2002

3-Methoxy-1'-phenyl-4'[beta],5-dihydro-1H-pyrazolo[4',3':16,17]estra-1,3,5(10)-triene

Veronica Konig
University of Göttingen

Thomas R. Schneider
University of Göttingen

E. Frank

Beatrix Aukszi
University of Szeged, ba285@nova.edu

Gyula Schneider
University of Szeged

See next page for additional authors

NSUWorks Citation

Konig, V., Schneider, T. R., Frank, E., Aukszi, B., Schneider, G., & Wolfling, J. (2002). 3-Methoxy-1'-phenyl-4'[beta],5-dihydro-1H-pyrazolo[4',3':16,17]estra-1,3,5(10)-triene. Acta Crystallographica Section E: Crystallographic Communications, 58, (8), o810 - 0811. https://doi.org/10.1107/S160053680201125X. Retrieved from https://nsuworks.nova.edu/cnso_chemphys_facarticles/3

Authors

Veronica Konig, Thomas R. Schneider, E. Frank, Beatrix Aukszi, Gyula Schneider, and Janos Wolfling

Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

3-Methoxy-1′-phenyl-4′β,5-dihydro-1*H*-pyrazolo[4′,3′:16,17]estra-1,3,5(10)-triene

Verena König,[a] Thomas R. Schneider,[a] Eva Frank,[b] Beatrix Aukszi,[b] Gyula Schneider[b] and János Wölfling[b]*

[a]Institute of Inorganic Chemistry, University of Göttingen, Tammannstraße 4, D-37077 Göttingen, Germany, and [b]Department of Organic Chemistry, University of Szeged, Dóm tér 8., H-6720 Szeged, Hungary

Correspondence e-mail:
wolfling@chem.u-szeged.hu

The regio- and stereochemistry of the title compound, $C_{26}H_{30}N_2O$, has been established by X-ray analysis. The configuration of the stereogenic centre at C-16 proved to be *S* and the H atom at C-16 adopts the β position.

Received 29 April 2002
Accepted 24 June 2002
Online 5 July 2002

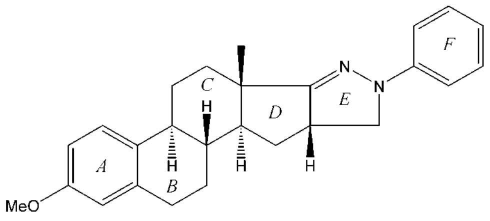
Key indicators

Single-crystal X-ray study
T = 133 K
Mean σ(C–C) = 0.004 Å
R factor = 0.038
wR factor = 0.092
Data-to-parameter ratio = 7.3

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

Comment

The synthesis of the title compound, (I), *via* a boron trifluoride diethyl etherate-induced 1,3-dipolar cycloaddition of the intermediate phenylhydrazone derived from the corresponding D-secoestrone aldehyde, will be published elsewhere (Frank *et al.*, 2002). The product has a newly formed stereogenic centre at the C-16 position, and the assignment of the stereochemistry at this position was the reason for the present study.



(I)

The structural study has shown that the H atom at the C-16 adopts the β position (Fig. 1). The *B*/*C* and *C*/*D* ring junctions are all-*trans*. Ring *A* is planar, ring *B* adopts a distorted half-chair conformation, and ring *C* displays a chair conformation. The *D* and *E* rings have envelope conformations, with atoms C13 and C16*A* displaced by 0.651 (4) and 0.436 (4) Å, respectively, from the planes of the remaining atoms of the corresponding rings.

For the crystal structures of some other related estrone derivatives, see Bes *et al.* (1997, 1998), Noltemeyer *et al.* (1996), Hooft & Kroon (1995), van Geerestein *et al.* (1987) and Duax *et al.* (1991).

