

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

5ba,6,7,13ba,14,15-Hexahydroacridino-[4,3-c]acridine

Jason Ashmore, Roger Bishop, Donald C. Craig and Marcia L. Scudder*

School of Chemistry, University of New South Wales, Sydney 2052, Australia
Correspondence e-mail: m.scudder@unsw.edu.au

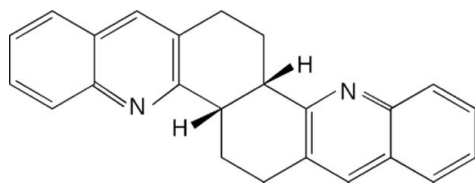
Received 3 May 2008; accepted 16 May 2008

Key indicators: single-crystal X-ray study; $T = 294$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.048; wR factor = 0.059; data-to-parameter ratio = 11.7.

The racemic title compound, $\text{C}_{24}\text{H}_{20}\text{N}_2$, gives spontaneous resolution with the formation of conglomerate crystals in the space group $P2_12_12_1$ when crystallized from ethyl acetate. The twisted molecules pack in parallel regions (ab plane) which then form a herringbone pattern along c .

Related literature

Condensation of two equivalents of 2-aminobenzaldehyde with one of *cis*-bicyclo[4.4.0]decane-2,7-dione affords the title compound by means of Friedländer condensation (Cheng & Yan, 1982). Substituted derivatives of molecules of this general V-shaped type frequently show inclusion properties (Bishop, 2006). For related literature, see: Collet *et al.* (1980); Jacques *et al.* (1981); Marjo *et al.* (1997); Peet & Cargill (1973); Smith & Opie (1955).



Experimental

Crystal data

 $\text{C}_{24}\text{H}_{20}\text{N}_2$ $M_r = 336.4$ Orthorhombic, $P2_12_12_1$
 $a = 8.863$ (3) Å
 $b = 9.759$ (4) Å
 $c = 20.071$ (8) Å
 $V = 1736$ (1) Å³ $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.07$ mm⁻¹
 $T = 294$ K
 $0.29 \times 0.27 \times 0.03$ mm

Data collection

Enraf–Nonius CAD-4
diffractometer
Absorption correction: none
1100 measured reflections
1100 independent reflections737 reflections with $I > 2\sigma(I)$
 $\theta_{\text{max}} = 21^\circ$
1 standard reflection
frequency: 30 min
intensity decay: none

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.059$
 $S = 1.64$
1100 reflections94 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.26$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.42$ e Å⁻³

Data collection: *CAD-4 Manual* (Schagen *et al.*, 1989); cell refinement: *CAD-4 Manual*; data reduction: local program; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *RAELS* (Rae, 2000); molecular graphics: *ORTEPII* (Johnson, 1976) and *CrystalMaker* (CrystalMaker, 2005); software used to prepare material for publication: local programs.

This research was supported by the UNSW Faculty Research Grants Program.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2079).

References

- Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Bishop, R. (2006). *Crystal Engineering of Halogenated Heteroaromatic Clathrate Systems*, in *Frontiers in Crystal Engineering*, edited by E. R. T. Tiekink & J. J. Vittal, ch. 5, pp. 91–116. Chichester: Wiley.
Cheng, C.-C. & Yan, S.-J. (1982). *Org. React.* **28**, 37–201.
Collet, A., Brienne, M.-J. & Jacques, J. (1980). *Chem. Rev.* **80**, 215–230.
CrystalMaker (2005). *CrystalMaker*. CrystalMaker Software Ltd, Yarnton, Oxfordshire, England. www.CrystalMaker.co.uk.
Jacques, J., Collet, A. & Wilen, S. H. (1981). *Enantiomers, Racemates, and Resolutions*. New York: Wiley.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Marjo, C. E., Scudder, M. L., Craig, D. C. & Bishop, R. (1997). *J. Chem. Soc., Perkin Trans. 2*, pp. 2099–2104.
Peet, N. P. & Cargill, R. G. (1973). *J. Org. Chem.* **38**, 4281–4285.
Rae, A. D. (2000). *RAELS*. Australian National University.
Schagen, J. D., Straver, L., van Meurs, F. & Williams, G. (1989). *CAD-4 Manual*. Enraf–Nonius, Delft, The Netherlands.
Smith, L. I. & Opie, J. W. (1955). *Org. Synth. Coll.* **3**, 56–58.

supporting information

Acta Cryst. (2008). E64, o1136 [doi:10.1107/S1600536808014803]

