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# (1*S*,3*R*,8*S*,9*R*,10*S*)-2,2-Dichloro-3,7,7,10-tetramethyl-9,10-epoxy-tricyclo[6.4.0.0$^{1,3}$]dodecane

**Ahmed Benharref,[a]* Lahcen El Ammari,[b] Daniel Avignant,[c] Abdelghani Oudahmane[c] and Moha Berraho[a]**

[a]Laboratoire de Chimie Biomoléculaires, Substances Naturelles et Réactivité, URAC16, Faculté des Sciences, Semlalia, BP 2390 Bd My Abdellah, 40000 Marrakech, Morocco, [b]Laboratoire de Chimie du Solide Appliquée, Faculté des Sciences, Avenue Ibn Battouta, BP 1014 Rabat, Morocco, and [c]Université Blaise Pascal, Laboratoire des Matériaux Inorganiques, UMR CNRS 6002, 24 Avenue des Landais, 63177 Aubière, France
Correspondence e-mail: abenharref@yahoo.fr

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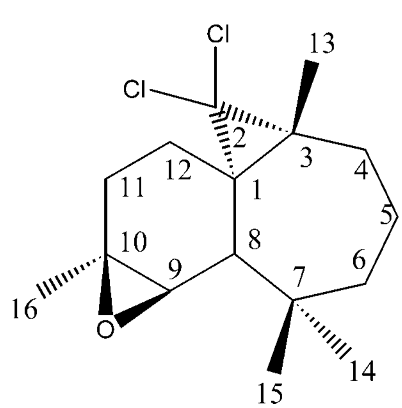
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.040; $wR$ factor = 0.106; data-to-parameter ratio = 19.0.

The title compound, $C_{16}H_{24}Cl_2O$, 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 forms an extended sheet of two fused rings which exhibit different conformations. The six-membered ring has a half-chair conformation, while the seven-membered ring displays a chair conformation; the dihedral angle between the two rings is 38.2 (1)°.

## Related literature

For the isolation of $\beta$-himachalene, see: Joseph & Dev (1968); Plattier & Teiseire (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 ring puckering parameters, see: Cremer & Pople (1975).




## Experimental

*Crystal data*

| | |
|---|---|
| $C_{16}H_{24}Cl_2O$ | $V$ = 1581.98 (10) Å$^3$ |
| $M_r$ = 303.24 | $Z$ = 4 |
| Orthorhombic, $P2_12_12_1$ | Mo $K\alpha$ radiation |
| $a$ = 8.4995 (3) Å | $\mu$ = 0.40 mm$^{-1}$ |
| $b$ = 10.2461 (4) Å | $T$ = 298 K |
| $c$ = 18.1656 (6) Å | 0.67 × 0.41 × 0.26 mm |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD diffractometer | 7171 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2008) | 3369 independent reflections |
| $T_{min}$ = 0.609, $T_{max}$ = 0.745 | 2830 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.025 |

*Refinement*

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.040 | $\Delta\rho_{max}$ = 0.22 e Å$^{-3}$ |
| $wR(F^2)$ = 0.106 | $\Delta\rho_{min}$ = −0.29 e Å$^{-3}$ |
| $S$ = 1.01 | Absolute structure: Flack & Bernardinelli (2000), 1423 Friedel pairs |
| 3369 reflections | Flack parameter: 0.04 (7) |
| 177 parameters | |
| H-atom parameters constrained | |

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, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2241).

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# supporting information

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## (1*S*,3*R*,8*S*,9*R*,10*S*)-2,2-Dichloro-3,7,7,10-tetramethyl-9,10-epoxytricyclo-[6.4.0.0$^{1,3}$]dodecane

Ahmed Benharref, Lahcen El Ammari, Daniel Avignant, Abdelghani Oudahmane and Moha Berraho

