06550 (18)	0.0302 (8)
O2	0.5016 (5)	0.41693 (15)	0.19878 (12)	0.0353 (6)
O3	0.4298 (5)	0.51232 (18)	0.10996 (14)	0.0588 (8)
C16	0.3724 (7)	0.4812 (2)	0.1662 (2)	0.0378 (9)

C17	0.1550 (7)	0.5111 (2)	0.2049 (2)	0.0425 (10)
H17A	0.1996	0.5655	0.2300	0.064*
H17B	0.1148	0.4670	0.2398	0.064*
H17C	0.0077	0.5206	0.1704	0.064*
H1N	0.748 (6)	0.405 (2)	−0.0237 (19)	0.034 (10)*
H2N	0.651 (7)	0.446 (3)	0.045 (2)	0.054 (12)*
H1	0.639 (7)	0.394 (3)	0.168 (2)	0.069 (13)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0502 (16)	0.0310 (14)	0.0239 (14)	0.0104 (12)	0.0007 (11)	−0.0023 (11)
N1	0.0389 (17)	0.0192 (15)	0.0227 (16)	0.0021 (13)	0.0026 (13)	−0.0008 (12)
N2	0.060 (2)	0.0302 (18)	0.0265 (19)	0.0166 (16)	0.0036 (16)	0.0037 (15)
C1	0.032 (2)	0.0286 (19)	0.025 (2)	0.0085 (16)	0.0036 (16)	−0.0005 (15)
C2	0.041 (2)	0.0265 (19)	0.034 (2)	0.0043 (17)	0.0023 (17)	0.0041 (16)
C3	0.049 (2)	0.036 (2)	0.036 (2)	0.0054 (19)	0.0129 (19)	0.0094 (18)
C4	0.060 (3)	0.037 (2)	0.023 (2)	0.013 (2)	0.0055 (19)	−0.0003 (18)
C5	0.054 (3)	0.030 (2)	0.028 (2)	0.0061 (18)	−0.0047 (18)	−0.0022 (17)
C6	0.036 (2)	0.027 (2)	0.026 (2)	0.0050 (16)	−0.0037 (16)	−0.0007 (15)
C7	0.039 (2)	0.033 (2)	0.035 (2)	−0.0004 (17)	−0.0015 (17)	−0.0048 (17)
C8	0.037 (2)	0.028 (2)	0.033 (2)	−0.0027 (16)	0.0076 (16)	−0.0039 (16)
C9	0.037 (2)	0.030 (2)	0.0217 (18)	−0.0002 (17)	0.0110 (16)	−0.0035 (15)
C10	0.049 (2)	0.025 (2)	0.029 (2)	−0.0012 (17)	0.0092 (18)	−0.0013 (16)
C11	0.047 (2)	0.035 (2)	0.026 (2)	0.0090 (19)	0.0043 (17)	0.0059 (17)
C12	0.037 (2)	0.042 (2)	0.0250 (19)	0.0036 (18)	0.0008 (16)	−0.0018 (18)
C13	0.042 (2)	0.0252 (19)	0.029 (2)	0.0006 (17)	0.0040 (17)	−0.0022 (16)
C14	0.031 (2)	0.0233 (19)	0.0239 (18)	0.0027 (15)	0.0064 (15)	0.0007 (15)
C15	0.039 (2)	0.0253 (19)	0.026 (2)	−0.0005 (17)	0.0006 (16)	−0.0044 (17)
O2	0.0461 (16)	0.0282 (14)	0.0317 (14)	0.0075 (12)	0.0035 (12)	0.0018 (12)
O3	0.089 (2)	0.0520 (19)	0.0378 (17)	0.0340 (16)	0.0187 (15)	0.0141 (14)
C16	0.050 (2)	0.030 (2)	0.032 (2)	0.0059 (19)	−0.0056 (18)	−0.0054 (18)
C17	0.048 (2)	0.034 (2)	0.045 (2)	0.0091 (19)	0.0025 (19)	−0.0023 (19)

Geometric parameters (Å, º)

O1—C15	1.252 (4)	C8—C9	1.510 (4)
N1—C15	1.366 (4)	C8—H8A	0.9900
N1—C1	1.439 (4)	C8—H8B	0.9900
N1—C14	1.445 (4)	C9—C14	1.398 (4)
N2—C15	1.335 (4)	C9—C10	1.409 (5)
N2—H1N	0.88 (3)	C10—C11	1.373 (5)
N2—H2N	0.95 (4)	C10—H10	0.9500
C1—C2	1.383 (4)	C11—C12	1.395 (5)
C1—C6	1.397 (4)	C11—H11	0.9500
C2—C3	1.385 (5)	C12—C13	1.385 (5)
C2—H2	0.9500	C12—H12	0.9500
C3—C4	1.381 (5)	C13—C14	1.386 (4)

C3—H3	0.9500	C13—H13	0.9500
C4—C5	1.388 (5)	O2—C16	1.324 (4)
C4—H4	0.9500	O2—H1	1.03 (4)
C5—C6	1.401 (5)	O3—C16	1.221 (4)
C5—H5	0.9500	C16—C17	1.489 (5)
C6—C7	1.497 (5)	C17—H17A	0.9800
C7—C8	1.530 (5)	C17—H17B	0.9800
C7—H7A	0.9900	C17—H17C	0.9800
C7—H7B	0.9900		