5b α ,6,7,13b α ,14,15-Hexahydroacridino[4,3-*c*]acridine

Jason Ashmore, Roger Bishop, Donald C. Craig and Marcia L. Scudder

S1. Comment

The title compound was prepared as racemic material by Friedländer condensation (Cheng & Yan, 1982), but the crystallization process resulted in self-resolution and formation of a conglomerate (Collet *et al.*, 1980; Jacques *et al.*, 1981) (Fig 1). The two aromatic extremities of the molecule are essentially planar but are not coplanar, instead they exhibit a relative twist with the angle between the normals to the planes of 29.5 (2)°. These awkwardly shaped molecules pack in parallel regions in the *ab* plane. These regions then interact in herringbone fashion along *c* (Fig 2). Within the *ab* plane, molecules take part in edge-face aromatic interactions with H $\cdots\pi$ distance of about 3.4 Å. Because of the twisted nature of the molecule, it is not possible for them to take part in edge-edge C—H \cdots N interactions that we have previously observed (Marjo *et al.*, 1997). The crystals do not exhibit solvent inclusion, in contrast to other derivatives, which are V-shaped (Bishop, 2006).

S2. Experimental

Racemic *cis*-bicyclo[4.4.0]decane-2,7-dione (Peet & Cargill, 1973) (0.54 g, 3.25 mmol) and 2-aminobenzaldehyde (Smith & Opie, 1955) (0.88 g, 7.26 mmol) were dissolved in methanol (15 mL) with heating. To the cooled solution was added sodium hydroxide solution (2M; 2.5 mL) and the mixture stirred at rt for 2 days. The solid precipitate was filtered, and then recrystallised from ethyl acetate to yield the title compound (0.63 g, 58%) as pale yellow plates. ¹³C NMR (75.5 MHz, CDCl₃) δ : 27.9 (CH₂), 29.5 (CH₂), 42.7 (CH), 126.2 (CH), 127.3 (CH), 127.6 (C), 128.7 (CH), 128.9 (CH), 130.4 (C), 135.6 (CH), 147.5 (C), 161.4 (C); ¹H NMR (300 MHz, CDCl₃) δ : 2.09-2.23 (m, 2H), 2.45-2.50 (m, 2H), 3.07-3.16 (m, 2H), 3.23-3.34 (m, 2H), 3.70 (d, *J* = 9.6 Hz, 2H), 7.44-7.49 (m, 2H), 7.61-7.65 (m, 2H), 7.74 (d, *J* = 8.3 Hz, 2H), 7.86-7.90 (m, 2H), 8.05 (d, *J* = 8.7 Hz, 2H). X-ray quality crystals were obtained from ethyl acetate solution. The identical product is obtained if *trans*-bicyclo[4.4.0]decane-2,7-dione is used but the reaction takes longer.

S3. Refinement

Hydrogen atoms attached to C were included at calculated positions (C—H = 1.0 Å) and were refined with isotropic thermal parameters equivalent to those of the atom to which they were bonded.

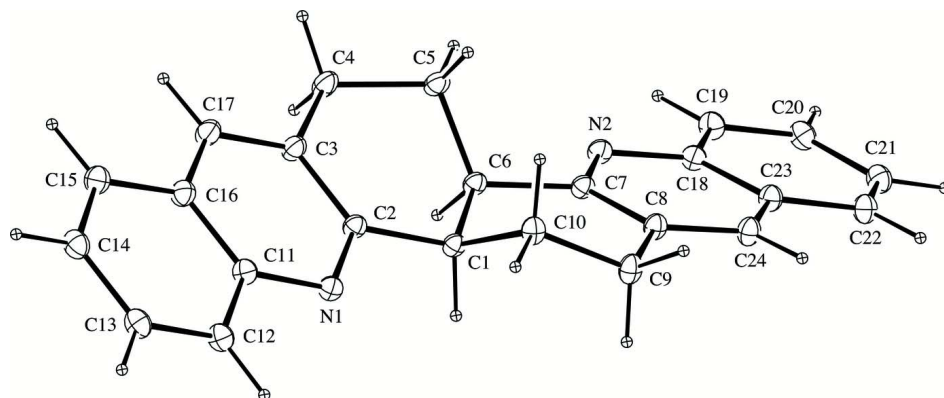


Figure 1

Molecular structure of the compound, with ellipsoids drawn at 30% probability level.

