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

**Najia Ourhriss,[a]* Ahmed Benharref,[a] Mohamed Saadi,[b] Moha Berraho[a] and Lahcen El Ammari[b]**

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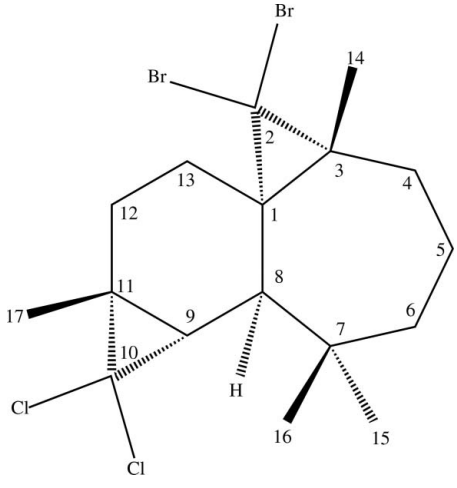
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.007 Å; $R$ factor = 0.038; $wR$ factor = 0.092; data-to-parameter ratio = 19.6.

The title compound, $C_{17}H_{24}Br_2Cl_2$, 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 contains fused six-, seven- and two three-membered rings. The six-membered ring has a half-chair conformation, while the seven-membered ring displays a boat conformation. The absolute structure was unambiguously established from anomalous dispersion effects. The crystal packing exhibits no short intermolecular contacts.

## Related literature

For the crystal structures of related compounds, see: Ourhriss *et al.* (2013); Oukhrib *et al.* (2013*a*,*b*). For puckering parameters, see: Cremer & Pople (1975).




## Experimental

### Crystal data

$C_{17}H_{24}Br_2Cl_2$
$M_r$ = 459.08
Monoclinic, $P2_1$
$a$ = 9.0112 (6) Å
$b$ = 11.6772 (8) Å
$c$ = 9.0849 (6) Å
$\beta$ = 108.045 (5)°
$V$ = 908.94 (11) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 4.75 mm$^{-1}$
$T$ = 296 K
0.45 × 0.34 × 0.29 mm

### Data collection

Bruker X8 APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008)
$T_{min}$ = 0.739, $T_{max}$ = 0.867
6676 measured reflections
3720 independent reflections
2910 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.034

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.092
$S$ = 1.03
3720 reflections
190 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.64 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.79 e Å$^{-3}$
Absolute structure: Flack & Bernardinelli (2000), 1096 Friedel pairs
Flack parameter: 0.039 (10)

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 *publCIF* (Westrip, 2010).

The authors thank the Unit of Support for Technical and Scientific Research (UATRS, CNRST) for the X-ray measurements.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5397).

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# supporting information

*Acta Cryst.* (2013). E**69**, o724 [https://doi.org/10.1107/S1600536813009070]

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

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

### S1. Comment

As a continuation of our structural study of *β*-himachalene derivatives isolated from the essential oil of the Atlas cedar (Cedrus Atlantica) (Ourhriss *et al.*, 2013; Oukhrib *et al.*, 2013*a,b*), we present here the crystal structure of the title compound, (1*S*,3*R*,8*R*,9S,11*R*)-2,2-dibromo-10,10-dichloro-3,7,7,11- tetramethyltetracyclo[6.5.0.0$^{1,3}$.0$^{9,11}$]tridecane, (I).

In (I) (Fig. 1), the molecule contains a fused six- and seven-membered rings, which are fused to two three-membered rings. The six-membered ring has a half chair conformation as indicated by the total puckering amplitude QT = 0.446 (5) Å and spherical polar angle $\theta$ = 140.8 (6)° and $\varphi$2 = 143 (1)°, whereas the seven-membered ring displays a boat conformation with QT = 1.122 (5) Å, $\theta$2 = 87.4 (3)°, $\varphi$2 = -48.2 (3)° and $\varphi$3 = -118 (5)° (Cremer & Pople, 1975). The three-membered rings (C1/C2/C3) and (C9/C10/C11) are nearly perpendicular to the six and seven-membered rings (C1/C8–C13)and (C1/C3–C8), with a dihedral angles of 84.1 (4) and 80.6 (4), respectively. Owing to the presence of Br and Cl atoms, the absolute configuration could be fully confirmed from anomalous dispersion effects, by refining the Flack parameter as C1(S),C3(*R*),C8(*R*),C9(S), and C11(*R*). The crystal packing exhibits no short intermolecular contacts.