C15—N1—C1	122.9 (3)	C7—C8—H8B	107.6
C15—N1—C14	119.1 (3)	H8A—C8—H8B	107.0
C1—N1—C14	117.3 (3)	C14—C9—C10	116.0 (3)
C15—N2—H1N	126 (2)	C14—C9—C8	127.0 (3)
C15—N2—H2N	117 (2)	C10—C9—C8	117.1 (3)
H1N—N2—H2N	117 (3)	C11—C10—C9	123.0 (3)
C2—C1—C6	121.3 (3)	C11—C10—H10	118.5
C2—C1—N1	120.7 (3)	C9—C10—H10	118.5
C6—C1—N1	117.9 (3)	C10—C11—C12	119.5 (3)
C1—C2—C3	119.6 (3)	C10—C11—H11	120.2
C1—C2—H2	120.2	C12—C11—H11	120.2
C3—C2—H2	120.2	C13—C12—C11	119.2 (3)
C4—C3—C2	120.5 (3)	C13—C12—H12	120.4
C4—C3—H3	119.8	C11—C12—H12	120.4
C2—C3—H3	119.8	C12—C13—C14	120.6 (3)
C3—C4—C5	119.9 (3)	C12—C13—H13	119.7
C3—C4—H4	120.1	C14—C13—H13	119.7
C5—C4—H4	120.1	C13—C14—C9	121.8 (3)
C4—C5—C6	120.8 (3)	C13—C14—N1	117.1 (3)
C4—C5—H5	119.6	C9—C14—N1	121.1 (3)
C6—C5—H5	119.6	O1—C15—N2	122.0 (3)
C1—C6—C5	118.0 (3)	O1—C15—N1	119.6 (3)
C1—C6—C7	118.4 (3)	N2—C15—N1	118.4 (3)
C5—C6—C7	123.6 (3)	C16—O2—H1	111 (2)
C6—C7—C8	114.3 (3)	O3—C16—O2	122.2 (3)
C6—C7—H7A	108.7	O3—C16—C17	124.2 (3)
C8—C7—H7A	108.7	O2—C16—C17	113.6 (3)
C6—C7—H7B	108.7	C16—C17—H17A	109.5
C8—C7—H7B	108.7	C16—C17—H17B	109.5
H7A—C7—H7B	107.6	H17A—C17—H17B	109.5
C9—C8—C7	118.8 (3)	C16—C17—H17C	109.5
C9—C8—H8A	107.6	H17A—C17—H17C	109.5
C7—C8—H8A	107.6	H17B—C17—H17C	109.5
C9—C8—H8B	107.6		

C15—N1—C1—C2	83.9 (4)	C14—C9—C10—C11	−0.4 (5)
C14—N1—C1—C2	−105.5 (3)	C8—C9—C10—C11	179.5 (3)
C15—N1—C1—C6	−99.1 (4)	C9—C10—C11—C12	−0.3 (5)

C14—N1—C1—C6	71.4 (4)	C10—C11—C12—C13	0.5 (5)
C6—C1—C2—C3	−0.3 (5)	C11—C12—C13—C14	−0.1 (5)
N1—C1—C2—C3	176.6 (3)	C12—C13—C14—C9	−0.6 (5)
C1—C2—C3—C4	0.1 (5)	C12—C13—C14—N1	−178.8 (3)
C2—C3—C4—C5	0.4 (5)	C10—C9—C14—C13	0.8 (5)
C3—C4—C5—C6	−0.8 (5)	C8—C9—C14—C13	−179.0 (3)
C2—C1—C6—C5	−0.1 (5)	C10—C9—C14—N1	178.9 (3)
N1—C1—C6—C5	−177.1 (3)	C8—C9—C14—N1	−0.9 (5)
C2—C1—C6—C7	178.9 (3)	C15—N1—C14—C13	−69.1 (4)
N1—C1—C6—C7	2.0 (4)	C1—N1—C14—C13	120.0 (3)
C4—C5—C6—C1	0.7 (5)	C15—N1—C14—C9	112.7 (4)
C4—C5—C6—C7	−178.3 (3)	C1—N1—C14—C9	−58.2 (4)
C1—C6—C7—C8	−69.5 (4)	C1—N1—C15—O1	174.6 (3)
C5—C6—C7—C8	109.5 (4)	C14—N1—C15—O1	4.2 (5)
C6—C7—C8—C9	53.4 (4)	C1—N1—C15—N2	−5.8 (5)
C7—C8—C9—C14	1.7 (5)	C14—N1—C15—N2	−176.2 (3)
C7—C8—C9—C10	−178.2 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1···O1	1.03 (4)	1.53 (4)	2.547 (3)	167 (4)
N2—H1*N*···O3^{i}	0.88 (4)	2.20 (3)	2.894 (4)	136 (3)
N2—H2*N*···O3	0.95 (4)	2.04 (4)	2.970 (4)	164 (4)

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