

Spiro[cyclopentane-1,11'-hexacyclo-[7.6.0.0^{1,6}.0^{6,13}.0^{8,12}.0^{10,14}]pentadecane]-7',15'-dione

Sambasivarao Kotha,* Rama Gunta, Subba Rao Cheekatla and Darshan S. Mhatre

Department of Chemistry, Indian Institute of Technology - Bombay, Powai, Mumbai, 400 076, India. *Correspondence e-mail: srk@chem.iitb.ac.in

Received 18 September 2018

Accepted 9 November 2018

Edited by I. Brito, University of Antofagasta, Chile

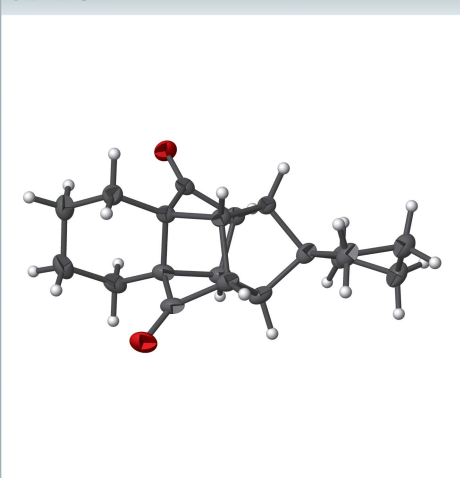
Keywords: crystal structure; cage molecule; trishomocubane; Lewis acid.

CCDC reference: 1878138

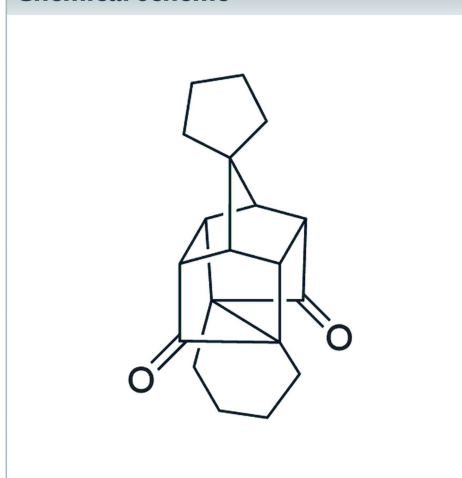
Structural data: full structural data are available from iucrdata.iucr.org

An unusual rearrangement of spiro cage dione to a trishomocubane derivatives is reported by acid-catalysed rearrangement with the aid of $\text{BF}_3 \cdot \text{OEt}_2$ in benzene (solvent) reflux conditions. Here, the molecular structure of cage molecule $\text{C}_{19}\text{H}_{22}\text{O}_2$ (major product) consists of five-membered rings, which adopt an *envelope* conformation and six-membered rings adopt a *chair* or *boat* conformation. The Cremer & Pople puckering parameters of all four six-membered rings are calculated.

3D view



Chemical scheme



Structure description

D_3 -Trishomocubane and its derivatives are of interest for their use as targets for pharmaceutical applications (Liu *et al.*, 2001), in medicinal chemistry (Oliver *et al.*, 1991) as well as in asymmetric catalysis (Levandovsky *et al.*, 2010; Sharapa *et al.*, 2012). Several amino functionalized D_3 -trishomocubane derivatives show significant biological activity and are NMDA receptor antagonists. In addition, some of them exhibit potent anti-TB activity, act as P_2X_7 receptor antagonists and exhibit anti-Parkinson's activity (Geldenhuis *et al.*, 2005).

As part of our major program on cage molecules, which involves the design of unusual polycyclic cage frameworks, for example, D_3 -trishomocubanes by the rearrangement approach (Kotha *et al.*, 2018) and we present herein the synthesis of the title cage compound **II** (Fig. 1), which was prepared (Fig. 2) from cheap and commercially available starting materials such as 1,4-hydroquinone in eight steps *via* Claisen rearrangement, Diels–Alder reaction and ring-closing metathesis (RCM) followed by acid-promoted rearrangement with Lewis acid (Kotha & Dipak, 2006).