### S1. Comment

The bicyclic sesquiterpene *β*-himachalene is the main constituent of the essential oil of the Atlas cedar (*Cedrus atlantica*) (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; 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 one equivalent of dichlorocarbene, generated *in situ* from chloroform in the presence of sodium hydroxide as base and n-benzyltriethylammonium chloride as catalyst, on *β*-himachalene produces only (1*S*,3*R*,8*S*)-2,2-dichloro-3,7,7,10- tetramethyltricyclo[6,4,0,0$^{1,3}$]dodec-9-ene (*X*) (El Jamili *et al.*, 2002). Treatement of (*X*) with one equivalent of *meta*-chloroperbenzoic acid (mCPBA) leads to a mixture of two diastereisomers: (1*S*, 3*R*, 8S, 9S, 10*R*)-2,2-dichloro-9–10-epoxy-3,7,7,10-tetramethyl- tricyclo[6.4.0.0$^{1,3}$]dodecane (*Y*) and its isomer (1*S*, 3*R*, 8S, 9*R*, 10S)-2,2-di-chloro-9–10-epoxy-3,7,7,10-tetramethyl-tricyclo[6.4.0.0$^{1,3}$]dodecane (*Z*) in an over-all yield of 80% and 30:70 ratio. In a previous work (Sbai *et al.*, 2002), we have determined the structure and the stereochemistry of *Y.* In this paper we present the absolute configuration of *Z* established by single-crystal X-ray diffraction analysis. The molecule is built up from two fused six-membered and seven-membered rings (Fig. 1). The six-membered ring has a half chair conformation, as indicated by the total puckering amplitude QT = 0.513 (2) Å and spherical polar angle $\theta$ = 125.9 (2)° with $\varphi$ = 138.1 (4)°, whereas the seven-membered ring displays an aproximate chair conformation with QT = 0.783 (3) Å, $\theta$ = 31.9 (3)°, $\varphi2$ = -50.3 (4)° and $\varphi3$ =-78.3 (2)° (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*), C8(S), C9(*R*) and C10(*S*).

### S2. Experimental

For the synthesis of compounds (1*S*, 3*R*, 8S, 9S, 10*R*)-2,2-dichloro-9–10- epoxy-3,7,7,10-tetramethyl-tricyclo-[6.4.0.0$^{1,3}$]dodecane (*Y*) and its isomer (1*S*, 3*R*, 8S, 9*R*, 10S)-2,2-dichloro-9–10-epoxy-3,7,7,10- tetramethyl-tricyclo-[6.4.0.0$^{1,3}$]dodecane (*Z*), a stoichiometric quantity of *m*-chloroperbenzoic acid (*m*-CPBA) was added to a 100 ml flask containing a solution of (1*S*,3*R*,8*S*)-2,2-dicchloro-3,7,7,10- tetramethyltricyclo[6,4,0,0$^{1,3}$]dodec-9-ene (*X*) (500 mg, 1.74 mmol) in $CH_2Cl_2$ (30 ml). The reaction mixture was stirred at ambient temperature for 2 h, then treated with a 10% solution of sodium hydrogencarbonate. The aqueous phase was extracted with ether and the organic phases were dried and concentrated. Chromatography of the residue on silica (hexane/ethyl acetate 97/3) allowed the isolation of both isomers *Y* and *Z* in a pure state. Crystallization of *Z* was carried out at room temperature from a hexane solution.

## S3. Refinement

All H atoms were fixed geometrically and treated as riding with C—H = 0.96 Å (methyl), 0.97 Å (methylene), 0.98Å (methine) with $U_{iso}(H) = 1.2U_{eq}$ (methylene, methine) or $U_{iso}(H) = 1.5U_{eq}$ (methyl).