Experimental

For the synthesis of the title compound, (I), 16,17-seco-3-methoxy-estra-1,3,5(10)16-tetraen-17-al (298 mg, 1.00 mmol), phenylhydrazine (0.10 ml, 109 mg) and 2 drops of glacial acetic acid were reacted in ethanol (10 ml). The mixture was stirred for 2 h at room temperature. The resulting phenylhydrazone derivative (369 mg, 95%), when treated (after purification) with a catalytic amount of 48% $BF_3\cdot OEt_2$ (0.07 ml, 0.25 mmol) in ice-cold CH_2Cl_2 (5 ml), undergoes intramolecular cyclization to afford (I) as a main product (290 mg, 79%). After purification by column chromatography (CH_2Cl_2) on silica gel, the product was crystallized from a 1:1 mixture of CH_2Cl_2/light petroleum at 298 K (m.p. 451–453 K). Spectroscopic analysis, ^{1}H

o810 Verena König *et al.* • $C_{26}H_{30}N_2O$ DOI: 10.1107/S160053680201125X *Acta Cryst.* (2002). E**58**, o810–o811

NMR ($CDCl_3$, δ, p.p.m.): 1.10 (*s*, 3H, $18H_3$), 2.84 (*m*, 2H, $6H_2$), 2.96 (*dd*, 1H, J = 13.3 Hz, J = 10.5 Hz, 16*aβ*–H), 3.36 (*m*, 1H, 16H), 3.77 (*s*, 3H, 3–OMe), 4.20 (*dd*, 1H, J = 10.5 Hz, J = 9.6 Hz, 16*aα*–H), 6.63 (*d*, 1H, J = 2.4 Hz, 4H), 6.72 (*dd*, J = 8.6 Hz, J = 2.4 Hz, 2H), 6.84 (*t*, 1H, J = 7.4 Hz, 4′–H), 7.07 (*d*, 2H, J = 8.2 Hz, 2′–H and 6′–H), 7.23 (*m*, 3H, 1H, 3′–H and 5′–H); ^{13}C NMR ($CDCl_3$, δ, p.p.m): 14.7 (C-18), 25.9, 26.7, 26.8, 29.6, 32.9, 38.6, 40.8, 44.2, 45.0, 54.8 (C-16), 55.2 (3–OMe), 58.4 (C-16*a*), 111.5 (C-2), 113.9 (3C, C-4, C-2′ and C-6′), 119.3 (C-4′), 126.3 (C-1), 128.9 (2C, C-3′ and C-5′), 132.1 (C-10), 137.6 (C-5), 148.9 (C-1′), 157.6 (C-3), 172.1 (C-17); analysis calculated for $C_{26}H_{30}N_2O$: C 80.79, H 7.82, N 7.25%; found: C 80.62, H 7.96, N 7.45%.

Crystal data

$C_{26}H_{30}N_2O$
M_r = 386.52
Orthorhombic, $P2_12_12_1$
a = 6.120 (1) Å
b = 8.950 (1) Å
c = 37.622 (4) Å
V = 2060.7 (5) Å^3
Z = 4
D_x = 1.246 Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 3250 reflections
θ = 2.2–24.7°
μ = 0.08 mm^{-1}
T = 133 (2) K
Block, colourless
0.3 × 0.2 × 0.2 mm

Data collection

Locally modified Stoe–Siemens–Huber four-circle diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
$T_{\min}$ = 0.978, $T_{\max}$ = 0.985
23229 measured reflections

1939 independent reflections
1669 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.047
$\theta_{\max}$ = 24.7°
$h = -6 \rightarrow 6$
$k = 0 \rightarrow 10$
$l = 0 \rightarrow 43$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.092$
S = 1.09
1939 reflections
264 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2 + 0.5351P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max}$ = 0.13 e Å^{-3}
$\Delta\rho_{\min}$ = −0.16 e Å^{-3}

Friedel pairs were merged, because of the lack of significant anomalous scattering. H atoms were included in calculated positions and refined using a riding model. The $U_{\rm eq}$ values of the H atoms were set to 1.5 times the $U_{\rm eq}$ values of the attached atom for methyl groups and 1.2 times the $U_{\rm eq}$ values of the attached atom for all the remaining H atoms.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

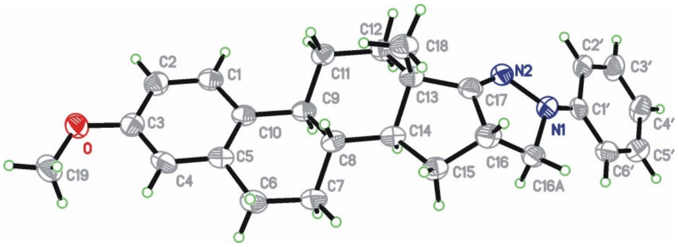


Figure 1
View of the molecule of the title compound, with the atomic numbering scheme and 50% probability displacement ellipsoids.