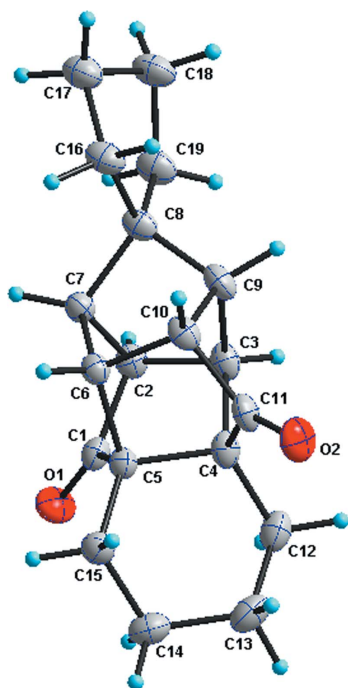


Figure 1
The molecular structure of the title compound **II** with displacement ellipsoids drawn at the 50% probability level.

The molecular structure of **II** is made up of fused five- and six-membered rings that are joined into a compact cage system. All five-membered rings adopt an *envelope* conformation, whereas the six-membered rings are in *chair* or *boat* conformations. The Cremer & Pople puckering parameters of three six-membered rings, namely, C2–C7, C2/C3/C9/C10/C6/C7 and C3–C6/C10/C9 are $Q = 1.110$ (2) Å, $\theta = 89.25$ (10)° and $\varphi = 15.37$ (12)°; $Q = 1.112$ (2) Å, $\theta = 89.98$ (10)° and $\varphi = 285.71$ (12)°; and $Q = 1.114$ (2) Å, $\theta = 90.57$ (10)° and $\varphi = 44.48$ (12)° respectively. These six-membered rings all exhibit a *boat* conformation. The other six-membered ring C4/C5/C12–C15 is in a *chair* conformation with puckering parameters $Q = 0.530$ (3) Å, $\theta = 7.1$ (3)° and $\varphi = 216$ (2)°.

Synthesis and crystallization

Compound **II** can be prepared *via* Lewis acid-promoted rearrangement (Fig. 2) of the cage [4.4.2]propellane **I** with the aid of $\text{BF}_3 \cdot \text{OEt}_2$ in the presence of benzene as a solvent. Spiro cage dione **I** (200 mg, 0.70 mmol) was added to a stirred

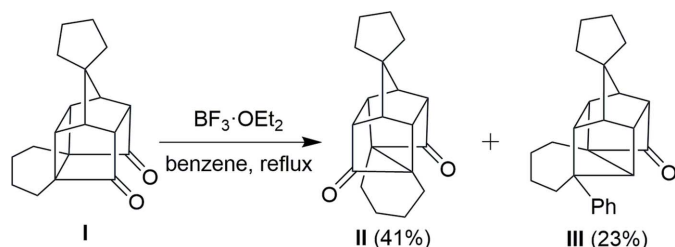


Figure 2
Lewis acid-promoted rearrangement of the cage dione **I**.

Table 1
Experimental details.

Crystal data	
Chemical formula	$\text{C}_{19}\text{H}_{22}\text{O}_2$
M_r	282.36
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, b, c (Å)	10.8650 (8), 14.3936 (9), 9.8008 (8)
β (°)	111.680 (9)
V (Å ³)	1424.3 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.08
Crystal size (mm)	0.14 × 0.11 × 0.09
Data collection	
Diffractometer	Rigaku Saturn724+
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Rigaku OD, 2018)
T_{\min} , T_{\max}	0.740, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	4407, 2470, 1877
R_{int}	0.050
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.594
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.052, 0.140, 1.05
No. of reflections	2470
No. of parameters	190
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.25, -0.28

Computer programs: *CrysAlis PRO* (Rigaku OD, 2018), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b) and *OLEX2* (Dolomanov *et al.*, 2009).

solution of anhydrous $\text{BF}_3 \cdot \text{OEt}_2$ (1 mL) in dry benzene (10 mL) at room temperature. Next, the resulting reaction mixture was refluxed for two days. After completion of the reaction (TLC monitoring), the reaction mixture was quenched with a saturated aqueous NaHCO_3 solution and extracted with benzene. The combined organic layers were washed with water and brine solution then dried over anhydrous Na_2SO_4 . After removal of the solvent under vacuum, the resulting crude residue was subjected to silica gel column chromatography by using 5% ethyl acetate in petroleum ether as an eluent to deliver the desired rearranged cage ketone **III** (57 mg, 23%) containing a phenyl group as a colourless liquid. Continuous elution with 10% ethyl acetate in petroleum ether delivered the rearranged cage dione **II** (82 mg, 41%) as a colourless crystalline solid. Recrystallization of a column-purified **II** from a mixture of ethyl acetate and hexane (1:2) solvents gave crystals suitable for X-ray analysis. M.p. 409–411 K. IR (neat, cm^{-1}) 2926, 2857, 1751, 1450, 1294, 1076; ¹H NMR (500 MHz, CDCl_3 p.p.m.): δ 2.23–2.26 (*m*, 6H), 1.83 (*d*, $J = 13.5$ Hz, 2H), 1.69–1.62 (*m*, 2H), 1.49–1.42 (*m*, 10H), 1.15–1.12 (*m*, 2H); ¹³C NMR (125 MHz, CDCl_3 , p.p.m.): δ 213.1, 60.5, 50.6, 48.6, 48.4, 42.8, 32.5, 26.1, 22.2, 21.9; HRMS (ESI, Q-TOF) m/z calculated for $\text{C}_{19}\text{H}_{22}\text{O}_2$ [$M + \text{Na}$]⁺ 305.1512; found: 305.1514.

