

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

(1*S*,3*R*,8*R*,9*S*,11*R*)-2,2,10,10-Tetrachloro-3,7,7,11-tetramethyltetracyclo-[6.5.0.0^{1,3}.0^{9,11}]tridecane

 Najia Ourhiss,^{a*} Ahmed Benharref,^a Mohamed Saadi,^b Lahcen El Ammari^b and Moha Berraho^a

^aLaboratoire de Chimie Biomoléculaire, Substances Naturelles et Réactivité "Unité Associée au CNRST(URAC16)", Faculté des Sciences Semlalia, BP 2390, Bd My Abdellah, 40000 Marrakech, Morocco, and ^bLaboratoire de Chimie du Solide Appliquée, Faculté des Sciences, Avenue Ibn Battouta, BP 1014 Rabat, Morocco
Correspondence e-mail: berraho@uca.ma

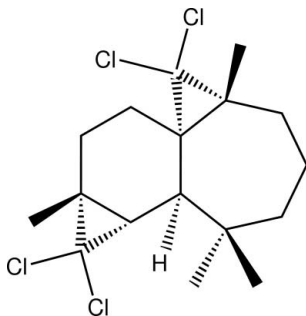
Received 14 January 2013; accepted 16 January 2013

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.032; wR factor = 0.085; data-to-parameter ratio = 28.5.

The title compound, $\text{C}_{17}\text{H}_{24}\text{Cl}_4$, was synthesized from β -himachalene (3,5,5,9-tetramethyl-2,4a,5,6,7,8-hexahydro-1*H*-benzocycloheptene), which was isolated from the essential oil of the Atlas cedar (*Cedrus Atlantica*). The molecule is built up from fused six- and seven-membered rings and two three-membered rings from the reaction of β -himachalene with dichlorocarbene. The six-membered ring shows a chair conformation, whereas the seven-membered ring displays a boat conformation.

Related literature

For the isolation of β -himachalene, see: Joseph & Dev (1968); Plattier & Teisseire (1974). For the reactivity of this sesquiterpene, see: Lassaba *et al.* (1998); Chekroun *et al.* (2000); El Jamili *et al.* (2002); Sbai *et al.* (2002); Dakir *et al.* (2004). For its biological activity, see: Daoubi *et al.* (2004). For puckering parameters, see: Cremer & Pople (1975).



Experimental

Crystal data

$\text{C}_{17}\text{H}_{24}\text{Cl}_4$	$V = 891.42(10) \text{ \AA}^3$
$M_r = 370.16$	$Z = 2$
Monoclinic, $P2_1$	Mo $K\alpha$ radiation
$a = 8.8807(6) \text{ \AA}$	$\mu = 0.66 \text{ mm}^{-1}$
$b = 11.6280(8) \text{ \AA}$	$T = 296 \text{ K}$
$c = 9.0596(6) \text{ \AA}$	$0.41 \times 0.35 \times 0.27 \text{ mm}$
$\beta = 107.665(2)^\circ$	

Data collection

Bruker X8 APEX diffractometer	4910 reflections with $I > 2\sigma(I)$
15112 measured reflections	$R_{\text{int}} = 0.019$
5419 independent reflections	

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$	H-atom parameters constrained
$wR(F^2) = 0.085$	$\Delta\rho_{\text{max}} = 0.32 \text{ e \AA}^{-3}$
$S = 1.03$	$\Delta\rho_{\text{min}} = -0.19 \text{ e \AA}^{-3}$
5419 reflections	Absolute structure: Flack (1983)
190 parameters	Flack parameter: 0.04 (4)
1 restraint	

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2009) and *pubCIF* (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT6883).