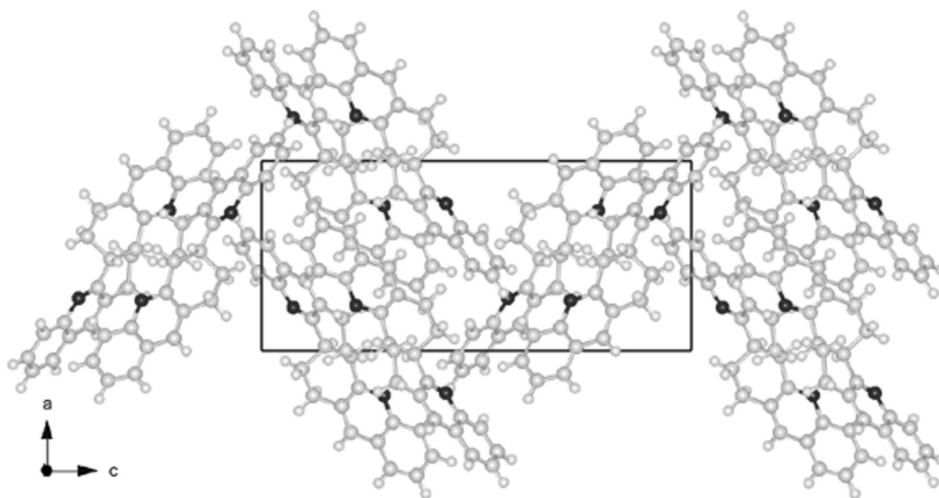


Figure 2

Cell diagram showing the parallel regions (in the *ab* plane) which pack in a herringbone pattern.

5ba,6,7,13ba,14,15-Hexahydroacridino[4,3-c]acridine

Crystal data

$C_{24}H_{20}N_2$

$M_r = 336.4$

Orthorhombic, $P2_12_12_1$

$a = 8.863$ (3) Å

$b = 9.759$ (4) Å

$c = 20.071$ (8) Å

$V = 1736$ (1) Å³

$Z = 4$

$F(000) = 712.0$

$D_x = 1.29$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 11 reflections

$\theta = 10\text{--}11^\circ$

$\mu = 0.08$ mm⁻¹

$T = 294$ K

Plate, colourless

$0.29 \times 0.27 \times 0.03$ mm

Data collection

Enraf–Nonius CAD-4

diffractometer

ω - 2θ scans

1100 measured reflections

1100 independent reflections

737 reflections with $I > 2\sigma(I)$

$\theta_{\max} = 21^\circ$

$h = 0 \rightarrow 8$

$k = 0 \rightarrow 9$
 $l = 0 \rightarrow 20$

1 standard reflections every 30 min
 intensity decay: none

Refinement

Refinement on F
 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.059$
 $S = 1.64$
 1100 reflections
 94 parameters

0 restraints
 H-atom parameters constrained
 $w = 1/[\sigma^2(F) + 0.0004F^2]$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.26 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.42 \text{ e } \text{\AA}^{-3}$