Melting points were recorded on a Veego VMP-CMP melting point apparatus and are uncorrected. Nuclear Magnetic Resonance (NMR) spectra were recorded on a Bruker (Avance IIITM500) spectrometer operated at 500 MHz for ¹H and 125.7 MHz for ¹³C nuclei.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Funding information

We thank the Defence Research and Development Organization (DRDO, No. ARDB/01/1041849/M/1), New Delhi, for financial assistance. SK thanks the Department of Science and Technology (DST, No. SR/S2/JCB-33/2010) for the award of a J. C. Bose fellowship and Praj industries for the Pramod Chaudhari Chair Professorship (Green Chemistry). RG thanks Indian Institute of Technology (IIT) - Bombay, Mumbai for financial support as an Institute Research Associate (RA) and SRC thanks the University Grants Commission (UGC), New Delhi, for the award of a research fellowship.

References

- Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
- Geldenhuis, W. J., Malan, S. F., Bloomquist, J. R., Marchand, A. P. & Van der Schyf, C. J. (2005). *Med. Res. Rev.* **25**, 21–48.
- Kotha, S., Cheekatla, S. R. & Gunta, R. (2018). *IUCrData*, **3**, x180090.
- Kotha, S. & Dipak, M. K. (2006). *Chem. Eur. J.* **12**, 4446–4450.
- Levandovsky, I. A., Sharapa, D. I., Cherenkova, O. A., Gaidai, A. V. & Shubina, T. E. (2010). *Russ. Chem. Rev.* **79**, 1005–1026.
- Liu, X., Nuwayhid, S., Christie, M. J., Kassiou, M. & Werling, L. L. (2001). *Eur. J. Pharmacol.* **422**, 39–45.
- Oliver, D. W., Dekker, T. G., Snyckers, F. O. & Fourie, T. G. (1991). *J. Med. Chem.* **34**, 851–854.
- Rigaku OD (2018). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.
- Sharapa, D. I., Levandovskiy, I. A. & Shubina, T. E. (2012). *Curr. Org. Chem.* **16**, 2632–2660.
- Sheldrick, G. M. (2015a). *Acta Cryst.* **A71**, 3–8.
- Sheldrick, G. M. (2015b). *Acta Cryst.* **C71**, 3–8.

full crystallographic data

IUCrData (2018). 3, x181590 [https://doi.org/10.1107/S2414314618015900]

Spiro[cyclopentane-1,11'-hexacyclo[7.6.0.0^{1,6}.0^{6,13}.0^{8,12}.0^{10,14}]penta-decane]-7',15'-dione

Sambasivarao Kotha, Rama Gunta, Subba Rao Cheekatla and Darshan S. Mhatre

Spiro[cyclopentane-1,11'-hexacyclo[7.6.0.0^{1,6}.0^{6,13}.0^{8,12}.0^{10,14}]penta-decane]-7',15'-dione

Crystal data

C₁₉H₂₂O₂

$M_r = 282.36$

Monoclinic, $P2_1/c$

$a = 10.8650$ (8) Å

$b = 14.3936$ (9) Å

$c = 9.8008$ (8) Å

$\beta = 111.680$ (9)°

$V = 1424.3$ (2) Å³

$Z = 4$

$F(000) = 608$

$D_x = 1.317$ Mg m⁻³

Melting point = 409–411 K

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

Cell parameters from 2620 reflections

$\theta = 2.5$ – 31.0 °

$\mu = 0.08$ mm⁻¹

$T = 150$ K

Block, colourless

0.14 × 0.11 × 0.09 mm

Data collection

Rigaku Saturn724+
diffractometer

Radiation source: fine-focus sealed X-ray tube

Graphite monochromator

ω scans

Absorption correction: multi-scan
(CrysAlisPro; Rigaku OD, 2018)