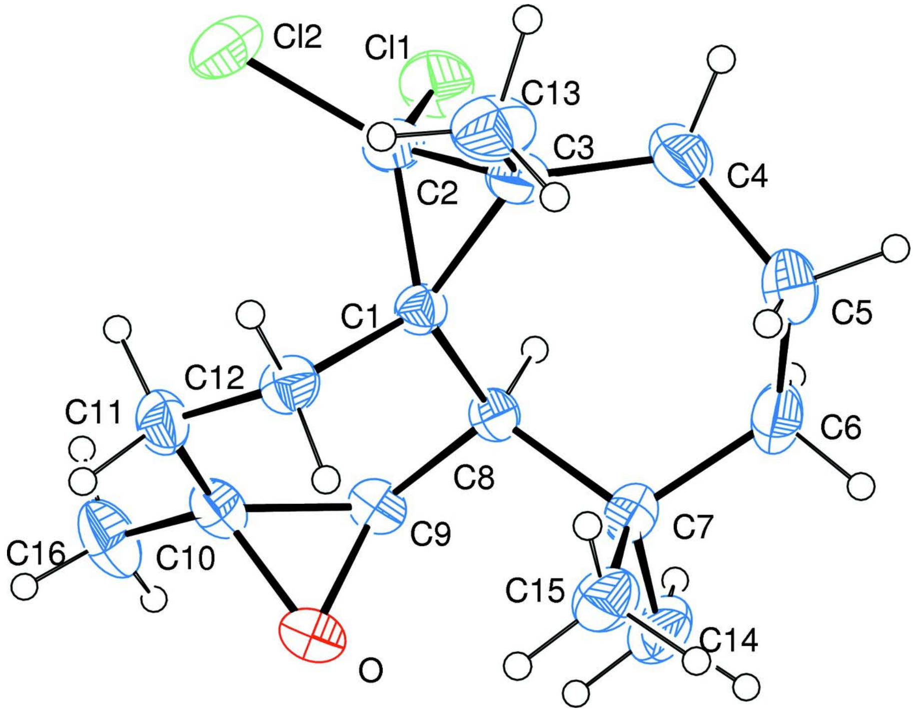


**Figure 1**

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.

## (1*S*,3*R*,8*S*,9*R*,10*S*)-2,2-Dichloro- 3,7,7,10-tetramethyl-9,10-epoxytricyclo[6.4.0.0$^{1,3}$]dodecane

### *Crystal data*

$C_{16}H_{24}Cl_2O$
$M_r = 303.24$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 8.4995$ (3) Å
$b = 10.2461$ (4) Å
$c = 18.1656$ (6) Å
$V = 1581.98$ (10) Å$^3$
$Z = 4$
$F(000) = 648$
$D_x = 1.273$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3372 reflections
$\theta = 2.3–26.9°$
$\mu = 0.40$ mm$^{-1}$
$T = 298$ K
Prism, colourless
0.67 × 0.41 × 0.26 mm

### *Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm$^{-1}$
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min} = 0.609$, $T_{max} = 0.745$
7171 measured reflections
3369 independent reflections
2830 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 26.9°$, $\theta_{min} = 2.3°$
$h = -9 \rightarrow 10$
$k = -13 \rightarrow 10$
$l = -16 \rightarrow 22$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.106$
$S = 1.01$
3369 reflections
177 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
$w = 1/[\sigma^2(F_o^2) + (0.0568P)^2 + 0.1767P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.22$ e Å$^{-3}$
$\Delta\rho_{min} = -0.29$ e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.073 (4)
Absolute structure: Flack & Bernardinelli (2000), 1423 Friedel pairs
Absolute structure parameter: 0.04 (7)

*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.

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

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.6413 (2) | 0.5366 (2) | 0.38517 (10) | 0.0356 (4) |
| C2 | 0.5713 (3) | 0.5121 (2) | 0.46043 (13) | 0.0457 (5) |
| C3 | 0.6259 (3) | 0.3964 (2) | 0.41628 (12) | 0.0460 (5) |
| C4 | 0.7701 (3) | 0.3249 (3) | 0.44259 (15) | 0.0630 (7) |
| H4A | 0.7375 | 0.2445 | 0.4663 | 0.076* |
| H4B | 0.8230 | 0.3780 | 0.4792 | 0.076* |
| C5 | 0.8864 (3) | 0.2922 (3) | 0.38160 (18) | 0.0675 (8) |
| H5A | 0.9496 | 0.2180 | 0.3967 | 0.081* |
| H5B | 0.8285 | 0.2671 | 0.3378 | 0.081* |
| C6 | 0.9941 (3) | 0.4052 (3) | 0.36304 (16) | 0.0622 (7) |
| H6A | 1.0759 | 0.3720 | 0.3308 | 0.075* |
| H6B | 1.0451 | 0.4322 | 0.4083 | 0.075* |
| C7 | 0.9253 (3) | 0.5290 (2) | 0.32646 (13) | 0.0464 (5) |
| C8 | 0.8050 (2) | 0.59920 (19) | 0.37903 (11) | 0.0359 (4) |
| H8 | 0.8509 | 0.5936 | 0.4284 | 0.043* |
| C9 | 0.7899 (3) | 0.7442 (2) | 0.36270 (12) | 0.0417 (5) |
| H9 | 0.8687 | 0.7990 | 0.3871 | 0.050* |
| C10 | 0.6401 (3) | 0.8106 (2) | 0.34700 (12) | 0.0472 (5) |
| C11 | 0.4936 (3) | 0.7314 (2) | 0.34176 (14) | 0.0513 (6) |
| H11A | 0.4293 | 0.7650 | 0.3019 | 0.062* |
| H11B | 0.4344 | 0.7408 | 0.3871 | 0.062* |
| C12 | 0.5260 (3) | 0.5877 (2) | 0.32837 (12) | 0.0438 (5) |
| H12A | 0.4284 | 0.5389 | 0.3314 | 0.053* |
| H12B | 0.5692 | 0.5760 | 0.2794 | 0.053* |
| C13 | 0.5035 (4) | 0.3054 (3) | 0.38394 (17) | 0.0677 (8) |

