Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# (1*S*,3*R*,8*R*)-2,2-Dichloro-3,7,7,10-tetramethyltricyclo[6.4.0.0$^{1,3}$]dodec-9-en-11-one

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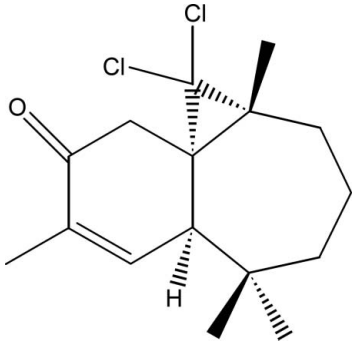
Received 29 April 2013; accepted 30 April 2013

Key indicators: single-crystal X-ray study; $T$ = 180 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.028; $wR$ factor = 0.065; data-to-parameter ratio = 10.4.

The title compound, $C_{16}H_{22}Cl_2O$, was synthesized from $\beta$-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 an additional three-membered ring arising from the reaction of himachalene with dichlorocarbene. The six-membered ring has an envelope conformation, with the C atom belonging to the three-membered ring forming the flap, whereas the seven-membered ring displays a screw-boat conformation; the dihedral angle between the rings (all atoms) is 59.65 (14)°.

## Related literature

For background to the essential oil of the Alas cedar (*Cedrus atlantica*), see: Joseph & Dev (1968); Plattier & Teiseire (1974). For the reactivity and biological properties of $\beta$-himachalene, see: Benharref *et al.* (2012); Chekroun *et al.* (2000); El Jamili *et al.* (2002); Lassaba *et al.* (1998); Dakir *et al.* (2004); Daoubi *et al.* (2004). For conformational analysis, see: Cremer & Pople (1975).




## Experimental

### Crystal data

$C_{16}H_{22}Cl_2O$
$M_r$ = 301.24
Monoclinic, $P2_1$
$a$ = 8.8780 (3) Å
$b$ = 10.3340 (3) Å
$c$ = 8.9230 (3) Å
$\beta$ = 108.805 (4)°
$V$ = 774.94 (4) Å$^3$
$Z$ = 2
Cu $K\alpha$ radiation
$\mu$ = 3.67 mm$^{-1}$
$T$ = 180 K
0.30 × 0.25 × 0.21 mm

### Data collection

Agilent Xcalibur (Eos, Gemini ultra) diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
$T_{min}$ = 0.761, $T_{max}$ = 1.000
2787 measured reflections
1835 independent reflections
1779 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027
$\theta_{max}$ = 60.6°

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.065
$S$ = 1.03
1835 reflections
176 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$
Absolute structure: Flack & Bernardinelli (2000), 614 Friedel pairs
Flack parameter: 0.014 (15)

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; 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) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK5222).

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# supplementary materials

*Acta Cryst.* (2013). E**69**, o830 [doi:10.1107/S1600536813011781]