### S2. Experimental

A solution containing 4 g (10 mmol) of (1*S*,3*R*,8*S*)-2,2-dibromo- 3,7,7,10- tetramethyltricyclo[6.4.0.01,3]dodec-9-ene and 1 ml (12.4 mmol) of $CHCl_3$ in 40 ml of dichloromethane was added dropwise at 273 K over 30 min to 1 g (25 mmol) of pulverized sodium hydroxide and 40 mg of *N*–benzyltriethylam monium 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 (96–4) used as eluent. The two diastereoisomers (1*S*,3*R*,8*S*,9S,11*R*)- 2,2-Dibromo-10,10-di-chloro-3,7,7,11-tetramethyltetracyclo[6.5.0.0$^{1,3}$.0 $^{9,11}$]tridecane(*X*) and its isomer (1*S*,3*R*,8*S*,9*R*,11*S*)-2,2-Dibromo-10,10-dichloro-3,7,7,11-tetramethyltetracyclo[6.5.0.0$^{1,3}$.0$^{9,11}$]tridecane(Y) were obtained by this procedure in a 80/20 ratio and a combined yield of 65% (3 g; 6.5 mmol). The title compound (isomer *X*) was recrystallized from hexane.

### 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 $U_{iso}$(H) = 1.2 $U_{eq}$(methylene, methine) and $U_{iso}$(H) = 1.5 $U_{eq}$(methyl). The space group is non-centrosymmetric and the polar axis restraint is generated automatically by *SHELXL* program. The 1096 Friedel opposites reflections are not merged.

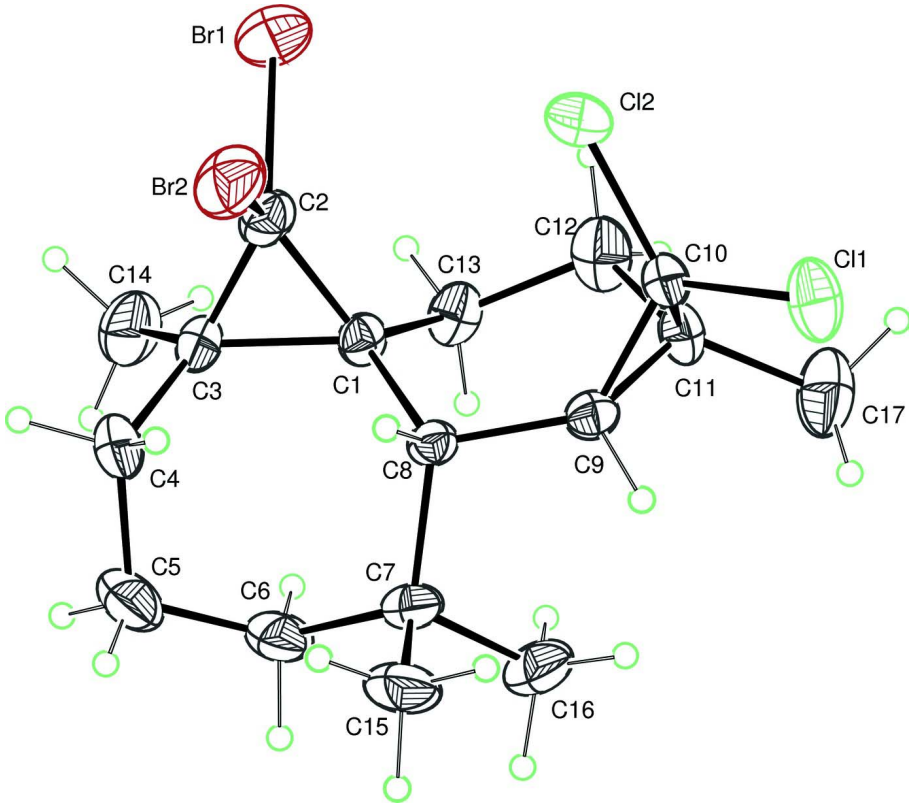


**Figure 1**

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-Dibromo-10,10-dichloro-3,7,7,11-tetramethyltetracyclo[6.5.0.0$^{1,3}$.0$^{9,11}$]tridecane**