| | | | | |
|---|---|---|---|---|
| H13A | 0.4747 | 0.2411 | 0.4199 | 0.102* |
| H13B | 0.5462 | 0.2627 | 0.3413 | 0.102* |
| H13C | 0.4121 | 0.3547 | 0.3701 | 0.102* |
| C14 | 1.0652 (3) | 0.6208 (3) | 0.31365 (18) | 0.0665 (8) |
| H14A | 1.1444 | 0.5764 | 0.2855 | 0.100* |
| H14B | 1.1083 | 0.6469 | 0.3602 | 0.100* |
| H14C | 1.0303 | 0.6966 | 0.2872 | 0.100* |
| C15 | 0.8565 (3) | 0.4933 (3) | 0.25117 (13) | 0.0575 (6) |
| H15A | 0.8199 | 0.5710 | 0.2271 | 0.086* |
| H15B | 0.7702 | 0.4340 | 0.2577 | 0.086* |
| H15C | 0.9362 | 0.4527 | 0.2216 | 0.086* |
| C16 | 0.6208 (4) | 0.9531 (3) | 0.36539 (17) | 0.0711 (8) |
| H16A | 0.7209 | 0.9961 | 0.3619 | 0.107* |
| H16B | 0.5809 | 0.9617 | 0.4146 | 0.107* |
| H16C | 0.5484 | 0.9924 | 0.3314 | 0.107* |
| O | 0.7511 (2) | 0.78441 (15) | 0.28799 (9) | 0.0529 (4) |
| Cl1 | 0.66972 (9) | 0.56107 (8) | 0.54165 (3) | 0.0691 (2) |
| Cl2 | 0.36713 (8) | 0.53272 (8) | 0.47590 (4) | 0.0698 (2) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0372 (10) | 0.0357 (10) | 0.0339 (9) | 0.0002 (9) | 0.0019 (9) | −0.0013 (8) |
| C2 | 0.0485 (11) | 0.0517 (13) | 0.0369 (11) | −0.0012 (10) | 0.0050 (10) | 0.0004 (10) |
| C3 | 0.0565 (13) | 0.0393 (12) | 0.0423 (11) | −0.0039 (10) | 0.0074 (11) | 0.0030 (9) |
| C4 | 0.0839 (18) | 0.0461 (14) | 0.0591 (16) | 0.0145 (13) | 0.0087 (14) | 0.0109 (12) |
| C5 | 0.0754 (18) | 0.0448 (14) | 0.0822 (19) | 0.0203 (13) | 0.0098 (16) | 0.0030 (13) |
| C6 | 0.0529 (15) | 0.0563 (16) | 0.0774 (17) | 0.0187 (12) | 0.0092 (14) | −0.0024 (13) |
| C7 | 0.0389 (11) | 0.0482 (13) | 0.0521 (12) | 0.0031 (10) | 0.0054 (10) | −0.0031 (11) |
| C8 | 0.0356 (10) | 0.0379 (11) | 0.0342 (10) | −0.0006 (9) | −0.0059 (9) | −0.0004 (8) |
| C9 | 0.0470 (12) | 0.0384 (11) | 0.0396 (11) | −0.0050 (9) | −0.0071 (10) | −0.0009 (9) |
| C10 | 0.0595 (14) | 0.0389 (12) | 0.0432 (11) | 0.0053 (10) | −0.0069 (11) | 0.0019 (9) |
| C11 | 0.0449 (13) | 0.0572 (15) | 0.0517 (14) | 0.0121 (11) | −0.0082 (11) | 0.0051 (11) |
| C12 | 0.0353 (11) | 0.0537 (13) | 0.0424 (11) | −0.0042 (10) | −0.0034 (9) | −0.0007 (10) |
| C13 | 0.081 (2) | 0.0477 (14) | 0.0743 (18) | −0.0225 (13) | 0.0173 (16) | −0.0033 (13) |
| C14 | 0.0397 (13) | 0.0759 (19) | 0.084 (2) | −0.0028 (12) | 0.0119 (14) | 0.0010 (15) |
| C15 | 0.0643 (15) | 0.0617 (15) | 0.0467 (13) | 0.0046 (13) | 0.0106 (12) | −0.0106 (11) |
| C16 | 0.095 (2) | 0.0450 (14) | 0.0737 (17) | 0.0165 (14) | −0.0216 (17) | 0.0008 (13) |
| O | 0.0632 (11) | 0.0497 (10) | 0.0458 (9) | −0.0048 (8) | −0.0006 (8) | 0.0107 (8) |
| Cl1 | 0.0888 (5) | 0.0842 (5) | 0.0342 (3) | 0.0068 (4) | −0.0030 (3) | −0.0063 (3) |
| Cl2 | 0.0547 (4) | 0.0862 (5) | 0.0683 (4) | −0.0017 (3) | 0.0248 (3) | 0.0005 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.512 (3) | C9—O | 1.456 (3) |
| C1—C12 | 1.517 (3) | C9—C10 | 1.472 (3) |
| C1—C8 | 1.536 (3) | C9—H9 | 0.9800 |
| C1—C3 | 1.550 (3) | C10—O | 1.453 (3) |