## (1*S*,3*R*,8*R*)-2,2-Dichloro-3,7,7,10-tetramethyltricyclo[6.4.0.0$^{1,3}$]dodec-9-en-11-one

**Naja Ourhriss, Ahmed Benharref, Abdelouahd Oukhrib, Jean-Claude Daran and Moha Berraho**

### Comment

The essential oil of the Alas cedar (*Cedrus atlantica*) consist mainly (50%) of a bicyclic hydrocarbon called essential oil of the Alas cedar (*Cedrus atlantica*) consist mainly (50%) of a bicyclic hydrocarbon called (Joseph & Dev, 1968; Plattier & Teiseire, 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; Dakir *et al.*, 2004; Benharref *et al.* 2012). Indeed, these compounds were tested, using the food poisoning technique, for their potential antifungal activity against phytopathogen *Botrytis cinerea* (Daoubi *et al.*, 2004). We present here the crystal structure of the title compound, (1*S*,3*R*,8*R*)-2,2-dichloro-3,7,7,10-tetramethyltricyclo [6.4.0.0$^{1}$,$^{3}$]dodec-9-en-10-one. The molecule is built up from two fused six-and seven- membered rings and an additional three-membered ring from the reaction with the carbene (Fig. 1). The six-membered ring has an envelope conformation, as indicated by the total puckering amplitude QT = 0.453 (3) Å and spherical polar angle $\theta$ = 123.4 (4)° with $\varphi$ = 170.0 (4)°, whereas the seven-membered ring display a boat conformation with QT = 1.1545 (3) Å, $\theta$ = 87.74 (2)°, $\varphi$2 = -48.13 (14)° and $\varphi$3 = -134.45 (4)° (Cremer & Pople, 1975). Owing to the presence of Cl atoms, the absolute configuration could be fully confirmed, by refining the Flack parameter (Flack & Bernardinelli, 2000) as C1(*S*), C3(*R*) and C8(*R*).

### Experimental

In a reactor containing a solution of (1*S*, 3*R*, 8*R*)-2,2- dichloro-3,7,7,10 tetramethyltricyclo [6.4.0.0$^{1}$,$^{3}$] dodec-9-ene (1 g, 3.48 mmol) (El Jamili *et al.*, 2002) in 50 ml tetrahydrofuran and water (THF/$H_2O$) (4:1) cooled to 273 K and kept in the dark, was added in small portions 1.23 g (6.96 mmol) of *N*-bromosccinimide (NBS). The reaction mixture was left stirring for 1 h, after which 20 ml of a saturated solution of $NaHCO_3$ was added. Subsequently, the extraction was performed three times with diethyl ether (3x 20 ml). The organic extracts were dried over $Na_2SO_4$, filtered, concentrated, and chromatographed. The title compound was obtained with a yield of 80% and was recrystallized from its hexane solution.

### 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 $U_{iso}$(H) = 1.2$U_{eq}$(methylene, methine) or $U_{iso}$(H) = 1.5$U_{eq}$(methyl). Owing to the tiny size of the crystal and to define the correct absolute structure determination, the data were collected using Cu radiation.

### Computing details

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO* (Agilent, 2010); data reduction: *CrysAlis PRO* (Agilent, 2010); 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) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