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

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-------|-------------|------------|------------|----------------------------------|
| N1 | -0.2254 (5) | 0.4393 (4) | 0.4278 (2) | 0.0464 (9) |
| N2 | 0.2369 (5) | 0.5930 (4) | 0.2179 (2) | 0.0470 (7) |
| C1 | -0.0205 (6) | 0.4796 (5) | 0.3538 (3) | 0.0427 (9) |
| C2 | -0.1687 (6) | 0.5253 (6) | 0.3840 (3) | 0.0442 (8) |
| C3 | -0.2383 (6) | 0.6509 (6) | 0.3667 (3) | 0.0517 (6) |
| C4 | -0.1694 (6) | 0.7391 (5) | 0.3130 (3) | 0.060 (1) |
| C5 | 0.0008 (6) | 0.7137 (5) | 0.3058 (3) | 0.0535 (6) |
| C6 | 0.0323 (6) | 0.5681 (5) | 0.2944 (3) | 0.0438 (8) |
| C7 | 0.1968 (6) | 0.5402 (5) | 0.2756 (3) | 0.0435 (8) |
| C8 | 0.2927 (6) | 0.4617 (6) | 0.3160 (3) | 0.0478 (8) |
| C9 | 0.2386 (7) | 0.3999 (6) | 0.3811 (3) | 0.055 (1) |
| C10 | 0.0995 (6) | 0.4728 (6) | 0.4075 (2) | 0.0500 (9) |
| C11 | -0.3538 (6) | 0.4784 (6) | 0.4617 (3) | 0.0491 (9) |
| C12 | -0.4120 (7) | 0.3867 (6) | 0.5090 (3) | 0.055 (1) |
| C13 | -0.5368 (6) | 0.4207 (6) | 0.5461 (3) | 0.059 (1) |
| C14 | -0.6080 (7) | 0.5469 (6) | 0.5353 (3) | 0.061 (1) |
| C15 | -0.5551 (7) | 0.6374 (6) | 0.4883 (3) | 0.062 (1) |
| C16 | -0.4254 (7) | 0.6036 (5) | 0.4505 (3) | 0.0541 (7) |
| C17 | -0.3670 (7) | 0.6883 (6) | 0.4001 (3) | 0.0587 (9) |
| C18 | 0.3795 (6) | 0.5649 (5) | 0.1950 (3) | 0.0481 (7) |
| C19 | 0.4207 (7) | 0.6142 (6) | 0.1309 (3) | 0.0553 (9) |
| C20 | 0.5578 (7) | 0.5824 (6) | 0.1045 (3) | 0.058 (1) |
| C21 | 0.6593 (6) | 0.4985 (6) | 0.1403 (3) | 0.057 (1) |
| C22 | 0.6250 (7) | 0.4515 (6) | 0.2028 (3) | 0.057 (1) |
| C23 | 0.4821 (6) | 0.4854 (6) | 0.2310 (3) | 0.0502 (8) |
| C24 | 0.4353 (6) | 0.4356 (6) | 0.2941 (3) | 0.053 (1) |
| HC1 | -0.0355 | 0.3843 | 0.3367 | 0.045 |
| H1C4 | -0.1862 | 0.8376 | 0.3246 | 0.074 |
| H2C4 | -0.2198 | 0.7180 | 0.2696 | 0.065 |
| H1C5 | 0.0530 | 0.7439 | 0.3474 | 0.057 |
| H2C5 | 0.0397 | 0.7679 | 0.2671 | 0.061 |
| HC6 | -0.0302 | 0.5398 | 0.2553 | 0.047 |
| H1C9 | 0.3212 | 0.4072 | 0.4149 | 0.066 |
| H2C9 | 0.2136 | 0.3011 | 0.3736 | 0.060 |
| H1C10 | 0.1275 | 0.5679 | 0.4214 | 0.054 |