| | | | |
|---|---|---|---|
| C2—C3 | 1.505 (3) | C10—C11 | 1.489 (3) |
| C2—Cl1 | 1.769 (2) | C10—C16 | 1.507 (3) |
| C2—Cl2 | 1.770 (2) | C11—C12 | 1.517 (3) |
| C3—C4 | 1.506 (3) | C11—H11A | 0.9700 |
| C3—C13 | 1.516 (4) | C11—H11B | 0.9700 |
| C4—C5 | 1.522 (4) | C12—H12A | 0.9700 |
| C4—H4A | 0.9700 | C12—H12B | 0.9700 |
| C4—H4B | 0.9700 | C13—H13A | 0.9600 |
| C5—C6 | 1.515 (4) | C13—H13B | 0.9600 |
| C5—H5A | 0.9700 | C13—H13C | 0.9600 |
| C5—H5B | 0.9700 | C14—H14A | 0.9600 |
| C6—C7 | 1.546 (3) | C14—H14B | 0.9600 |
| C6—H6A | 0.9700 | C14—H14C | 0.9600 |
| C6—H6B | 0.9700 | C15—H15A | 0.9600 |
| C7—C15 | 1.532 (3) | C15—H15B | 0.9600 |
| C7—C14 | 1.534 (4) | C15—H15C | 0.9600 |
| C7—C8 | 1.574 (3) | C16—H16A | 0.9600 |
| C8—C9 | 1.521 (3) | C16—H16B | 0.9600 |
| C8—H8 | 0.9800 | C16—H16C | 0.9600 |