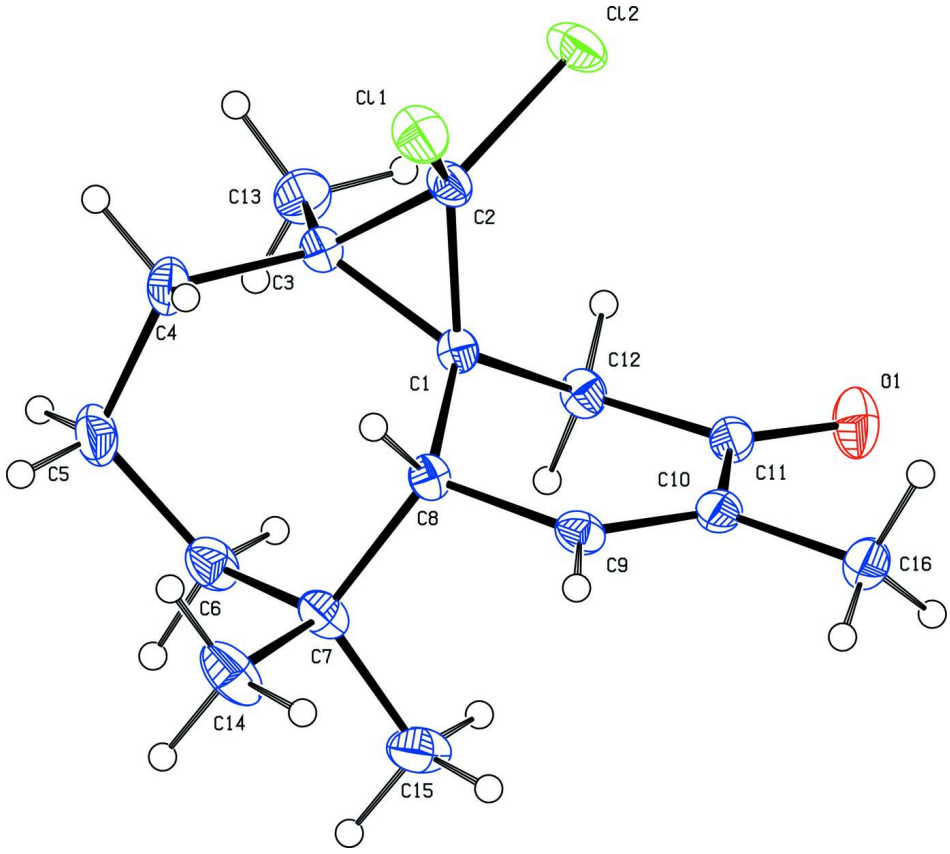


**Figure 1**

Molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability. level. H atoms are represented as small spheres of arbitrary radii.

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*Crystal data*

$C_{16}H_{22}Cl_2O$
$M_r$ = 301.24
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a$ = 8.8780 (3) Å
$b$ = 10.3340 (3) Å
$c$ = 8.9230 (3) Å
$\beta$ = 108.805 (4)°
$V$ = 774.94 (4) Å$^3$
$Z$ = 2
$F(000)$ = 320
$D_x$ = 1.291 Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda$ = 1.5418 Å
Cell parameters from 1955 reflections
$\theta$ = 4.3–60.5°
$\mu$ = 3.67 mm$^{-1}$
$T$ = 180 K
Block, colourless
0.30 × 0.25 × 0.21 mm

*Data collection*

Agilent Xcalibur (Eos, Gemini ultra) diffractometer
Radiation source: Enhance Ultra (Cu) X-ray Source
Mirror monochromator
Detector resolution: 16.1978 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
$T_{min}$ = 0.761, $T_{max}$ = 1.000

2787 measured reflections
1835 independent reflections
1779 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 60.6°$, $\theta_{min} = 5.2°$
$h = -9 \rightarrow 8$
$k = -11 \rightarrow 11$
$l = -8 \rightarrow 10$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.065$
$S = 1.03$
1835 reflections
176 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
$w = 1/[\sigma^2(F_o^2) + (0.0268P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å$^{-3}$
$\Delta\rho_{min} = -0.17$ e Å$^{-3}$
Absolute structure: Flack & Bernardinelli (2000), 614 Friedel pairs
Flack parameter: 0.014 (15)

*Special details*

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.37702 (8) | 0.87301 (6) | 0.63481 (9) | 0.04024 (19) |
| Cl2 | 0.53172 (8) | 0.67535 (7) | 0.51438 (9) | 0.0422 (2) |
| O1 | 0.7317 (2) | 0.4592 (2) | 0.9131 (3) | 0.0472 (6) |
| C1 | 0.3527 (3) | 0.6081 (2) | 0.7144 (3) | 0.0230 (6) |
| C2 | 0.3817 (3) | 0.7052 (2) | 0.6004 (3) | 0.0278 (6) |
| C3 | 0.2321 (3) | 0.6249 (2) | 0.5493 (3) | 0.0280 (6) |
| C4 | 0.0763 (3) | 0.6914 (3) | 0.5429 (3) | 0.0367 (7) |
| H4A | 0.0196 | 0.7190 | 0.4329 | 0.044* |
| H4B | 0.1000 | 0.7696 | 0.6105 | 0.044* |
| C5 | −0.0311 (3) | 0.6006 (3) | 0.5995 (4) | 0.0417 (8) |
| H5A | −0.1098 | 0.6536 | 0.6294 | 0.050* |
| H5B | −0.0906 | 0.5446 | 0.5100 | 0.050* |
| C6 | 0.0567 (3) | 0.5144 (3) | 0.7398 (3) | 0.0366 (7) |
| H6A | 0.1202 | 0.4510 | 0.7025 | 0.044* |
| H6B | −0.0241 | 0.4650 | 0.7708 | 0.044* |
| C7 | 0.1685 (3) | 0.5800 (3) | 0.8897 (3) | 0.0310 (6) |
| C8 | 0.3075 (3) | 0.6569 (3) | 0.8553 (3) | 0.0249 (6) |
| H8 | 0.2677 | 0.7473 | 0.8285 | 0.030* |
| C9 | 0.4529 (3) | 0.6672 (3) | 0.9982 (3) | 0.0276 (6) |
| H9 | 0.4453 | 0.7195 | 1.0830 | 0.033* |