References

- Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Chekroun, A., Jarid, A., Benharref, A. & Boutalib, A. (2000). *J. Org. Chem.* **65**, 4431–4434.
- Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
- Dakir, M., Auhmani, A., Ait Itto, M. Y., Mazoir, N., Akssira, M., Pierrot, M. & Benharref, A. (2004). *Synth. Commun.* **34**, 2001–2008.
- Daoubi, M., Duran -Patron, R., Hmamouchi, M., Hernandez -Galan, R., Benharref, A. & Isidro, G. C. (2004). *Pest Manag. Sci.* **60**, 927–932.
- El Jamili, H., Auhmani, A., Dakir, M., Lassaba, E., Benharref, A., Pierrot, M., Chiaroni, A. & Riche, C. (2002). *Tetrahedron Lett.* **43**, 6645–6648.
- Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Joseph, T. C. & Dev, S. (1968). *Tetrahedron*, **24**, 3841–3859.
- Lassaba, E., Eljamili, H., Chekroun, A., Benharref, A., Chiaroni, A., Riche, C. & Laverigne, J.-P. (1998). *Synth. Commun.* **28**, 2641–2651.
- Plattier, M. & Teisseire, P. (1974). *Recherche*, **19**, 131–144.
- Sbai, F., Dakir, M., Auhmani, A., El Jamili, H., Akssira, M., Benharref, A., Kenz, A. & Pierrot, M. (2002). *Acta Cryst.* **C58**, o518–o520.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2013). E69, o275 [doi:10.1107/S1600536813001700]

(1*S*,3*R*,8*R*,9*S*,11*R*)-2,2,10,10-Tetrachloro-3,7,7,11-tetramethyltetracyclo-[6.5.0.0^{1,3}.0^{9,11}]tridecane

Najia Ourhriss, Ahmed Benharref, Mohamed Saadi, Lahcen El Ammari and Moha Berraho

S1. Comment

The bicyclic sesquiterpene, β -himachalene is the main constituent (50%) of the essential oil of the Atlas cedar (*Cedrus atlantica*) (Joseph & Dev, 1968; Plattier & Teisseire, 1974). The reactivity of this sesquiterpene and its derivatives has been studied extensively by our team in order to prepare new products having biological proprieties (Lassaba *et al.*, 1998; Chekroun *et al.*, 2000; El Jamili *et al.*, 2002; Sbai *et al.*, 2002; Dakir *et al.*, 2004). Indeed, these compounds were tested, using the food poisoning technique, for their potential antifungal activity against phytopathogen *Botrytis cinerea* (Daoubi *et al.*, 2004). Thus the action of two equivalents of dichlorocarbene, generated *in situ* from chloroform in the presence of sodium hydroxide as base and *n*-benzyltriethylammonium chloride as catalyst, on β -himachalene leads to a mixture of two diastereoisomers: (1*S*,3*R*,8*R*,9*S*,11*R*)-2,2,10,10-tetrachloro-3,7,7,11-tetraméthyletetracyclo [6,5,0,01.2,09.11] tridecane (*X*) and its isomer (1*S*,3*R*,8*R*,9*R*,11*S*)-2,2,10,10-tetrachloro-3,7,7,11-tetraméthyletetracyclo [6,5,0,01.2,09.11]tridecane (*Y*), in an over-all yield of 80% and 85/15 ratio. By single-crystal X-ray diffraction analysis, we have determined the absolute configuration of *X* and we deduced that from its isomer *Y*.

The molecule contains a fused six- and seven-membered rings, which is fused to two three-membered rings as shown in Fig. 1. The six-membered ring has a chair conformation, with as indicated by the total puckering amplitude $QT = 0.4518(19)$ Å and spherical polar angle $\theta = 140.4(2)^\circ$ with $\varphi_2 = 141.5(4)^\circ$, whereas the seven-membered ring displays a boat conformation with $QT = 1.1323(2)$ Å, $\theta_2 = 87.3(1)$, $\varphi_2 = -48.94(9)^\circ$ and $\varphi_3 = -125(2)^\circ$ (Cremer & Pople, 1975). The dihedral angle between the five- and seven-membered rings is $55.89(9)^\circ$. The three-membered ring (C1, C2, C3) ring is nearly perpendicular to the six-membered ring (C1, C8, C9, C11, C12, C13) with a dihedral angle of $84.24(19)^\circ$. Owing to the presence of Cl atoms, the absolute configuration could be determined from anomalous dispersion effects, by refining the Flack parameter (Flack, 1983) as C1(*S*), C3(*R*), C8(*R*), C9(*S*), and C11(*R*).