This research was supported by the Hungarian Scientific Research Fund (OTKA T032265), the Hungarian Ministry of Education (FKFP 0110/2000) and the Hungarian–German Intergovernmental S&T Cooperation Program (project No. UNG-43/00).

References

Bes, T., Hajnal, A., Schneider, Gy., Noltemeyer, M. & Wölfling, J. (1997). *Acta Cryst.* C**54**, 372–373.
Bes, M. T., Wölfling J., Usón, I., Pelikán, Sz., Tietze, L. F., Frank, É. & Schneider, Gy. (1998). *Acta Cryst.* C**54**, 1341–1343.
Bruker (1997). *SAINT*. Version 5.000. Bruker AXS Inc., Madison, Wisconsin, USA.
Duax, W. L., Griffin, J. F. & Strong, P. D. (1991). *Acta Cryst.* C**47**, 1096–1097.
Frank, É., Wölfling J., Aukszi, B., König, V., Schneider, T. R. & Schneider, Gy. (2002). *Tetrahedron.* Submitted.
Geerestein, V. J. van, Kanters, J. A. & Kroon, J. (1987). *Acta Cryst.* C**43**, 319–322.
Hooft, R. W. W. & Kroon, J. (1995). *Acta Cryst.* C**51**, 721–723.
Noltemeyer, M., Tietze, L. F., Wölfling J., Frank, É. & Schneider, Gy. (1996). *Acta Cryst.* C**52**, 2258.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997*a*). *SHELXL*97. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2000). *SADABS*. University of Göttingen, Germany.
Siemens (1996). *SMART*. Version 4.202. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Acta Cryst. (2002). E**58**, o810–o811 Verena König *et al.* • $C_{26}H_{30}N_2O$ **o811**

supporting information

Acta Cryst. (2002). E**58**, o810–o811   [https://doi.org/10.1107/S160053680201125X]

3-Methoxy-1′-phenyl-4′*β*,5-dihydro-1*H*-pyrazolo[4′,3′:16,17]estra-1,3,5(10)-triene

Verena König, Thomas R. Schneider, Eva Frank, Beatrix Aukszi, Gyula Schneider and János Wölfling

3-methoxy-1′-phenyl-4′*β*,5-dihydro-1*H*-pyrazolo [4′,3′:16,17]estra-1,3,5(10)-triene

Crystal data

$C_{26}H_{30}N_2O$
$M_r = 386.52$
Orthorhombic, $P2_12_12_1$
$a = 6.120$ (1) Å
$b = 8.950$ (1) Å
$c = 37.622$ (4) Å
$V = 2060.7$ (5) Å^3
$Z = 4$
$F(000) = 832$
$D_x = 1.246$ Mg m^{-3}
Melting point = 451–453 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3250 reflections
$\theta = 2.2$–24.7°
$\mu = 0.08$ mm^{-1}
$T = 133$ K
Block, colourless
0.3 × 0.2 × 0.2 mm

Data collection

Locally modified Stoe-Siemens-Huber four-circles diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2000)
$T_{\min} = 0.978$, $T_{\max} = 0.985$
23229 measured reflections
1939 independent reflections
1669 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.047$
$\theta_{\max} = 24.7°$, $\theta_{\min} = 2.2°$
$h = -6 \rightarrow 6$
$k = 0 \rightarrow 10$
$l = 0 \rightarrow 43$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.092$
$S = 1.09$
1939 reflections
264 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2 + 0.5351P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.13$ e Å^{-3}
$\Delta\rho_{\min} = -0.16$ e Å^{-3}
Absolute structure: Flack (1983); Friedel pairs were merged due to the lack of anomalous scatterers
Absolute structure parameter: −1 (3)

Special details

Experimental. intnesities were measured with a SIEMENS CCD area-detector

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 hydrogen atoms were included in calculated positions and refined using a riding model.