$T_{\min} = 0.740$, $T_{\max} = 1.000$

4407 measured reflections

2470 independent reflections

1877 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.050$

$\theta_{\max} = 25.0$ °, $\theta_{\min} = 2.7$ °

$h = -12 \rightarrow 8$

$k = -11 \rightarrow 17$

$l = -10 \rightarrow 11$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.052$

$wR(F^2) = 0.140$

$S = 1.05$

2470 reflections

190 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0668P)^2 + 0.4068P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.25$ e Å⁻³

$\Delta\rho_{\min} = -0.28$ e Å⁻³

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. All H atoms were placed in geometrically calculated positions and refined using a riding model with C–H distances of 1.00 Å for all H atoms bound to tertiary C(sp^3) atoms and 0.99 Å for H atoms bound to secondary C(sp^3) atoms. Isotropic displacement parameters for H atoms were calculated as $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.66123 (15)	0.57866 (10)	0.78083 (19)	0.0336 (4)
O2	0.67492 (16)	0.18936 (11)	0.86490 (19)	0.0361 (5)
C1	0.6053 (2)	0.50462 (15)	0.7681 (2)	0.0228 (5)
C2	0.4704 (2)	0.48099 (15)	0.7682 (2)	0.0236 (5)
H2	0.420116	0.532032	0.793568	0.028*
C3	0.4940 (2)	0.39008 (14)	0.8618 (3)	0.0250 (5)
H3	0.481313	0.397490	0.957203	0.030*
C4	0.6387 (2)	0.35801 (14)	0.8782 (2)	0.0252 (5)
C5	0.6500 (2)	0.40821 (14)	0.7433 (2)	0.0217 (5)
C6	0.5219 (2)	0.36927 (14)	0.6173 (2)	0.0218 (5)
H6	0.531107	0.361861	0.520102	0.026*
C7	0.4066 (2)	0.43687 (14)	0.6154 (2)	0.0224 (5)
H7	0.375903	0.481631	0.531443	0.027*
C8	0.2984 (2)	0.37374 (15)	0.6313 (3)	0.0254 (5)
C9	0.3986 (2)	0.31667 (15)	0.7546 (2)	0.0269 (6)
H9	0.359305	0.269925	0.802299	0.032*
C10	0.4915 (2)	0.27694 (14)	0.6830 (3)	0.0251 (5)
H10	0.457245	0.223742	0.613611	0.030*
C11	0.6139 (2)	0.25960 (15)	0.8169 (2)	0.0259 (5)
C12	0.7534 (2)	0.37557 (16)	1.0209 (3)	0.0313 (6)
H12A	0.747001	0.333189	1.097601	0.038*
H12B	0.749162	0.440225	1.053410	0.038*
C13	0.8851 (2)	0.35997 (18)	1.0017 (3)	0.0364 (6)
H13A	0.958731	0.376379	1.094051	0.044*
H13B	0.893859	0.293352	0.981774	0.044*
C14	0.8961 (2)	0.41781 (17)	0.8765 (3)	0.0335 (6)
H14A	0.982037	0.404682	0.866980	0.040*
H14B	0.894383	0.484567	0.900056	0.040*
C15	0.7839 (2)	0.39734 (16)	0.7303 (3)	0.0273 (5)
H15A	0.790035	0.440386	0.654310	0.033*
H15B	0.793140	0.333131	0.699164	0.033*
C16	0.2179 (2)	0.31748 (16)	0.4922 (3)	0.0308 (6)
H16A	0.255017	0.326049	0.414784	0.037*
H16B	0.219347	0.250448	0.515439	0.037*
C17	0.0770 (2)	0.35547 (18)	0.4420 (3)	0.0346 (6)
H17A	0.066801	0.411673	0.380529	0.041*
H17B	0.011547	0.308245	0.385971	0.041*
C18	0.0616 (2)	0.37849 (18)	0.5865 (3)	0.0366 (6)
H18A	0.048415	0.321521	0.636087	0.044*
H18B	−0.013808	0.421180	0.571085	0.044*
C19	0.1933 (2)	0.42530 (17)	0.6750 (3)	0.0320 (6)