| | | | |
|---|---|---|---|
| C2—C1—C12 | 114.70 (17) | O—C9—C8 | 118.51 (17) |
| C2—C1—C8 | 119.45 (17) | C10—C9—C8 | 124.23 (19) |
| C12—C1—C8 | 113.09 (17) | O—C9—H9 | 114.5 |
| C2—C1—C3 | 58.86 (14) | C10—C9—H9 | 114.5 |
| C12—C1—C3 | 120.89 (19) | C8—C9—H9 | 114.5 |
| C8—C1—C3 | 119.35 (18) | O—C10—C9 | 59.71 (14) |
| C3—C2—C1 | 61.81 (14) | O—C10—C11 | 113.26 (19) |
| C3—C2—Cl1 | 121.47 (17) | C9—C10—C11 | 118.93 (18) |
| C1—C2—Cl1 | 121.38 (16) | O—C10—C16 | 114.4 (2) |
| C3—C2—Cl2 | 118.75 (17) | C9—C10—C16 | 120.0 (2) |
| C1—C2—Cl2 | 120.64 (16) | C11—C10—C16 | 116.8 (2) |
| Cl1—C2—Cl2 | 107.30 (12) | C10—C11—C12 | 112.81 (18) |
| C2—C3—C4 | 117.7 (2) | C10—C11—H11A | 109.0 |
| C2—C3—C13 | 118.7 (2) | C12—C11—H11A | 109.0 |
| C4—C3—C13 | 112.5 (2) | C10—C11—H11B | 109.0 |
| C2—C3—C1 | 59.33 (14) | C12—C11—H11B | 109.0 |
| C4—C3—C1 | 119.9 (2) | H11A—C11—H11B | 107.8 |
| C13—C3—C1 | 119.2 (2) | C1—C12—C11 | 110.06 (18) |
| C3—C4—C5 | 113.9 (2) | C1—C12—H12A | 109.6 |
| C3—C4—H4A | 108.8 | C11—C12—H12A | 109.6 |
| C5—C4—H4A | 108.8 | C1—C12—H12B | 109.6 |
| C3—C4—H4B | 108.8 | C11—C12—H12B | 109.6 |
| C5—C4—H4B | 108.8 | H12A—C12—H12B | 108.2 |
| H4A—C4—H4B | 107.7 | C3—C13—H13A | 109.5 |
| C6—C5—C4 | 112.7 (2) | C3—C13—H13B | 109.5 |
| C6—C5—H5A | 109.0 | H13A—C13—H13B | 109.5 |
| C4—C5—H5A | 109.0 | C3—C13—H13C | 109.5 |
| C6—C5—H5B | 109.0 | H13A—C13—H13C | 109.5 |

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| C4—C5—H5B | 109.0 | H13B—C13—H13C | 109.5 |
| H5A—C5—H5B | 107.8 | C7—C14—H14A | 109.5 |
| C5—C6—C7 | 119.6 (2) | C7—C14—H14B | 109.5 |
| C5—C6—H6A | 107.4 | H14A—C14—H14B | 109.5 |
| C7—C6—H6A | 107.4 | C7—C14—H14C | 109.5 |
| C5—C6—H6B | 107.4 | H14A—C14—H14C | 109.5 |
| C7—C6—H6B | 107.4 | H14B—C14—H14C | 109.5 |
| H6A—C6—H6B | 107.0 | C7—C15—H15A | 109.5 |
| C15—C7—C14 | 107.9 (2) | C7—C15—H15B | 109.5 |
| C15—C7—C6 | 109.4 (2) | H15A—C15—H15B | 109.5 |
| C14—C7—C6 | 106.0 (2) | C7—C15—H15C | 109.5 |
| C15—C7—C8 | 113.74 (18) | H15A—C15—H15C | 109.5 |
| C14—C7—C8 | 108.4 (2) | H15B—C15—H15C | 109.5 |
| C6—C7—C8 | 111.10 (19) | C10—C16—H16A | 109.5 |
| C9—C8—C1 | 110.22 (17) | C10—C16—H16B | 109.5 |
| C9—C8—C7 | 112.54 (18) | H16A—C16—H16B | 109.5 |
| C1—C8—C7 | 116.23 (17) | C10—C16—H16C | 109.5 |
| C9—C8—H8 | 105.6 | H16A—C16—H16C | 109.5 |
| C1—C8—H8 | 105.6 | H16B—C16—H16C | 109.5 |
| C7—C8—H8 | 105.6 | C10—O—C9 | 60.78 (14) |
| O—C9—C10 | 59.51 (14) | | |