S2. Experimental

A solution containing 6 g (29 mmol) of β -himachalene and 6 mL (75 mmol) of CHCl_3 in 40 ml of dichloromethane was added dropwise at 273 K over 30 min to 1.6 g (40 mmol) of pulverized sodium hydroxide and 60 mg of *N*-benzyltriethylammonium chloride placed in a 100 ml three-necked flask. After stirring at room temperature for 2 h, the mixture was filtered on celite and concentrated in vacuum. The residue obtained was chromatographed on silicagel column impregnated with silver nitrate (10%) with a mixture of hexane - ethyl acetate (98–2) used as eluent. The two diastereoisomers (1*S*,3*R*,8*R*,9*S*,11*R*)-2,2,10,10-tetrachloro-3,7,7,11-tetraméthyletetracyclo [6,5,0,01.2,09.11] tridecane (*X*) and (1*S*,3*R*,8*R*,9*R*,11*S*)-2,2,10,10-tetrachloro-3,7,7,11-tetraméthyletetracyclo [6,5,0,01.2,09.11]tridecane (*Y*), were obtained by this procedure in a 85/15 ratio and a combined yield of 80% (8,5 g; 23,2 mmol). The title compound (isomer *X*) was recrystallized from pentane.

S3. Refinement

All H atoms were fixed geometrically and treated as riding with C—H = 0.96 Å (methyl), 0.97 Å (methylene), 0.98 Å (methine) with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$ (methylene, methine) or $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}$ (methyl). The space group is not centrosymmetric and the polar axis restraint is generated automatically by the *SHELXL* program. Friedel pairs were not merged.

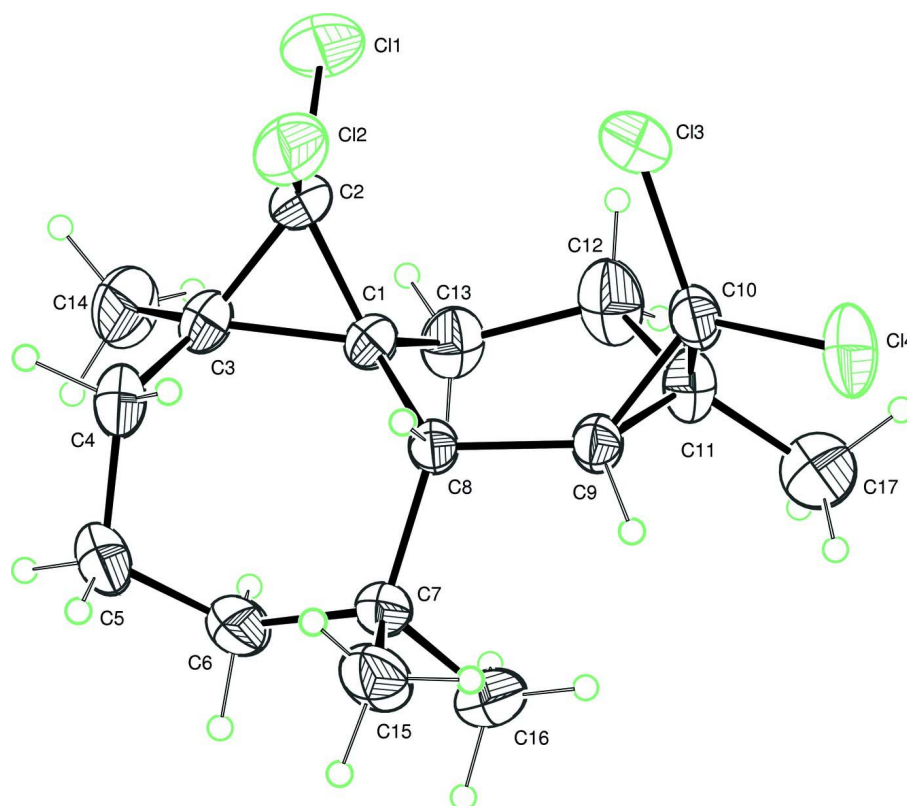


Figure 1

Molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

(1*S*,3*R*,8*R*,9*S*,11*R*)-2,2,10,10-Tetrachloro-3,7,7,11-tetramethyltetracyclo[6.5.0.0^{1,3}.0^{9,11}]tridecane

*Crystal data*C₁₇H₂₄Cl₄ $M_r = 370.16$ Monoclinic, *P*2₁Hall symbol: *P* 2y_b $a = 8.8807$ (6) Å $b = 11.6280$ (8) Å $c = 9.0596$ (6) Å $\beta = 107.665$ (2)° $V = 891.42$ (10) Å³ $Z = 2$ $F(000) = 388$ $D_x = 1.379$ Mg m⁻³Mo *K*α radiation, $\lambda = 0.71073$ Å