*Crystal data*

$C_{17}H_{24}Br_2Cl_2$
$M_r$ = 459.08
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a$ = 9.0112 (6) Å
$b$ = 11.6772 (8) Å
$c$ = 9.0849 (6) Å
$\beta$ = 108.045 (5)°
$V$ = 908.94 (11) Å$^3$
$Z$ = 2
$F(000)$ = 460
$D_x$ = 1.677 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 3720 reflections
$\theta$ = 2.8–29.6°
$\mu$ = 4.75 mm$^{-1}$
$T$ = 296 K
Block, colourless
0.45 × 0.34 × 0.29 mm

*Data collection*

Bruker X8 APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2008)
$T_{min}$ = 0.739, $T_{max}$ = 0.867
6676 measured reflections
3720 independent reflections
2910 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.034
$\theta_{max}$ = 29.6°, $\theta_{min}$ = 2.8°
$h$ = −12→12
$k$ = −16→15
$l$ = −12→12

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.092$
$S = 1.03$
3720 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
$w = 1/[\sigma^2(F_o^2) + (0.0333P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.64$ e Å$^{-3}$
$\Delta\rho_{min} = -0.79$ e Å$^{-3}$
Absolute structure: Flack & Bernardinelli (2000), 1096 Friedel pairs
Absolute structure parameter: 0.039 (10)

*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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.8734 (5) | 0.4080 (3) | 0.7265 (5) | 0.0211 (8) |
| C2 | 0.9989 (5) | 0.3302 (4) | 0.6990 (6) | 0.0288 (10) |
| C3 | 1.0234 (4) | 0.3775 (4) | 0.8568 (5) | 0.0275 (9) |
| C4 | 1.0081 (6) | 0.2965 (4) | 0.9812 (5) | 0.0357 (11) |
| H4A | 1.1102 | 0.2657 | 1.0363 | 0.043* |
| H4B | 0.9413 | 0.2330 | 0.9329 | 0.043* |
| C5 | 0.9408 (6) | 0.3542 (5) | 1.0962 (6) | 0.0442 (13) |
| H5A | 1.0232 | 0.3954 | 1.1721 | 0.053* |
| H5B | 0.9014 | 0.2960 | 1.1507 | 0.053* |
| C6 | 0.8095 (6) | 0.4372 (5) | 1.0187 (5) | 0.0387 (12) |
| H6A | 0.8567 | 0.5027 | 0.9849 | 0.046* |
| H6B | 0.7670 | 0.4645 | 1.0981 | 0.046* |
| C7 | 0.6702 (5) | 0.3992 (4) | 0.8798 (5) | 0.0301 (9) |
| C8 | 0.7181 (4) | 0.3573 (3) | 0.7345 (5) | 0.0206 (8) |
| H8 | 0.7319 | 0.2741 | 0.7439 | 0.025* |
| C9 | 0.5812 (4) | 0.3798 (4) | 0.5883 (4) | 0.0224 (8) |
| H9 | 0.4807 | 0.3749 | 0.6086 | 0.027* |
| C10 | 0.5657 (5) | 0.3530 (4) | 0.4239 (5) | 0.0261 (9) |
| C11 | 0.5826 (5) | 0.4755 (4) | 0.4748 (5) | 0.0278 (9) |
| C12 | 0.7378 (6) | 0.5328 (4) | 0.4939 (6) | 0.0373 (11) |
| H12A | 0.7190 | 0.6125 | 0.4639 | 0.045* |
| H12B | 0.7856 | 0.4970 | 0.4234 | 0.045* |
| C13 | 0.8528 (5) | 0.5277 (3) | 0.6570 (5) | 0.0277 (9) |