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

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
O	0.0061 (4)	−0.5755 (2)	−0.06171 (4)	0.0400 (5)
N1	0.1372 (4)	−0.1795 (2)	0.23953 (5)	0.0379 (6)
C1	0.2376 (5)	−0.3910 (3)	0.01525 (7)	0.0359 (7)
H1	0.3548	−0.3242	0.0199	0.043*
C1′	0.2936 (5)	−0.1872 (3)	0.26636 (7)	0.0348 (7)
N2	0.2147 (4)	−0.1367 (2)	0.20503 (6)	0.0372 (6)
C2	0.2025 (5)	−0.4380 (3)	−0.01926 (7)	0.0384 (7)
H2	0.2949	−0.4038	−0.0378	0.046*
C2′	0.4724 (5)	−0.0914 (3)	0.26608 (7)	0.0389 (7)
H2′	0.4921	−0.0239	0.2469	0.047*
C3	0.0318 (5)	−0.5355 (3)	−0.02674 (7)	0.0349 (7)
C3′	0.6211 (6)	−0.0938 (4)	0.29356 (7)	0.0476 (8)
H3′	0.7416	−0.0269	0.2933	0.057*
C4	−0.1009 (5)	−0.5840 (3)	0.00060 (7)	0.0385 (7)
H4	−0.2186	−0.6500	−0.0043	0.046*
C4′	0.5972 (5)	−0.1927 (4)	0.32168 (7)	0.0465 (8)
H4′	0.7019	−0.1953	0.3403	0.056*
C5	−0.0633 (5)	−0.5362 (3)	0.03582 (7)	0.0364 (7)
C5′	0.4206 (6)	−0.2867 (3)	0.32223 (8)	0.0458 (8)
H5′	0.4025	−0.3539	0.3415	0.055*
C6	−0.2191 (6)	−0.5950 (3)	0.06378 (7)	0.0460 (8)
H6A	−0.2337	−0.7045	0.0609	0.055*
H6B	−0.3649	−0.5500	0.0599	0.055*
C6′	0.2672 (6)	−0.2850 (3)	0.29488 (7)	0.0403 (7)
H6′	0.1450	−0.3504	0.2957	0.048*
C7	−0.1462 (6)	−0.5618 (3)	0.10172 (7)	0.0416 (8)
H7A	−0.2707	−0.5754	0.1182	0.050*
H7B	−0.0290	−0.6321	0.1087	0.050*
C8	−0.0625 (5)	−0.4022 (3)	0.10416 (7)	0.0329 (7)
H8	−0.1757	−0.3341	0.0939	0.039*
C9	0.1472 (5)	−0.3875 (3)	0.08187 (7)	0.0309 (7)
H9	0.2555	−0.4589	0.0923	0.037*
C10	0.1070 (5)	−0.4381 (3)	0.04355 (7)	0.0317 (7)