| | | | | |
|---|---|---|---|---|
| C10 | 0.5923 (3) | 0.6092 (3) | 1.0171 (3) | 0.0289 (7) |
| C11 | 0.6079 (3) | 0.5170 (3) | 0.8973 (3) | 0.0289 (6) |
| C12 | 0.4618 (3) | 0.4911 (2) | 0.7555 (3) | 0.0276 (6) |
| H12A | 0.4028 | 0.4166 | 0.7788 | 0.033* |
| H12B | 0.4953 | 0.4681 | 0.6633 | 0.033* |
| C13 | 0.2113 (4) | 0.5220 (3) | 0.4243 (3) | 0.0410 (7) |
| H13A | 0.1623 | 0.5602 | 0.3193 | 0.061* |
| H13B | 0.1426 | 0.4530 | 0.4411 | 0.061* |
| H13C | 0.3154 | 0.4858 | 0.4313 | 0.061* |
| C14 | 0.0742 (4) | 0.6748 (4) | 0.9559 (4) | 0.0483 (8) |
| H14A | 0.0328 | 0.7447 | 0.8794 | 0.072* |
| H14B | 0.1439 | 0.7114 | 1.0555 | 0.072* |
| H14C | −0.0145 | 0.6294 | 0.9753 | 0.072* |
| C15 | 0.2324 (4) | 0.4722 (3) | 1.0132 (3) | 0.0422 (8) |
| H15A | 0.3011 | 0.5103 | 1.1123 | 0.063* |
| H15B | 0.2937 | 0.4101 | 0.9733 | 0.063* |
| H15C | 0.1429 | 0.4277 | 1.0326 | 0.063* |
| C16 | 0.7361 (3) | 0.6288 (3) | 1.1612 (4) | 0.0395 (8) |
| H16A | 0.8121 | 0.6856 | 1.1345 | 0.059* |
| H16B | 0.7863 | 0.5450 | 1.1974 | 0.059* |
| H16C | 0.7034 | 0.6686 | 1.2456 | 0.059* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0401 (4) | 0.0234 (3) | 0.0606 (5) | 0.0026 (3) | 0.0209 (3) | 0.0072 (3) |
| Cl2 | 0.0418 (4) | 0.0447 (4) | 0.0518 (4) | 0.0023 (3) | 0.0313 (3) | 0.0049 (4) |
| O1 | 0.0303 (11) | 0.0442 (12) | 0.0622 (14) | 0.0111 (10) | 0.0081 (9) | 0.0002 (11) |
| C1 | 0.0221 (13) | 0.0210 (12) | 0.0259 (15) | 0.0004 (10) | 0.0077 (10) | −0.0016 (11) |
| C2 | 0.0249 (14) | 0.0268 (14) | 0.0358 (16) | 0.0033 (10) | 0.0153 (11) | 0.0027 (12) |
| C3 | 0.0240 (14) | 0.0314 (15) | 0.0292 (15) | 0.0012 (11) | 0.0093 (11) | 0.0024 (11) |
| C4 | 0.0246 (15) | 0.0439 (17) | 0.0376 (17) | 0.0060 (12) | 0.0046 (11) | 0.0013 (14) |
| C5 | 0.0207 (14) | 0.0578 (19) | 0.0425 (18) | −0.0052 (13) | 0.0044 (12) | −0.0043 (16) |
| C6 | 0.0323 (16) | 0.0418 (16) | 0.0368 (17) | −0.0130 (13) | 0.0126 (12) | −0.0085 (13) |
| C7 | 0.0290 (15) | 0.0355 (15) | 0.0319 (16) | −0.0079 (12) | 0.0146 (11) | −0.0076 (13) |
| C8 | 0.0224 (13) | 0.0252 (14) | 0.0273 (14) | 0.0002 (11) | 0.0084 (10) | −0.0021 (13) |
| C9 | 0.0299 (15) | 0.0271 (13) | 0.0277 (14) | −0.0078 (12) | 0.0119 (10) | −0.0036 (13) |
| C10 | 0.0274 (16) | 0.0276 (14) | 0.0301 (16) | −0.0066 (12) | 0.0073 (11) | 0.0058 (12) |
| C11 | 0.0249 (15) | 0.0258 (13) | 0.0362 (16) | 0.0015 (11) | 0.0100 (11) | 0.0087 (12) |
| C12 | 0.0279 (14) | 0.0232 (13) | 0.0333 (15) | 0.0039 (11) | 0.0121 (11) | −0.0018 (12) |
| C13 | 0.0425 (17) | 0.0523 (18) | 0.0275 (16) | −0.0021 (14) | 0.0105 (13) | −0.0078 (14) |
| C14 | 0.0409 (17) | 0.0547 (19) | 0.061 (2) | −0.0082 (16) | 0.0327 (15) | −0.0181 (18) |
| C15 | 0.0506 (19) | 0.0452 (18) | 0.0344 (17) | −0.0140 (15) | 0.0189 (13) | 0.0004 (15) |
| C16 | 0.0299 (16) | 0.0473 (19) | 0.0361 (17) | −0.0025 (12) | 0.0033 (12) | 0.0105 (14) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C2 | 1.764 (3) | C8—C9 | 1.497 (3) |
| Cl2—C2 | 1.766 (3) | C8—H8 | 1.0000 |
| O1—C11 | 1.218 (3) | C9—C10 | 1.336 (4) |