| | | | | |
|-------|---------|--------|--------|-------|
| H2C10 | 0.0591 | 0.4215 | 0.4468 | 0.056 |
| HC12 | -0.3622 | 0.2958 | 0.5159 | 0.062 |
| HC13 | -0.5765 | 0.3559 | 0.5804 | 0.066 |
| HC14 | -0.6987 | 0.5716 | 0.5624 | 0.067 |
| HC15 | -0.6080 | 0.7266 | 0.4808 | 0.073 |
| HC17 | -0.4193 | 0.7760 | 0.3886 | 0.072 |
| HC19 | 0.3487 | 0.6726 | 0.1051 | 0.064 |
| HC20 | 0.5867 | 0.6184 | 0.0596 | 0.065 |
| HC21 | 0.7581 | 0.4731 | 0.1197 | 0.062 |
| HC22 | 0.6988 | 0.3943 | 0.2282 | 0.066 |
| HC24 | 0.5066 | 0.3815 | 0.3224 | 0.065 |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|------------|------------|------------|-------------|-------------|-------------|
| N1 | 0.0488 (6) | 0.048 (1) | 0.0427 (8) | 0.0013 (6) | 0.0019 (6) | 0.0061 (6) |
| N2 | 0.0502 (7) | 0.047 (1) | 0.0444 (9) | 0.0024 (6) | 0.0029 (7) | 0.0088 (7) |
| C1 | 0.0464 (7) | 0.041 (1) | 0.0409 (9) | 0.0038 (7) | 0.0000 (6) | 0.0070 (8) |
| C2 | 0.0470 (7) | 0.043 (1) | 0.0429 (9) | 0.0032 (6) | 0.0012 (7) | 0.0052 (7) |
| C3 | 0.0523 (7) | 0.0458 (8) | 0.057 (1) | 0.0085 (8) | 0.0076 (7) | 0.0085 (9) |
| C4 | 0.061 (1) | 0.049 (1) | 0.072 (2) | 0.015 (1) | 0.015 (1) | 0.019 (2) |
| C5 | 0.058 (1) | 0.0405 (9) | 0.062 (1) | 0.0067 (8) | 0.0120 (9) | 0.0108 (9) |
| C6 | 0.0476 (7) | 0.041 (1) | 0.0431 (9) | 0.0047 (7) | 0.0011 (7) | 0.0084 (8) |
| C7 | 0.0470 (7) | 0.042 (1) | 0.0418 (9) | 0.0028 (6) | 0.0007 (7) | 0.0061 (7) |
| C8 | 0.0464 (7) | 0.053 (1) | 0.0440 (8) | 0.0058 (6) | 0.0002 (6) | 0.0085 (7) |
| C9 | 0.0490 (7) | 0.068 (2) | 0.0476 (9) | 0.0108 (8) | 0.0007 (7) | 0.0178 (8) |
| C10 | 0.0475 (7) | 0.061 (2) | 0.041 (1) | 0.0037 (7) | -0.0006 (7) | 0.0095 (7) |
| C11 | 0.0493 (7) | 0.054 (1) | 0.0445 (9) | -0.0010 (6) | 0.0033 (6) | 0.0019 (6) |
| C12 | 0.0547 (9) | 0.064 (2) | 0.047 (1) | -0.0039 (9) | 0.0065 (9) | 0.0055 (8) |
| C13 | 0.055 (1) | 0.074 (2) | 0.049 (1) | -0.008 (1) | 0.008 (1) | -0.001 (1) |
| C14 | 0.053 (1) | 0.073 (2) | 0.056 (2) | -0.006 (1) | 0.010 (1) | -0.010 (1) |
| C15 | 0.055 (1) | 0.065 (2) | 0.067 (2) | 0.002 (1) | 0.014 (1) | -0.005 (1) |
| C16 | 0.0513 (8) | 0.0549 (9) | 0.056 (1) | 0.0030 (8) | 0.0080 (8) | -0.0006 (9) |
| C17 | 0.0559 (9) | 0.0520 (9) | 0.068 (2) | 0.011 (1) | 0.013 (1) | 0.007 (1) |
| C18 | 0.0497 (7) | 0.050 (1) | 0.0442 (9) | -0.0004 (6) | 0.0032 (7) | 0.0044 (6) |
| C19 | 0.055 (1) | 0.064 (2) | 0.047 (1) | -0.0023 (9) | 0.006 (1) | 0.009 (1) |
| C20 | 0.055 (1) | 0.070 (2) | 0.048 (1) | -0.007 (1) | 0.007 (1) | 0.001 (1) |
| C21 | 0.0507 (8) | 0.068 (2) | 0.052 (1) | -0.0038 (8) | 0.0070 (9) | -0.005 (1) |
| C22 | 0.0484 (7) | 0.068 (2) | 0.054 (1) | 0.0035 (7) | 0.0051 (7) | 0.001 (1) |
| C23 | 0.0473 (7) | 0.056 (1) | 0.0470 (8) | 0.0025 (6) | 0.0025 (6) | 0.0027 (7) |
| C24 | 0.0471 (7) | 0.064 (2) | 0.0490 (8) | 0.0082 (6) | 0.0015 (6) | 0.0097 (7) |

Geometric parameters (Å, °)

| | | | |
|--------|-----------|-----------|-----------|
| N1—C2 | 1.316 (6) | C10—H2C10 | 1.000 |
| N1—C11 | 1.378 (6) | C11—C12 | 1.404 (7) |
| N2—C7 | 1.316 (6) | C11—C16 | 1.395 (7) |
| N2—C18 | 1.373 (6) | C12—C13 | 1.373 (7) |