H19A	0.213210	0.419146	0.781667	0.038*
H19B	0.190743	0.492109	0.650138	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0352 (10)	0.0194 (9)	0.0443 (11)	-0.0054 (7)	0.0125 (8)	-0.0020 (7)
O2	0.0463 (10)	0.0204 (9)	0.0435 (11)	0.0061 (8)	0.0188 (8)	0.0057 (8)
C1	0.0275 (12)	0.0199 (12)	0.0184 (12)	0.0011 (9)	0.0057 (9)	0.0006 (9)
C2	0.0281 (12)	0.0189 (11)	0.0262 (12)	0.0020 (9)	0.0127 (10)	-0.0013 (9)
C3	0.0349 (13)	0.0208 (11)	0.0242 (12)	-0.0009 (9)	0.0168 (10)	-0.0018 (9)
C4	0.0339 (13)	0.0193 (11)	0.0246 (13)	0.0014 (9)	0.0132 (10)	0.0019 (9)
C5	0.0245 (12)	0.0215 (11)	0.0194 (12)	0.0000 (9)	0.0083 (9)	0.0006 (9)
C6	0.0246 (11)	0.0214 (11)	0.0209 (12)	-0.0015 (9)	0.0102 (10)	-0.0010 (9)
C7	0.0223 (11)	0.0219 (11)	0.0242 (12)	-0.0001 (9)	0.0100 (9)	0.0006 (9)
C8	0.0256 (12)	0.0253 (12)	0.0294 (13)	-0.0034 (9)	0.0150 (10)	-0.0055 (10)
C9	0.0336 (13)	0.0234 (12)	0.0309 (14)	-0.0071 (10)	0.0203 (11)	-0.0031 (10)
C10	0.0304 (12)	0.0187 (11)	0.0297 (13)	-0.0029 (9)	0.0154 (10)	-0.0031 (9)
C11	0.0358 (13)	0.0186 (12)	0.0283 (13)	-0.0004 (10)	0.0177 (11)	0.0033 (10)
C12	0.0409 (14)	0.0274 (12)	0.0225 (13)	0.0024 (10)	0.0082 (11)	0.0015 (10)
C13	0.0333 (13)	0.0368 (14)	0.0301 (15)	0.0059 (11)	0.0012 (11)	0.0015 (11)
C14	0.0246 (13)	0.0370 (14)	0.0339 (14)	0.0003 (10)	0.0051 (11)	-0.0046 (11)
C15	0.0262 (12)	0.0287 (12)	0.0278 (13)	0.0004 (10)	0.0108 (10)	0.0001 (10)
C16	0.0291 (13)	0.0308 (13)	0.0360 (14)	-0.0068 (10)	0.0161 (11)	-0.0080 (11)
C17	0.0302 (13)	0.0396 (14)	0.0362 (15)	-0.0073 (11)	0.0150 (11)	-0.0056 (11)
C18	0.0279 (13)	0.0429 (15)	0.0438 (16)	-0.0055 (11)	0.0190 (12)	-0.0070 (12)
C19	0.0297 (13)	0.0350 (13)	0.0364 (15)	-0.0006 (10)	0.0181 (11)	-0.0052 (11)

Geometric parameters (Å, °)

O1—C1	1.210 (3)	C12—H12A	0.9900
O2—C11	1.205 (3)	C12—H12B	0.9900
C1—C2	1.505 (3)	C12—C13	1.528 (3)
C1—C5	1.519 (3)	C13—H13A	0.9900
C2—H2	1.0000	C13—H13B	0.9900
C2—C3	1.564 (3)	C14—C13	1.523 (3)
C2—C7	1.536 (3)	C14—H14A	0.9900
C3—H3	1.0000	C14—H14B	0.9900
C3—C4	1.589 (3)	C15—C5	1.514 (3)
C3—C9	1.578 (3)	C15—C14	1.528 (3)
C4—C12	1.512 (3)	C15—H15A	0.9900
C5—C4	1.550 (3)	C15—H15B	0.9900
C5—C6	1.583 (3)	C16—H16A	0.9900
C6—H6	1.0000	C16—H16B	0.9900
C6—C7	1.580 (3)	C16—C17	1.527 (3)
C6—C10	1.564 (3)	C17—H17A	0.9900
C7—H7	1.0000	C17—H17B	0.9900
C7—C8	1.538 (3)	C18—C17	1.523 (3)