| | | | | |
|---|---|---|---|---|
| H13A | 0.9534 | 0.5556 | 0.6546 | 0.033* |
| H13B | 0.8168 | 0.5784 | 0.7235 | 0.033* |
| C14 | 1.1485 (6) | 0.4682 (5) | 0.9207 (7) | 0.0432 (13) |
| H14A | 1.1495 | 0.4896 | 1.0230 | 0.065* |
| H14B | 1.1262 | 0.5343 | 0.8546 | 0.065* |
| H14C | 1.2486 | 0.4377 | 0.9247 | 0.065* |
| C15 | 0.5843 (6) | 0.2992 (5) | 0.9266 (6) | 0.0453 (13) |
| H15A | 0.4981 | 0.2763 | 0.8394 | 0.068* |
| H15B | 0.5463 | 0.3228 | 1.0096 | 0.068* |
| H15C | 0.6547 | 0.2360 | 0.9601 | 0.068* |
| C16 | 0.5593 (6) | 0.5035 (5) | 0.8432 (6) | 0.0419 (12) |
| H16A | 0.6113 | 0.5673 | 0.8140 | 0.063* |
| H16B | 0.5305 | 0.5232 | 0.9333 | 0.063* |
| H16C | 0.4673 | 0.4849 | 0.7596 | 0.063* |
| C17 | 0.4417 (7) | 0.5546 (4) | 0.4175 (7) | 0.0479 (14) |
| H17A | 0.4693 | 0.6299 | 0.4593 | 0.072* |
| H17B | 0.3576 | 0.5255 | 0.4506 | 0.072* |
| H17C | 0.4095 | 0.5581 | 0.3065 | 0.072* |
| Cl1 | 0.37818 (14) | 0.30587 (10) | 0.30591 (14) | 0.0415 (3) |
| Cl2 | 0.70977 (16) | 0.28463 (12) | 0.36234 (14) | 0.0429 (3) |
| Br1 | 1.11977 (6) | 0.38295 (6) | 0.57096 (7) | 0.05382 (18) |
| Br2 | 0.97449 (6) | 0.16666 (4) | 0.66883 (6) | 0.04537 (16) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0167 (18) | 0.022 (2) | 0.023 (2) | −0.0038 (15) | 0.0039 (16) | −0.0013 (15) |
| C2 | 0.019 (2) | 0.034 (2) | 0.033 (3) | −0.0019 (17) | 0.0085 (19) | −0.0011 (18) |
| C3 | 0.0185 (18) | 0.035 (2) | 0.028 (2) | 0.005 (2) | 0.0054 (17) | 0.004 (2) |
| C4 | 0.028 (2) | 0.049 (3) | 0.024 (2) | 0.003 (2) | −0.0001 (19) | 0.003 (2) |
| C5 | 0.044 (3) | 0.066 (4) | 0.021 (3) | −0.004 (3) | 0.007 (2) | −0.002 (2) |
| C6 | 0.038 (3) | 0.057 (3) | 0.023 (3) | −0.001 (2) | 0.013 (2) | −0.010 (2) |
| C7 | 0.029 (2) | 0.038 (2) | 0.028 (2) | 0.0027 (19) | 0.0153 (19) | −0.004 (2) |
| C8 | 0.0199 (18) | 0.0217 (19) | 0.022 (2) | 0.0009 (15) | 0.0096 (17) | 0.0021 (15) |
| C9 | 0.0205 (18) | 0.0241 (18) | 0.024 (2) | −0.0013 (18) | 0.0093 (16) | 0.0001 (18) |
| C10 | 0.022 (2) | 0.035 (2) | 0.019 (2) | 0.0020 (17) | 0.0027 (17) | 0.0016 (16) |
| C11 | 0.029 (2) | 0.028 (2) | 0.023 (2) | 0.0031 (18) | 0.0021 (19) | 0.0076 (17) |
| C12 | 0.035 (3) | 0.030 (2) | 0.043 (3) | −0.006 (2) | 0.007 (2) | 0.011 (2) |
| C13 | 0.022 (2) | 0.022 (2) | 0.037 (3) | −0.0034 (17) | 0.0067 (19) | 0.0028 (18) |
| C14 | 0.023 (2) | 0.054 (3) | 0.047 (3) | −0.008 (2) | 0.004 (2) | −0.005 (2) |
| C15 | 0.043 (3) | 0.068 (3) | 0.033 (3) | −0.005 (3) | 0.024 (3) | 0.004 (3) |
| C16 | 0.036 (3) | 0.051 (3) | 0.044 (3) | 0.011 (2) | 0.019 (3) | −0.008 (2) |
