

(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}]dodecaneAhmed Benharref,^{a*} Lahcen El Ammari,^b Daniel Avignant,^c Abdelghani Oudahmane^c and Moha Berraho^a

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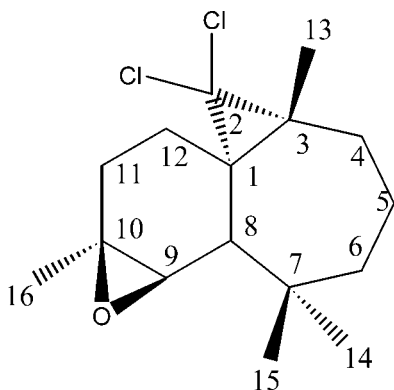
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.040; wR factor = 0.106; data-to-parameter ratio = 19.0.

The title compound, $\text{C}_{16}\text{H}_{24}\text{Cl}_2\text{O}$, 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 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 β -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*

$\text{C}_{16}\text{H}_{24}\text{Cl}_2\text{O}$
 $M_r = 303.24$
Orthorhombic, $P2_12_12_1$
 $a = 8.4995$ (3) Å
 $b = 10.2461$ (4) Å
 $c = 18.1656$ (6) Å

$V = 1581.98$ (10) Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.40$ mm⁻¹
 $T = 298$ K
 $0.67 \times 0.41 \times 0.26$ mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (SADABS; Bruker, 2008)
 $T_{\min} = 0.609$, $T_{\max} = 0.745$

7171 measured reflections
3369 independent reflections
2830 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.106$
 $S = 1.01$
3369 reflections
177 parameters
H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.22$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.29$ e Å⁻³
Absolute structure: Flack & Bernardinelli (2000), 1423 Friedel pairs
Flack parameter: 0.04 (7)

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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supplementary materials

Acta Cryst. (2010). E66, o3125 [doi:10.1107/S1600536810045344]

(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

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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). Treatment of (*X*) with one equivalent of *meta*-chloroperbenzoic acid (mCPBA) leads to a mixture of two diastereoisomers: (1*S*, 3*R*, 8*S*, 9*S*, 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*, 8*S*, 9*R*, 10*S*)-2,2-dichloro-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 $\phi = 138.1$ (4)°, whereas the seven-membered ring displays an approximate chair conformation with QT = 0.783 (3) Å, $\theta = 31.9$ (3)°, $\phi_2 = -50.3$ (4)° and $\phi_3 = -78.3$ (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*).

Experimental

For the synthesis of compounds (1*S*, 3*R*, 8*S*, 9*S*, 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*, 8*S*, 9*R*, 10*S*)-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 CH₂Cl₂ (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.

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).

Figures

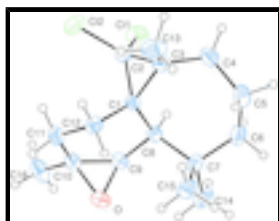


Fig. 1. Molecular structure of the title compound with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

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

Crystal data

$\text{C}_{16}\text{H}_{24}\text{Cl}_2\text{O}$	$F(000) = 648$
$M_r = 303.24$	$D_x = 1.273 \text{ Mg m}^{-3}$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: P 2ac 2ab	Cell parameters from 3372 reflections
$a = 8.4995 (3) \text{ \AA}$	$\theta = 2.3\text{--}26.9^\circ$
$b = 10.2461 (4) \text{ \AA}$	$\mu = 0.40 \text{ mm}^{-1}$
$c = 18.1656 (6) \text{ \AA}$	$T = 298 \text{ K}$
$V = 1581.98 (10) \text{ \AA}^3$	Prism, colourless
$Z = 4$	$0.67 \times 0.41 \times 0.26 \text{ mm}$

Data collection

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

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained

$R[F^2 > 2\sigma(F^2)] = 0.040$	$w = 1/[\sigma^2(F_o^2) + (0.0568P)^2 + 0.1767P]$
$wR(F^2) = 0.106$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{\max} < 0.001$
3369 reflections	$\Delta\rho_{\max} = 0.22 \text{ e } \text{\AA}^{-3}$
177 parameters	$\Delta\rho_{\min} = -0.29 \text{ e } \text{\AA}^{-3}$
0 restraints	Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.073 (4) Absolute structure: Flack & Bernardinelli (2000), 1423 Friedel pairs
Secondary atom site location: difference Fourier map	Flack 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
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*

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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 (\AA^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 (\AA , $^\circ$)

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—C12	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—C11	121.47 (17)	C9—C10—C11	118.93 (18)
C1—C2—C11	121.38 (16)	O—C10—C16	114.4 (2)
C3—C2—C12	118.75 (17)	C9—C10—C16	120.0 (2)
C1—C2—C12	120.64 (16)	C11—C10—C16	116.8 (2)
C11—C2—C12	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
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

supplementary materials

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)		

Fig. 1