| | | | |
|--------------|-----------|-----------------|-----------|
| C1—C2 | 1.514 (7) | C12—HC12 | 1.000 |
| C1—C6 | 1.544 (7) | C13—C14 | 1.400 (8) |
| C1—C10 | 1.516 (6) | C13—HC13 | 1.000 |
| C1—HC1 | 1.000 | C14—C15 | 1.376 (7) |
| C2—C3 | 1.415 (7) | C14—HC14 | 1.000 |
| C3—C4 | 1.508 (7) | C15—C16 | 1.417 (7) |
| C3—C17 | 1.373 (7) | C15—HC15 | 1.000 |
| C4—C5 | 1.536 (7) | C16—C17 | 1.405 (7) |
| C4—H1C4 | 1.000 | C17—HC17 | 1.000 |
| C4—H2C4 | 1.000 | C18—C19 | 1.422 (7) |
| C5—C6 | 1.466 (7) | C18—C23 | 1.397 (7) |
| C5—H1C5 | 1.000 | C19—C20 | 1.362 (7) |
| C5—H2C5 | 1.000 | C19—HC19 | 1.000 |
| C6—C7 | 1.531 (7) | C20—C21 | 1.413 (7) |
| C6—HC6 | 1.000 | C20—HC20 | 1.000 |
| C7—C8 | 1.403 (6) | C21—C22 | 1.370 (7) |
| C8—C9 | 1.517 (7) | C21—HC21 | 1.000 |
| C8—C24 | 1.362 (7) | C22—C23 | 1.426 (7) |
| C9—C10 | 1.519 (8) | C22—HC22 | 1.000 |
| C9—H1C9 | 1.000 | C23—C24 | 1.418 (7) |
| C9—H2C9 | 1.000 | C24—HC24 | 1.000 |
| C10—H1C10 | 1.000 | | |
| | | | |
| C2—N1—C11 | 117.9 (5) | C1—C10—H2C10 | 109.3 |
| C7—N2—C18 | 117.7 (5) | C9—C10—H1C10 | 109.3 |
| C2—C1—C6 | 114.0 (4) | C9—C10—H2C10 | 109.3 |
| C2—C1—C10 | 109.7 (4) | H1C10—C10—H2C10 | 109.5 |
| C2—C1—HC1 | 107.2 | N1—C11—C12 | 117.4 (5) |
| C6—C1—C10 | 111.1 (4) | N1—C11—C16 | 122.5 (5) |
| C6—C1—HC1 | 107.2 | C12—C11—C16 | 120.0 (5) |
| C10—C1—HC1 | 107.2 | C11—C12—C13 | 120.5 (6) |
| N1—C2—C1 | 114.3 (5) | C11—C12—HC12 | 119.7 |
| N1—C2—C3 | 123.3 (5) | C13—C12—HC12 | 119.7 |
| C1—C2—C3 | 122.3 (5) | C12—C13—C14 | 119.5 (6) |
| C2—C3—C4 | 119.6 (5) | C12—C13—HC13 | 120.2 |
| C2—C3—C17 | 118.2 (5) | C14—C13—HC13 | 120.2 |
| C4—C3—C17 | 122.2 (5) | C13—C14—C15 | 121.1 (5) |
| C3—C4—C5 | 111.9 (5) | C13—C14—HC14 | 119.4 |
| C3—C4—H1C4 | 108.8 | C15—C14—HC14 | 119.4 |
| C3—C4—H2C4 | 108.8 | C14—C15—C16 | 119.6 (6) |
| C5—C4—H1C4 | 108.8 | C14—C15—HC15 | 120.2 |
| C5—C4—H2C4 | 108.8 | C16—C15—HC15 | 120.2 |
| H1C4—C4—H2C4 | 109.5 | C11—C16—C15 | 119.1 (5) |
| C4—C5—C6 | 110.9 (5) | C11—C16—C17 | 117.7 (5) |
| C4—C5—H1C5 | 109.1 | C15—C16—C17 | 123.2 (5) |
| C4—C5—H2C5 | 109.1 | C3—C17—C16 | 120.1 (5) |
| C6—C5—H1C5 | 109.1 | C3—C17—HC17 | 120.0 |
| C6—C5—H2C5 | 109.1 | C16—C17—HC17 | 120.0 |