| C17 | 0.042 (3) | 0.038 (3) | 0.053 (3) | 0.012 (2) | −0.001 (3) | 0.003 (2) |
| Cl1 | 0.0330 (6) | 0.0449 (7) | 0.0341 (7) | −0.0066 (5) | −0.0077 (5) | −0.0011 (5) |
| Cl2 | 0.0438 (7) | 0.0613 (8) | 0.0262 (6) | 0.0125 (6) | 0.0144 (5) | −0.0040 (5) |
| Br1 | 0.0336 (3) | 0.0840 (4) | 0.0516 (3) | −0.0014 (3) | 0.0244 (3) | 0.0083 (3) |
| Br2 | 0.0452 (3) | 0.0386 (2) | 0.0525 (3) | 0.0134 (3) | 0.0156 (3) | −0.0033 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C13 | 1.522 (6) | C9—C11 | 1.524 (6) |
| C1—C2 | 1.530 (6) | C9—H9 | 0.9800 |
| C1—C3 | 1.537 (5) | C10—C11 | 1.496 (6) |
| C1—C8 | 1.542 (5) | C10—Cl2 | 1.756 (4) |
| C2—C3 | 1.488 (6) | C10—Cl1 | 1.785 (4) |
| C2—Br1 | 1.924 (4) | C11—C12 | 1.511 (6) |
| C2—Br2 | 1.932 (4) | C11—C17 | 1.525 (7) |
| C3—C4 | 1.513 (6) | C12—C13 | 1.524 (7) |
| C3—C14 | 1.524 (7) | C12—H12A | 0.9700 |
| C4—C5 | 1.519 (7) | C12—H12B | 0.9700 |
| C4—H4A | 0.9700 | C13—H13A | 0.9700 |
| C4—H4B | 0.9700 | C13—H13B | 0.9700 |
| C5—C6 | 1.523 (7) | C14—H14A | 0.9600 |
| C5—H5A | 0.9700 | C14—H14B | 0.9600 |
| C5—H5B | 0.9700 | C14—H14C | 0.9600 |
| C6—C7 | 1.544 (6) | C15—H15A | 0.9600 |
| C6—H6A | 0.9700 | C15—H15B | 0.9600 |
| C6—H6B | 0.9700 | C15—H15C | 0.9600 |
| C7—C15 | 1.531 (7) | C16—H16A | 0.9600 |
| C7—C16 | 1.545 (7) | C16—H16B | 0.9600 |
| C7—C8 | 1.587 (5) | C16—H16C | 0.9600 |
| C8—C9 | 1.529 (6) | C17—H17A | 0.9600 |
| C8—H8 | 0.9800 | C17—H17B | 0.9600 |
| C9—C10 | 1.490 (6) | C17—H17C | 0.9600 |
| | | | |
| C13—C1—C2 | 118.6 (3) | C10—C9—H9 | 111.8 |
| C13—C1—C3 | 119.8 (3) | C11—C9—H9 | 111.8 |
| C2—C1—C3 | 58.1 (3) | C8—C9—H9 | 111.8 |
| C13—C1—C8 | 112.1 (3) | C9—C10—C11 | 61.4 (3) |
| C2—C1—C8 | 120.5 (3) | C9—C10—Cl2 | 124.4 (3) |
| C3—C1—C8 | 118.0 (3) | C11—C10—Cl2 | 121.3 (3) |
| C3—C2—C1 | 61.2 (3) | C9—C10—Cl1 | 116.4 (3) |
| C3—C2—Br1 | 121.4 (3) | C11—C10—Cl1 | 117.8 (3) |
| C1—C2—Br1 | 119.6 (3) | Cl2—C10—Cl1 | 108.9 (2) |
| C3—C2—Br2 | 118.7 (3) | C10—C11—C12 | 117.4 (4) |
| C1—C2—Br2 | 123.5 (3) | C10—C11—C9 | 59.1 (3) |
| Br1—C2—Br2 | 106.9 (2) | C12—C11—C9 | 116.6 (4) |
| C2—C3—C4 | 117.9 (4) | C10—C11—C17 | 118.6 (4) |
| C2—C3—C14 | 119.7 (4) | C12—C11—C17 | 114.5 (4) |
| C4—C3—C14 | 112.2 (4) | C9—C11—C17 | 119.7 (4) |
| C2—C3—C1 | 60.7 (3) | C11—C12—C13 | 114.9 (4) |
| C4—C3—C1 | 117.3 (3) | C11—C12—H12A | 108.5 |
| C14—C3—C1 | 120.2 (4) | C13—C12—H12A | 108.5 |
| C3—C4—C5 | 112.6 (4) | C11—C12—H12B | 108.5 |
| C3—C4—H4A | 109.1 | C13—C12—H12B | 108.5 |
| C5—C4—H4A | 109.1 | H12A—C12—H12B | 107.5 |