C8—C9	1.532 (3)	C18—H18A	0.9900
C8—C16	1.548 (3)	C18—H18B	0.9900
C9—H9	1.0000	C19—C8	1.550 (3)
C10—C9	1.538 (3)	C19—C18	1.528 (3)
C10—H10	1.0000	C19—H19A	0.9900
C11—C4	1.523 (3)	C19—H19B	0.9900
C11—C10	1.505 (3)		
O1—C1—C2	130.6 (2)	C11—C10—C6	104.29 (17)
O1—C1—C5	130.0 (2)	C11—C10—C9	100.46 (18)
C2—C1—C5	99.37 (17)	C11—C10—H10	116.9
C1—C2—H2	117.1	O2—C11—C4	129.4 (2)
C1—C2—C3	103.90 (17)	O2—C11—C10	131.4 (2)
C1—C2—C7	100.46 (17)	C10—C11—C4	99.23 (17)
C3—C2—H2	117.1	C4—C12—H12A	109.5
C7—C2—H2	117.1	C4—C12—H12B	109.5
C7—C2—C3	98.24 (16)	C4—C12—C13	110.5 (2)
C2—C3—H3	114.2	H12A—C12—H12B	108.1
C2—C3—C4	104.15 (16)	C13—C12—H12A	109.5
C2—C3—C9	104.15 (18)	C13—C12—H12B	109.5
C4—C3—H3	114.2	C12—C13—H13A	109.2
C9—C3—H3	114.2	C12—C13—H13B	109.2
C9—C3—C4	104.79 (17)	H13A—C13—H13B	107.9
C5—C4—C3	99.51 (16)	C14—C13—C12	112.02 (19)
C11—C4—C3	101.89 (17)	C14—C13—H13A	109.2
C11—C4—C5	98.93 (17)	C14—C13—H13B	109.2
C12—C4—C3	119.41 (19)	C13—C14—H14A	109.2
C12—C4—C5	114.43 (18)	C13—C14—H14B	109.2
C12—C4—C11	119.06 (18)	C13—C14—C15	112.13 (19)
C1—C5—C4	99.11 (17)	H14A—C14—H14B	107.9
C1—C5—C6	101.95 (16)	C15—C14—H14A	109.2
C4—C5—C6	100.16 (16)	C15—C14—H14B	109.2
C15—C5—C1	118.81 (18)	C5—C15—C14	111.09 (19)
C15—C5—C4	113.84 (18)	C5—C15—H15A	109.4
C15—C5—C6	119.54 (18)	C5—C15—H15B	109.4
C5—C6—H6	114.3	C14—C15—H15A	109.4
C7—C6—C5	104.84 (16)	C14—C15—H15B	109.4
C7—C6—H6	114.3	H15A—C15—H15B	108.0
C10—C6—C5	103.79 (17)	C8—C16—H16A	110.6
C10—C6—H6	114.3	C8—C16—H16B	110.6
C10—C6—C7	103.97 (16)	H16A—C16—H16B	108.7
C2—C7—C6	99.94 (16)	C17—C16—C8	105.67 (18)
C2—C7—H7	115.4	C17—C16—H16A	110.6
C2—C7—C8	103.39 (17)	C17—C16—H16B	110.6
C6—C7—H7	115.4	C16—C17—H17A	111.2
C8—C7—C6	105.47 (16)	C16—C17—H17B	111.2
C8—C7—H7	115.4	H17A—C17—H17B	109.1
C7—C8—C16	115.11 (18)	C18—C17—C16	102.7 (2)

C7—C8—C19	114.46 (18)	C18—C17—H17A	111.2
C9—C8—C7	92.90 (17)	C18—C17—H17B	111.2
C9—C8—C16	114.81 (19)	C17—C18—H18A	111.2
C9—C8—C19	114.79 (19)	C17—C18—H18B	111.2
C16—C8—C19	105.03 (18)	C17—C18—C19	102.85 (19)
C3—C9—H9	115.4	H18A—C18—H18B	109.1
C8—C9—C3	105.47 (18)	C19—C18—H18A	111.2
C8—C9—H9	115.4	C19—C18—H18B	111.2
C8—C9—C10	103.50 (18)	C8—C19—H19A	110.7
C10—C9—C3	99.90 (17)	C8—C19—H19B	110.7
C10—C9—H9	115.4	C18—C19—C8	105.26 (19)
C6—C10—H10	116.9	C18—C19—H19A	110.7
C9—C10—C6	98.38 (16)	C18—C19—H19B	110.7
C9—C10—H10	116.9	H19A—C19—H19B	108.8