C11	0.2501 (5)	−0.2307 (3)	0.08453 (6)	0.0329 (7)
H11A	0.1577	−0.1590	0.0713	0.039*
H11B	0.3956	−0.2325	0.0730	0.039*
C12	0.2763 (5)	−0.1752 (3)	0.12311 (6)	0.0338 (7)
H12A	0.3888	−0.2359	0.1353	0.041*
H12B	0.3264	−0.0700	0.1229	0.041*
C13	0.0623 (5)	−0.1861 (3)	0.14338 (7)	0.0331 (7)
C14	−0.0145 (5)	−0.3523 (3)	0.14183 (7)	0.0314 (7)
H14	0.1131	−0.4133	0.1499	0.038*
C15	−0.1902 (5)	−0.3701 (3)	0.17088 (7)	0.0355 (7)
H15A	−0.1857	−0.4716	0.1813	0.043*
H15B	−0.3380	−0.3520	0.1611	0.043*
C16	−0.1316 (5)	−0.2510 (3)	0.19906 (7)	0.0389 (7)
H16	−0.2552	−0.1790	0.2020	0.047*
C16A	−0.0369 (5)	−0.2924 (3)	0.23511 (7)	0.0371 (7)
H16A	−0.1482	−0.2843	0.2541	0.044*
H16B	0.0237	−0.3950	0.2350	0.044*
C17	0.0650 (5)	−0.1723 (3)	0.18332 (7)	0.0355 (7)
C18	−0.1070 (5)	−0.0766 (3)	0.12888 (7)	0.0427 (8)
H18A	−0.0566	0.0260	0.1329	0.064*
H18B	−0.2465	−0.0919	0.1411	0.064*
H18C	−0.1264	−0.0935	0.1033	0.064*
C19	−0.1755 (6)	−0.6699 (3)	−0.06984 (8)	0.0459 (9)
H19A	−0.3116	−0.6194	−0.0632	0.069*
H19B	−0.1626	−0.7636	−0.0565	0.069*
H19C	−0.1769	−0.6916	−0.0954	0.069*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O	0.0492 (14)	0.0333 (10)	0.0376 (10)	0.0016 (11)	−0.0036 (10)	−0.0042 (9)
N1	0.0433 (16)	0.0369 (12)	0.0335 (12)	−0.0074 (13)	0.0108 (12)	−0.0024 (10)
C1	0.0304 (17)	0.0346 (14)	0.0428 (15)	−0.0052 (15)	0.0014 (14)	0.0016 (12)
C1′	0.041 (2)	0.0317 (14)	0.0319 (14)	−0.0019 (15)	0.0124 (14)	−0.0100 (12)
N2	0.0441 (17)	0.0315 (12)	0.0362 (12)	−0.0047 (12)	0.0096 (13)	−0.0021 (10)
C2	0.037 (2)	0.0389 (15)	0.0393 (15)	0.0008 (16)	0.0040 (14)	0.0018 (13)
C2′	0.0415 (19)	0.0409 (15)	0.0344 (14)	−0.0075 (16)	0.0149 (15)	−0.0057 (13)
C3	0.0400 (19)	0.0283 (13)	0.0363 (15)	0.0091 (15)	0.0020 (14)	0.0008 (12)
C3′	0.041 (2)	0.0625 (19)	0.0390 (16)	−0.0132 (18)	0.0128 (16)	−0.0093 (15)
C4	0.0400 (19)	0.0277 (13)	0.0480 (16)	−0.0063 (15)	−0.0068 (15)	−0.0027 (12)
C4′	0.039 (2)	0.063 (2)	0.0374 (15)	−0.0033 (19)	0.0044 (15)	−0.0028 (16)
C5	0.038 (2)	0.0294 (13)	0.0415 (15)	−0.0034 (15)	0.0015 (14)	0.0035 (12)
C5′	0.055 (2)	0.0425 (16)	0.0394 (16)	−0.0010 (18)	0.0033 (17)	0.0047 (13)
C6	0.046 (2)	0.0447 (17)	0.0479 (16)	−0.0188 (17)	0.0091 (16)	−0.0040 (14)
C6′	0.044 (2)	0.0323 (14)	0.0443 (16)	−0.0052 (15)	0.0094 (16)	−0.0026 (12)
C7	0.044 (2)	0.0359 (15)	0.0445 (16)	−0.0121 (16)	0.0059 (15)	0.0031 (13)
C8	0.0294 (18)	0.0331 (14)	0.0360 (14)	−0.0008 (14)	0.0022 (13)	0.0058 (12)
C9	0.0232 (16)	0.0305 (14)	0.0391 (14)	−0.0025 (13)	0.0015 (13)	0.0039 (12)

C10	0.0288 (17)	0.0267 (13)	0.0397 (14)	0.0007 (14)	−0.0001 (14)	0.0026 (11)
C11	0.0273 (17)	0.0359 (14)	0.0356 (13)	−0.0056 (14)	−0.0001 (14)	0.0040 (12)
C12	0.0278 (18)	0.0339 (14)	0.0396 (14)	−0.0059 (14)	−0.0032 (13)	0.0019 (12)
C13	0.0306 (19)	0.0303 (13)	0.0385 (15)	−0.0017 (14)	0.0025 (13)	0.0033 (12)
C14	0.0270 (18)	0.0275 (13)	0.0396 (14)	−0.0004 (14)	0.0010 (13)	0.0052 (12)
C15	0.0288 (18)	0.0356 (15)	0.0420 (15)	−0.0003 (13)	0.0046 (14)	0.0040 (12)
C16	0.0330 (18)	0.0372 (15)	0.0467 (16)	0.0013 (15)	0.0125 (15)	−0.0017 (13)
C16A	0.0358 (18)	0.0348 (14)	0.0406 (15)	−0.0051 (14)	0.0119 (14)	−0.0040 (13)
C17	0.039 (2)	0.0270 (13)	0.0400 (15)	−0.0007 (15)	0.0034 (15)	0.0006 (12)
C18	0.043 (2)	0.0350 (14)	0.0504 (17)	0.0031 (16)	0.0023 (16)	0.0049 (13)
C19	0.056 (2)	0.0346 (15)	0.0471 (16)	0.0048 (17)	−0.0088 (16)	−0.0064 (13)