| | | | |
|---|---|---|---|
| C1—C2 | 1.509 (4) | C9—H9 | 0.9500 |
| C1—C12 | 1.519 (3) | C10—C11 | 1.472 (4) |
| C1—C8 | 1.523 (4) | C10—C16 | 1.505 (4) |
| C1—C3 | 1.526 (3) | C11—C12 | 1.516 (4) |
| C2—C3 | 1.506 (4) | C12—H12A | 0.9900 |
| C3—C13 | 1.509 (4) | C12—H12B | 0.9900 |
| C3—C4 | 1.529 (4) | C13—H13A | 0.9800 |
| C4—C5 | 1.534 (4) | C13—H13B | 0.9800 |
| C4—H4A | 0.9900 | C13—H13C | 0.9800 |
| C4—H4B | 0.9900 | C14—H14A | 0.9800 |
| C5—C6 | 1.529 (4) | C14—H14B | 0.9800 |
| C5—H5A | 0.9900 | C14—H14C | 0.9800 |
| C5—H5B | 0.9900 | C15—H15A | 0.9800 |
| C6—C7 | 1.543 (4) | C15—H15B | 0.9800 |
| C6—H6A | 0.9900 | C15—H15C | 0.9800 |
| C6—H6B | 0.9900 | C16—H16A | 0.9800 |
| C7—C14 | 1.526 (4) | C16—H16B | 0.9800 |
| C7—C15 | 1.541 (4) | C16—H16C | 0.9800 |
| C7—C8 | 1.579 (4) | | |