Cell parameters from 5419 reflections

 $\theta = 2.8$ – 30.5 ° $\mu = 0.66$ mm⁻¹ $T = 296$ K

Block, colourless

 $0.41 \times 0.35 \times 0.27$ mm

Data collection

Bruker X8 APEX
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
 φ and ω scans
15112 measured reflections
5419 independent reflections

4910 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.019$
 $\theta_{\text{max}} = 30.5^\circ$, $\theta_{\text{min}} = 2.8^\circ$
 $h = -12 \rightarrow 12$
 $k = -16 \rightarrow 16$
 $l = -12 \rightarrow 12$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.085$
 $S = 1.03$
5419 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-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0491P)^2 + 0.074P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.32 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.19 \text{ e } \text{\AA}^{-3}$
Absolute structure: Flack (1983)
Absolute structure parameter: 0.04 (4)

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.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.38317 (6)	0.32772 (6)	0.92294 (6)	0.06701 (17)
C12	0.52164 (6)	0.12723 (5)	0.83384 (6)	0.05443 (13)
C13	0.78628 (6)	0.23092 (5)	1.13768 (5)	0.05374 (13)
C14	1.12169 (5)	0.25246 (4)	1.19453 (5)	0.04960 (12)
C1	0.62379 (15)	0.35612 (13)	0.77816 (16)	0.0288 (3)
C2	0.49711 (18)	0.27743 (16)	0.80650 (18)	0.0391 (4)
C3	0.47133 (16)	0.32604 (17)	0.64690 (18)	0.0380 (3)
C4	0.48758 (19)	0.24243 (18)	0.52377 (18)	0.0431 (4)
H4A	0.5552	0.1791	0.5733	0.052*
H4B	0.3845	0.2111	0.4692	0.052*
C5	0.5566 (2)	0.2997 (2)	0.40815 (19)	0.0518 (5)
H5A	0.4729	0.3396	0.3311	0.062*
H5B	0.5980	0.2408	0.3552	0.062*
C6	0.6879 (2)	0.38477 (18)	0.48244 (18)	0.0442 (4)
H6A	0.6393	0.4506	0.5156	0.053*

H6B	0.7306	0.4116	0.4019	0.053*
C7	0.82871 (16)	0.34716 (14)	0.62113 (16)	0.0324 (3)
C8	0.77955 (14)	0.30517 (11)	0.76794 (14)	0.0244 (2)
H8	0.7717	0.2249	0.7579	0.029*
C9	0.91820 (15)	0.32805 (12)	0.91322 (15)	0.0269 (2)
H9	1.0184	0.3143	0.8884	0.032*
C10	0.93290 (17)	0.29978 (13)	1.07857 (15)	0.0317 (3)
C11	0.91735 (18)	0.42382 (14)	1.02843 (17)	0.0350 (3)
C12	0.7581 (2)	0.48145 (17)	1.0110 (2)	0.0474 (4)
H12A	0.7766	0.5613	1.0420	0.057*
H12B	0.7095	0.4446	1.0812	0.057*
C13	0.64262 (19)	0.47670 (14)	0.84681 (19)	0.0377 (3)
H13A	0.5402	0.5044	0.8488	0.045*
H13B	0.6798	0.5277	0.7806	0.045*
C14	0.3446 (2)	0.4161 (2)	0.5839 (2)	0.0545 (5)
H14A	0.3648	0.4816	0.6516	0.082*
H14B	0.2430	0.3844	0.5775	0.082*
H14C	0.3457	0.4395	0.4826	0.082*
C15	0.9169 (2)	0.2471 (2)	0.57360 (19)	0.0469 (4)
H15A	0.8513	0.1798	0.5550	0.070*
H15B	1.0128	0.2318	0.6552	0.070*
H15C	0.9418	0.2672	0.4809	0.070*
C16	0.9411 (2)	0.45147 (18)	0.6573 (2)	0.0459 (4)
H16A	1.0290	0.4353	0.7471	0.069*
H16B	0.8854	0.5177	0.6767	0.069*
H16C	0.9789	0.4664	0.5704	0.069*
C17	1.0594 (2)	0.50220 (16)	1.0855 (2)	0.0529 (5)
H17A	1.0320	0.5781	1.0443	0.079*
H17B	1.1446	0.4729	1.0518	0.079*
H17C	1.0917	0.5053	1.1967	0.079*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0372 (2)	0.1166 (5)	0.0572 (3)	0.0018 (3)	0.0294 (2)	-0.0039 (3)
C12	0.0510 (2)	0.0575 (3)	0.0527 (3)	-0.0213 (2)	0.0126 (2)	0.0075 (2)
C13	0.0529 (2)	0.0783 (3)	0.03199 (18)	-0.0149 (2)	0.01578 (16)	0.00474 (19)
C14	0.0432 (2)	0.0512 (2)	0.03845 (19)	0.00492 (18)	-0.01151 (15)	0.00149 (18)
C1	0.0203 (5)	0.0383 (7)	0.0276 (6)	0.0004 (5)	0.0068 (5)	-0.0003 (5)
C2	0.0253 (6)	0.0579 (10)	0.0358 (7)	-0.0060 (6)	0.0120 (5)	-0.0007 (7)
C3	0.0202 (6)	0.0576 (10)	0.0339 (7)	-0.0013 (6)	0.0046 (5)	0.0000 (7)
C4	0.0305 (7)	0.0607 (10)	0.0318 (7)	-0.0065 (7)	-0.0001 (5)	-0.0055 (7)
C5	0.0408 (8)	0.0849 (15)	0.0247 (7)	-0.0039 (9)	0.0024 (6)	-0.0019 (8)
C6	0.0364 (8)	0.0666 (12)	0.0288 (7)	0.0003 (7)	0.0089 (6)	0.0111 (7)
C7	0.0268 (6)	0.0455 (8)	0.0260 (6)	-0.0005 (6)	0.0095 (5)	0.0001 (6)
C8	0.0209 (5)	0.0299 (6)	0.0212 (5)	0.0004 (5)	0.0049 (4)	-0.0022 (5)
C9	0.0220 (5)	0.0327 (6)	0.0244 (6)	0.0006 (5)	0.0048 (4)	-0.0024 (5)
C10	0.0295 (6)	0.0385 (7)	0.0234 (6)	0.0007 (6)	0.0023 (5)	-0.0018 (5)