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| C3—C4—H4B | 109.1 | C1—C13—C12 | 113.5 (4) |
| C5—C4—H4B | 109.1 | C1—C13—H13A | 108.9 |
| H4A—C4—H4B | 107.8 | C12—C13—H13A | 108.9 |
| C4—C5—C6 | 112.5 (4) | C1—C13—H13B | 108.9 |
| C4—C5—H5A | 109.1 | C12—C13—H13B | 108.9 |
| C6—C5—H5A | 109.1 | H13A—C13—H13B | 107.7 |
| C4—C5—H5B | 109.1 | C3—C14—H14A | 109.5 |
| C6—C5—H5B | 109.1 | C3—C14—H14B | 109.5 |
| H5A—C5—H5B | 107.8 | H14A—C14—H14B | 109.5 |
| C5—C6—C7 | 120.9 (4) | C3—C14—H14C | 109.5 |
| C5—C6—H6A | 107.1 | H14A—C14—H14C | 109.5 |
| C7—C6—H6A | 107.1 | H14B—C14—H14C | 109.5 |
| C5—C6—H6B | 107.1 | C7—C15—H15A | 109.5 |
| C7—C6—H6B | 107.1 | C7—C15—H15B | 109.5 |
| H6A—C6—H6B | 106.8 | H15A—C15—H15B | 109.5 |
| C15—C7—C6 | 110.2 (4) | C7—C15—H15C | 109.5 |
| C15—C7—C16 | 108.2 (4) | H15A—C15—H15C | 109.5 |
| C6—C7—C16 | 104.9 (4) | H15B—C15—H15C | 109.5 |
| C15—C7—C8 | 106.7 (4) | C7—C16—H16A | 109.5 |
| C6—C7—C8 | 114.0 (3) | C7—C16—H16B | 109.5 |
| C16—C7—C8 | 112.8 (4) | H16A—C16—H16B | 109.5 |
| C9—C8—C1 | 113.2 (3) | C7—C16—H16C | 109.5 |
| C9—C8—C7 | 108.4 (3) | H16A—C16—H16C | 109.5 |
| C1—C8—C7 | 113.9 (3) | H16B—C16—H16C | 109.5 |
| C9—C8—H8 | 107.0 | C11—C17—H17A | 109.5 |
| C1—C8—H8 | 107.0 | C11—C17—H17B | 109.5 |
| C7—C8—H8 | 107.0 | H17A—C17—H17B | 109.5 |
| C10—C9—C11 | 59.5 (3) | C11—C17—H17C | 109.5 |
| C10—C9—C8 | 129.4 (3) | H17A—C17—H17C | 109.5 |
| C11—C9—C8 | 122.7 (3) | H17B—C17—H17C | 109.5 |