| | | | |
|-----------------|------------|-------------------|------------|
| H1C5—C5—H2C5 | 109.5 | N2—C18—C19 | 118.1 (5) |
| C1—C6—C5 | 111.4 (5) | N2—C18—C23 | 122.5 (5) |
| C1—C6—C7 | 112.3 (4) | C19—C18—C23 | 119.3 (6) |
| C1—C6—HC6 | 106.5 | C18—C19—C20 | 120.3 (6) |
| C5—C6—C7 | 113.0 (5) | C18—C19—HC19 | 119.8 |
| C5—C6—HC6 | 106.5 | C20—C19—HC19 | 119.8 |
| C7—C6—HC6 | 106.5 | C19—C20—C21 | 120.1 (5) |
| N2—C7—C6 | 113.9 (5) | C19—C20—HC20 | 119.9 |
| N2—C7—C8 | 124.0 (5) | C21—C20—HC20 | 119.9 |
| C6—C7—C8 | 122.1 (5) | C20—C21—C22 | 121.2 (6) |
| C7—C8—C9 | 121.6 (5) | C20—C21—HC21 | 119.4 |
| C7—C8—C24 | 118.6 (5) | C22—C21—HC21 | 119.4 |
| C9—C8—C24 | 119.8 (5) | C21—C22—C23 | 118.9 (6) |
| C8—C9—C10 | 111.8 (5) | C21—C22—HC22 | 120.5 |
| C8—C9—H1C9 | 108.9 | C23—C22—HC22 | 120.5 |
| C8—C9—H2C9 | 108.9 | C18—C23—C22 | 120.1 (5) |
| C10—C9—H1C9 | 108.9 | C18—C23—C24 | 117.5 (5) |
| C10—C9—H2C9 | 108.9 | C22—C23—C24 | 122.4 (5) |
| H1C9—C9—H2C9 | 109.5 | C8—C24—C23 | 119.7 (5) |
| C1—C10—C9 | 110.0 (4) | C8—C24—HC24 | 120.2 |
| C1—C10—H1C10 | 109.3 | C23—C24—HC24 | 120.2 |
| | | | |
| C11—N1—C2—C1 | 174.9 (4) | C7—C8—C9—H1C9 | -141.1 |
| C11—N1—C2—C3 | -4.6 (7) | C7—C8—C9—H2C9 | 99.6 |
| C2—N1—C11—C12 | -179.0 (5) | C24—C8—C9—C10 | 162.6 (5) |
| C2—N1—C11—C16 | 0.9 (7) | C24—C8—C9—H1C9 | 42.3 |
| C18—N2—C7—C6 | -175.6 (4) | C24—C8—C9—H2C9 | -77.1 |
| C18—N2—C7—C8 | 2.6 (7) | C7—C8—C24—C23 | -1.2 (8) |
| C7—N2—C18—C19 | 176.1 (5) | C7—C8—C24—HC24 | 178.8 |
| C7—N2—C18—C23 | -1.1 (7) | C9—C8—C24—C23 | 175.6 (5) |
| C6—C1—C2—N1 | 170.4 (4) | C9—C8—C24—HC24 | -4.4 |
| C6—C1—C2—C3 | -10.1 (7) | C8—C9—C10—C1 | 52.2 (6) |
| C10—C1—C2—N1 | -64.2 (6) | C8—C9—C10—H1C10 | -67.9 |
| C10—C1—C2—C3 | 115.2 (6) | C8—C9—C10—H2C10 | 172.3 |
| HC1—C1—C2—N1 | 51.9 | H1C9—C9—C10—C1 | 172.6 |
| HC1—C1—C2—C3 | -128.6 | H1C9—C9—C10—H1C10 | 52.5 |
| C2—C1—C6—C5 | 38.9 (6) | H1C9—C9—C10—H2C10 | -67.4 |
| C2—C1—C6—C7 | 166.9 (4) | H2C9—C9—C10—C1 | -68.1 |
| C2—C1—C6—HC6 | -76.8 | H2C9—C9—C10—H1C10 | 171.8 |
| C10—C1—C6—C5 | -85.6 (6) | H2C9—C9—C10—H2C10 | 52.0 |
| C10—C1—C6—C7 | 42.4 (6) | N1—C11—C12—C13 | 178.0 (5) |
| C10—C1—C6—HC6 | 158.6 | N1—C11—C12—HC12 | -2.0 |
| HC1—C1—C6—C5 | 157.5 | C16—C11—C12—C13 | -1.9 (8) |
| HC1—C1—C6—C7 | -74.5 | C16—C11—C12—HC12 | 178.1 |
| HC1—C1—C6—HC6 | 41.7 | N1—C11—C16—C15 | -178.7 (5) |
| C2—C1—C10—C9 | 168.5 (5) | N1—C11—C16—C17 | 3.4 (8) |
| C2—C1—C10—H1C10 | -71.5 | C12—C11—C16—C15 | 1.2 (8) |
| C2—C1—C10—H2C10 | 48.4 | C12—C11—C16—C17 | -176.7 (5) |