Geometric parameters (Å, º)

O—C3	1.373 (3)	C5—C6	1.514 (4)
O—C19	1.430 (4)	C5′—C6′	1.393 (4)
N1—C1′	1.393 (3)	C6—C7	1.525 (4)
N1—N2	1.434 (3)	C7—C8	1.521 (4)
N1—C16A	1.478 (3)	C8—C14	1.514 (4)
C1—C2	1.382 (4)	C8—C9	1.539 (4)
C1—C10	1.397 (4)	C9—C10	1.531 (4)
C1′—C2′	1.390 (4)	C9—C11	1.542 (4)
C1′—C6′	1.395 (4)	C11—C12	1.543 (3)
N2—C17	1.268 (4)	C12—C13	1.519 (4)
C2—C3	1.390 (4)	C13—C17	1.508 (4)
C2′—C3′	1.378 (4)	C13—C18	1.527 (4)
C3—C4	1.381 (4)	C13—C14	1.562 (4)
C3′—C4′	1.387 (4)	C14—C15	1.542 (4)
C4—C5	1.411 (4)	C15—C16	1.546 (4)
C4′—C5′	1.369 (4)	C16—C17	1.514 (4)
C5—C10	1.393 (4)	C16—C16A	1.521 (4)
C3—O—C19	116.7 (2)	C7—C8—C9	109.2 (2)
C1′—N1—N2	116.2 (2)	C10—C9—C8	110.7 (2)
C1′—N1—C16A	122.9 (2)	C10—C9—C11	113.3 (2)
N2—N1—C16A	108.6 (2)	C8—C9—C11	112.5 (2)
C2—C1—C10	122.4 (3)	C5—C10—C1	117.3 (2)
C2′—C1′—N1	120.3 (2)	C5—C10—C9	120.2 (2)
C2′—C1′—C6′	119.0 (3)	C1—C10—C9	122.5 (2)
N1—C1′—C6′	120.6 (3)	C9—C11—C12	113.4 (2)
C17—N2—N1	106.1 (2)	C13—C12—C11	111.2 (2)
C1—C2—C3	119.9 (3)	C17—C13—C12	119.1 (2)
C3′—C2′—C1′	120.3 (3)	C17—C13—C18	108.1 (2)
O—C3—C4	124.4 (3)	C12—C13—C18	111.4 (2)
O—C3—C2	116.4 (2)	C17—C13—C14	96.8 (2)
C4—C3—C2	119.3 (2)	C12—C13—C14	107.6 (2)
C2′—C3′—C4′	120.9 (3)	C18—C13—C14	113.2 (2)
C3—C4—C5	120.5 (3)	C8—C14—C15	119.8 (2)

C5′—C4′—C3′	119.1 (3)	C8—C14—C13	112.0 (2)
C10—C5—C4	120.6 (3)	C15—C14—C13	106.4 (2)
C10—C5—C6	123.0 (2)	C14—C15—C16	104.7 (2)
C4—C5—C6	116.4 (3)	C17—C16—C16A	99.2 (2)
C4′—C5′—C6′	120.9 (3)	C17—C16—C15	103.7 (2)
C5—C6—C7	113.5 (3)	C16A—C16—C15	122.2 (2)
C5′—C6′—C1′	119.8 (3)	N1—C16A—C16	102.0 (2)
C8—C7—C6	109.8 (2)	N2—C17—C13	132.1 (3)
C14—C8—C7	113.5 (2)	N2—C17—C16	116.1 (2)
C14—C8—C9	108.8 (2)	C13—C17—C16	110.1 (2)