| | | | |
|---|---|---|---|
| C2—C1—C12 | 117.2 (2) | C1—C8—C7 | 115.1 (2) |
| C2—C1—C8 | 119.0 (2) | C9—C8—H8 | 106.2 |
| C12—C1—C8 | 112.4 (2) | C1—C8—H8 | 106.2 |
| C2—C1—C3 | 59.49 (16) | C7—C8—H8 | 106.2 |
| C12—C1—C3 | 121.2 (2) | C10—C9—C8 | 125.8 (2) |
| C8—C1—C3 | 118.0 (2) | C10—C9—H9 | 117.1 |
| C3—C2—C1 | 60.82 (17) | C8—C9—H9 | 117.1 |
| C3—C2—Cl1 | 121.74 (18) | C9—C10—C11 | 119.9 (2) |
| C1—C2—Cl1 | 121.15 (19) | C9—C10—C16 | 122.9 (3) |
| C3—C2—Cl2 | 119.2 (2) | C11—C10—C16 | 117.1 (2) |
| C1—C2—Cl2 | 119.59 (18) | O1—C11—C10 | 121.7 (2) |
| Cl1—C2—Cl2 | 108.11 (14) | O1—C11—C12 | 120.5 (2) |
| C2—C3—C13 | 119.9 (2) | C10—C11—C12 | 117.7 (2) |
| C2—C3—C1 | 59.68 (17) | C11—C12—C1 | 111.6 (2) |
| C13—C3—C1 | 120.9 (2) | C11—C12—H12A | 109.3 |
| C2—C3—C4 | 117.6 (2) | C1—C12—H12A | 109.3 |
| C13—C3—C4 | 113.3 (2) | C11—C12—H12B | 109.3 |
| C1—C3—C4 | 115.6 (2) | C1—C12—H12B | 109.3 |
| C3—C4—C5 | 111.3 (2) | H12A—C12—H12B | 108.0 |
| C3—C4—H4A | 109.4 | C3—C13—H13A | 109.5 |
| C5—C4—H4A | 109.4 | C3—C13—H13B | 109.5 |
| C3—C4—H4B | 109.4 | H13A—C13—H13B | 109.5 |
| C5—C4—H4B | 109.4 | C3—C13—H13C | 109.5 |
| H4A—C4—H4B | 108.0 | H13A—C13—H13C | 109.5 |
| C6—C5—C4 | 114.8 (2) | H13B—C13—H13C | 109.5 |
| C6—C5—H5A | 108.6 | C7—C14—H14A | 109.5 |
| C4—C5—H5A | 108.6 | C7—C14—H14B | 109.5 |
| C6—C5—H5B | 108.6 | H14A—C14—H14B | 109.5 |
| C4—C5—H5B | 108.6 | C7—C14—H14C | 109.5 |

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| H5A—C5—H5B | 107.6 | H14A—C14—H14C | 109.5 |
| C5—C6—C7 | 118.0 (3) | H14B—C14—H14C | 109.5 |
| C5—C6—H6A | 107.8 | C7—C15—H15A | 109.5 |
| C7—C6—H6A | 107.8 | C7—C15—H15B | 109.5 |
| C5—C6—H6B | 107.8 | H15A—C15—H15B | 109.5 |
| C7—C6—H6B | 107.8 | C7—C15—H15C | 109.5 |
| H6A—C6—H6B | 107.1 | H15A—C15—H15C | 109.5 |
| C14—C7—C15 | 108.0 (2) | H15B—C15—H15C | 109.5 |
| C14—C7—C6 | 109.7 (2) | C10—C16—H16A | 109.5 |
| C15—C7—C6 | 106.7 (2) | C10—C16—H16B | 109.5 |
| C14—C7—C8 | 108.2 (2) | H16A—C16—H16B | 109.5 |
| C15—C7—C8 | 111.9 (2) | C10—C16—H16C | 109.5 |
| C6—C7—C8 | 112.2 (2) | H16A—C16—H16C | 109.5 |
| C9—C8—C1 | 110.0 (2) | H16B—C16—H16C | 109.5 |
| C9—C8—C7 | 112.5 (2) | | |