C11	0.0321 (7)	0.0350 (7)	0.0317 (7)	0.0009 (6)	0.0006 (5)	-0.0070 (6)
C12	0.0456 (9)	0.0486 (9)	0.0434 (9)	0.0131 (7)	0.0066 (7)	-0.0172 (7)
C13	0.0319 (7)	0.0384 (8)	0.0412 (8)	0.0100 (6)	0.0087 (6)	-0.0023 (6)
C14	0.0264 (7)	0.0793 (14)	0.0513 (10)	0.0126 (8)	0.0020 (7)	0.0039 (10)
C15	0.0433 (8)	0.0676 (11)	0.0341 (7)	0.0100 (8)	0.0184 (6)	-0.0059 (8)
C16	0.0372 (8)	0.0578 (11)	0.0453 (9)	-0.0095 (7)	0.0162 (7)	0.0063 (8)
C17	0.0513 (10)	0.0410 (9)	0.0527 (10)	-0.0117 (8)	-0.0050 (8)	-0.0085 (8)

Geometric parameters (Å, °)

C11—C2	1.7682 (17)	C8—H8	0.9380
C12—C2	1.768 (2)	C9—C10	1.5001 (19)
C13—C10	1.7454 (16)	C9—C11	1.528 (2)
C14—C10	1.7744 (14)	C9—H9	0.9951
C1—C13	1.522 (2)	C10—C11	1.506 (2)
C1—C2	1.531 (2)	C11—C17	1.515 (2)
C1—C8	1.5332 (17)	C11—C12	1.529 (2)
C1—C3	1.5468 (19)	C12—C13	1.530 (2)
C2—C3	1.504 (2)	C12—H12A	0.9700
C3—C14	1.517 (2)	C12—H12B	0.9700
C3—C4	1.519 (2)	C13—H13A	0.9700
C4—C5	1.519 (3)	C13—H13B	0.9700
C4—H4A	0.9700	C14—H14A	0.9600
C4—H4B	0.9700	C14—H14B	0.9600
C5—C6	1.521 (3)	C14—H14C	0.9600
C5—H5A	0.9700	C15—H15A	0.9600
C5—H5B	0.9700	C15—H15B	0.9600
C6—C7	1.543 (2)	C15—H15C	0.9600
C6—H6A	0.9700	C16—H16A	0.9600
C6—H6B	0.9700	C16—H16B	0.9600
C7—C15	1.536 (2)	C16—H16C	0.9600
C7—C16	1.541 (2)	C17—H17A	0.9600
C7—C8	1.5970 (19)	C17—H17B	0.9600
C8—C9	1.5283 (17)	C17—H17C	0.9600
C13—C1—C2	118.50 (12)	C10—C9—H9	112.2
C13—C1—C8	113.04 (11)	C11—C9—H9	117.5
C2—C1—C8	120.10 (13)	C8—C9—H9	108.6
C13—C1—C3	118.97 (13)	C9—C10—C11	61.10 (10)
C2—C1—C3	58.50 (10)	C9—C10—C13	124.05 (10)
C8—C1—C3	117.48 (12)	C11—C10—C13	121.55 (11)
C3—C2—C1	61.28 (10)	C9—C10—C14	116.07 (10)
C3—C2—C12	118.84 (13)	C11—C10—C14	117.34 (11)