| | | | |
|------------------|------------|-------------------|------------|
| C6—C1—C10—C9 | -64.6 (6) | C11—C12—C13—C14 | 1.3 (8) |
| C6—C1—C10—H1C10 | 55.5 | C11—C12—C13—HC13 | -178.7 |
| C6—C1—C10—H2C10 | 175.3 | HC12—C12—C13—C14 | -178.7 |
| HC1—C1—C10—C9 | 52.3 | HC12—C12—C13—HC13 | 1.3 |
| HC1—C1—C10—H1C10 | 172.4 | C12—C13—C14—C15 | 0.1 (9) |
| HC1—C1—C10—H2C10 | -67.7 | C12—C13—C14—HC14 | -179.9 |
| N1—C2—C3—C4 | -176.5 (5) | HC13—C13—C14—C15 | -179.9 |
| N1—C2—C3—C17 | 3.9 (8) | HC13—C13—C14—HC14 | 0.1 |
| C1—C2—C3—C4 | 4.1 (8) | C13—C14—C15—C16 | -0.8 (9) |
| C1—C2—C3—C17 | -175.5 (5) | C13—C14—C15—HC15 | 179.2 |
| C2—C3—C4—C5 | -25.4 (7) | HC14—C14—C15—C16 | 179.2 |
| C2—C3—C4—H1C4 | -145.7 | HC14—C14—C15—HC15 | -0.8 |
| C2—C3—C4—H2C4 | 95.0 | C14—C15—C16—C11 | 0.2 (8) |
| C17—C3—C4—C5 | 154.2 (6) | C14—C15—C16—C17 | 178.0 (5) |
| C17—C3—C4—H1C4 | 33.8 | HC15—C15—C16—C11 | -179.8 |
| C17—C3—C4—H2C4 | -85.5 | HC15—C15—C16—C17 | -2.0 |
| C2—C3—C17—C16 | 0.6 (8) | C11—C16—C17—C3 | -4.0 (8) |
| C2—C3—C17—HC17 | -179.4 | C11—C16—C17—HC17 | 176.0 |
| C4—C3—C17—C16 | -179.0 (5) | C15—C16—C17—C3 | 178.2 (6) |
| C4—C3—C17—HC17 | 1.0 | C15—C16—C17—HC17 | -1.8 |
| C3—C4—C5—C6 | 54.8 (7) | N2—C18—C19—C20 | -176.2 (5) |
| C3—C4—C5—H1C5 | -65.5 | N2—C18—C19—HC19 | 3.8 |
| C3—C4—C5—H2C5 | 175.0 | C23—C18—C19—C20 | 1.0 (9) |
| H1C4—C4—C5—C6 | 175.1 | C23—C18—C19—HC19 | -179.0 |
| H1C4—C4—C5—H1C5 | 54.9 | N2—C18—C23—C22 | 175.6 (5) |
| H1C4—C4—C5—H2C5 | -64.6 | N2—C18—C23—C24 | -1.4 (8) |
| H2C4—C4—C5—C6 | -65.6 | C19—C18—C23—C22 | -1.6 (8) |
| H2C4—C4—C5—H1C5 | 174.2 | C19—C18—C23—C24 | -178.5 (5) |
| H2C4—C4—C5—H2C5 | 54.6 | C18—C19—C20—C21 | 0.8 (9) |
| C4—C5—C6—C1 | -61.8 (6) | C18—C19—C20—HC20 | -179.2 |
| C4—C5—C6—C7 | 170.6 (5) | HC19—C19—C20—C21 | -179.2 |
| C4—C5—C6—HC6 | 54.0 | HC19—C19—C20—HC20 | 0.8 |
| H1C5—C5—C6—C1 | 58.5 | C19—C20—C21—C22 | -2.2 (9) |
| H1C5—C5—C6—C7 | -69.2 | C19—C20—C21—HC21 | 177.8 |
| H1C5—C5—C6—HC6 | 174.2 | HC20—C20—C21—C22 | 177.8 |
| H2C5—C5—C6—C1 | 178.0 | HC20—C20—C21—HC21 | -2.2 |
| H2C5—C5—C6—C7 | 50.4 | C20—C21—C22—C23 | 1.6 (9) |
| H2C5—C5—C6—HC6 | -66.2 | C20—C21—C22—HC22 | -178.4 |
| C1—C6—C7—N2 | 167.5 (4) | HC21—C21—C22—C23 | -178.4 |
| C1—C6—C7—C8 | -10.7 (7) | HC21—C21—C22—HC22 | 1.6 |
| C5—C6—C7—N2 | -65.3 (6) | C21—C22—C23—C18 | 0.3 (8) |
| C5—C6—C7—C8 | 116.4 (6) | C21—C22—C23—C24 | 177.0 (5) |
| HC6—C6—C7—N2 | 51.3 | HC22—C22—C23—C18 | -179.7 |
| HC6—C6—C7—C8 | -127.0 | HC22—C22—C23—C24 | -3.0 |
| N2—C7—C8—C9 | -178.1 (5) | C18—C23—C24—C8 | 2.5 (8) |
| N2—C7—C8—C24 | -1.4 (8) | C18—C23—C24—HC24 | -177.5 |
| C6—C7—C8—C9 | -0.1 (8) | C22—C23—C24—C8 | -174.4 (5) |
| C6—C7—C8—C24 | 176.6 (5) | C22—C23—C24—HC24 | 5.6 |

C7—C8—C9—C10

−20.7 (7)