C1—C2—C12	123.25 (12)	C13—C10—C14	109.57 (8)
C3—C2—C11	120.10 (13)	C10—C11—C17	118.86 (14)
C1—C2—C11	119.01 (12)	C10—C11—C9	59.27 (9)
C12—C2—C11	108.16 (9)	C17—C11—C9	119.72 (15)
C2—C3—C14	120.05 (14)	C10—C11—C12	116.63 (15)

C2—C3—C4	116.41 (16)	C17—C11—C12	114.83 (15)
C14—C3—C4	112.99 (14)	C9—C11—C12	116.42 (12)
C2—C3—C1	60.23 (9)	C11—C12—C13	114.26 (13)
C14—C3—C1	120.64 (16)	C11—C12—H12A	108.7
C4—C3—C1	116.95 (12)	C13—C12—H12A	108.7
C5—C4—C3	111.97 (17)	C11—C12—H12B	108.7
C5—C4—H4A	109.2	C13—C12—H12B	108.7
C3—C4—H4A	109.2	H12A—C12—H12B	107.6
C5—C4—H4B	109.2	C1—C13—C12	112.86 (13)
C3—C4—H4B	109.2	C1—C13—H13A	109.0
H4A—C4—H4B	107.9	C12—C13—H13A	109.0
C4—C5—C6	113.30 (13)	C1—C13—H13B	109.0
C4—C5—H5A	108.9	C12—C13—H13B	109.0
C6—C5—H5A	108.9	H13A—C13—H13B	107.8
C4—C5—H5B	108.9	C3—C14—H14A	109.5
C6—C5—H5B	108.9	C3—C14—H14B	109.5
H5A—C5—H5B	107.7	H14A—C14—H14B	109.5
C5—C6—C7	119.92 (16)	C3—C14—H14C	109.5
C5—C6—H6A	107.3	H14A—C14—H14C	109.5
C7—C6—H6A	107.3	H14B—C14—H14C	109.5
C5—C6—H6B	107.3	C7—C15—H15A	109.5
C7—C6—H6B	107.3	C7—C15—H15B	109.5
H6A—C6—H6B	106.9	H15A—C15—H15B	109.5
C15—C7—C16	107.65 (13)	C7—C15—H15C	109.5
C15—C7—C6	110.06 (13)	H15A—C15—H15C	109.5
C16—C7—C6	105.23 (14)	H15B—C15—H15C	109.5
C15—C7—C8	107.07 (13)	C7—C16—H16A	109.5
C16—C7—C8	112.76 (12)	C7—C16—H16B	109.5
C6—C7—C8	113.95 (11)	H16A—C16—H16B	109.5
C9—C8—C1	112.74 (10)	C7—C16—H16C	109.5
C9—C8—C7	108.15 (10)	H16A—C16—H16C	109.5
C1—C8—C7	114.32 (11)	H16B—C16—H16C	109.5
C9—C8—H8	105.9	C11—C17—H17A	109.5
C1—C8—H8	110.4	C11—C17—H17B	109.5
C7—C8—H8	104.7	H17A—C17—H17B	109.5
C10—C9—C11	59.64 (10)	C11—C17—H17C	109.5
C10—C9—C8	128.69 (12)	H17A—C17—H17C	109.5
C11—C9—C8	123.06 (11)	H17B—C17—H17C	109.5