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# 1,2,3,4,5,6,7,8,13,13,14,14-Dodecachloro-1,4,4a,4b,5,8,8a,12b-octahydro-1,4:5,8-dimethanotriphenylene at 90 K[1]

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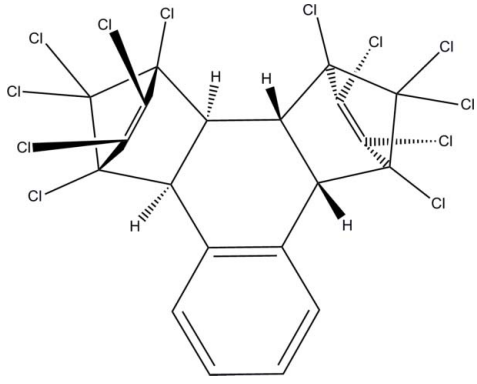
Key indicators: single-crystal X-ray study; $T$ = 90 K, $P$ = 0.0 kPa; mean $\sigma$(C–C) = 0.001 Å; $R$ factor = 0.032; $wR$ factor = 0.086; data-to-parameter ratio = 52.1.

The previously reported room-temperature crystal structure [Jaud Baldy, Negrel, Poite & Chanon (1993). *Z. Kristallogr.* **204**, 289–291] of the title compound, $C_{20}H_8Cl_{12}$, is monoclinic with $Z'$ = 1, whereas the 90 K structure reported herein is triclinic with $Z'$ = 2 and shows a 2% volume contraction. The crystallographically independent unit chosen consists of both enantiomers (Λ and Δ) of this propeller-like molecule. Both enantiomers display quasi-twofold symmetry, with average bond-length/bond-angle deviations of 0.0018 (4) Å and 0.41 (2)° for Λ, and 0.0026 (4) Å and 0.50 (2)° for Δ.

## Related literature

For the structure of the room-temperature polymorph, see: Jaud *et al.* (1993). For the preparation of the compound, see: Lacourcelle *et al.* (1993). For the Cambridge Structural Database, see: Allen (2002).




## Experimental

### Crystal data

$C_{20}H_8Cl_{12}$
$M_r$ = 673.66
Triclinic, $P\overline{1}$
$a$ = 9.6434 (1) Å
$b$ = 15.4287 (2) Å
$c$ = 16.4161 (2) Å
$\alpha$ = 92.1948 (6)°
$\beta$ = 98.2331 (7)°
$\gamma$ = 91.3097 (6)°
$V$ = 2414.53 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.39 mm$^{-1}$
$T$ = 90 K
0.40 × 0.35 × 0.15 mm

### Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
$T_{min}$ = 0.607, $T_{max}$ = 0.819
111692 measured reflections
30125 independent reflections
24699 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.026

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.086
$S$ = 1.03
30125 reflections
578 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.87 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.63 e Å$^{-3}$

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; 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).

The purchase of the diffractometer was made possible by Grant No. LEQSF(1999–2000)-ESH-TR-13, administered by the Louisiana Board of Regents. We thank Lee Shui and Mark McLaughlin for providing the sample.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZJ2089).

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[1] CAS 147730-93-6.

# supporting information

*Acta Cryst.* (2012). E**68**, o2538 [https://doi.org/10.1107/S1600536812032540]

## 1,2,3,4,5,6,7,8,13,13,14,14-Dodecachloro-1,4,4a,4b,5,8,8a,12b-octahydro-1,4:5,8-dimethanotriphenylene at 90 K

**Brandon W. Jenkins, Frank R. Fronczek and Steven F. Watkins**

### S1. Comment

The crystal structure of the title compound at 298 K is monoclinic, $P2_1/c$, $Z = 4$, a = 9.743 (3), b = 15.523 (3), c = 16.575 (2) Å, $\beta = 100.11$ (2)°, in agreement with the published room-temperature structure (Jaud *et al.*, 1993. CCDC refcode YASKOS, Allen, 2002). Upon cooling to 90 K, the material undergoes a phase change to triclinic ($P\overline{1}$) and a volume contraction of 2%. The two crystallographically independent enantiomers chosen for the asymmetric unit are propeller-like with opposite pitch (Δ, **Ia** and Λ, **Ib**). Both display near twofold symmetry, with average off-symmetry bond-length/bond-angle deviations of 0.0018 (4) Å/0.41 (2)° (**Ia**) and 0.0026 (4) Å/0.50 (2)° (**Ib**). The bond lengths and bond angles are normal and are essentially as described by Jaud *et al.* (1993).

### S2. Experimental

The compound was prepared by Lee Shui and Mark McLaughlin using the method described by Lacourcelle *et al.* (1993). A sample suitable for diffraction was recrystallized from ethyl acetate.

### S3. Refinement

All H atoms were placed in calculated positions, guided by difference maps, with C—H bond distances 0.95 (aromatic C) and 1.00 (alkyl C) Å, $U_{iso} = 1.2U_{eq}$, and thereafter refined as riding.

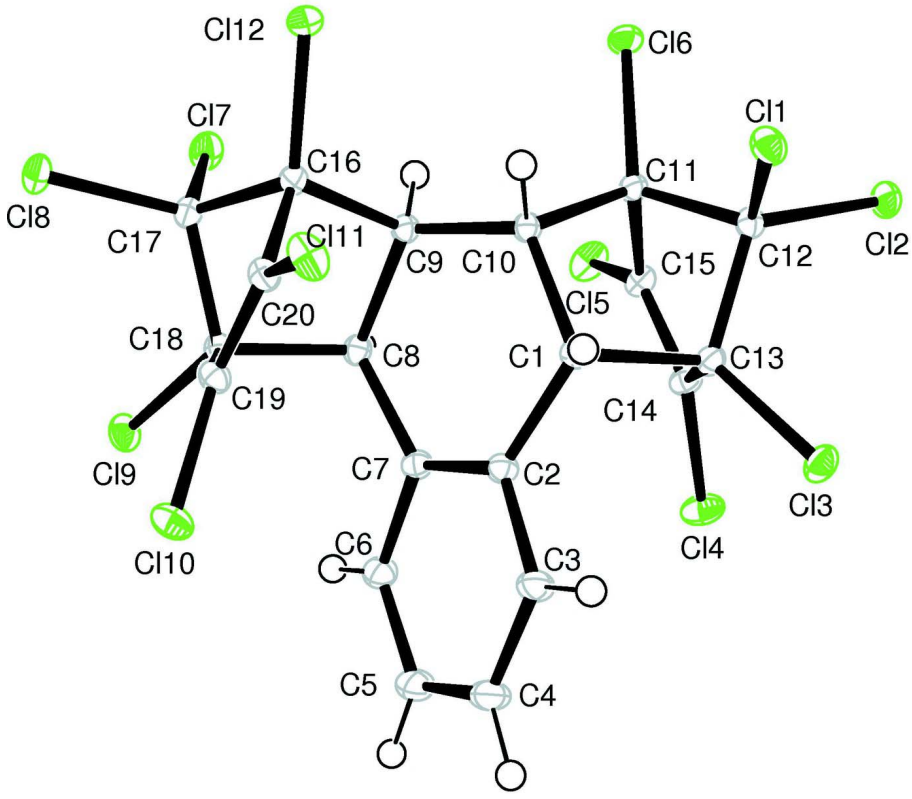


**Figure 1**

View of **Ia** (Δ, 50% probability displacement ellipsoids)

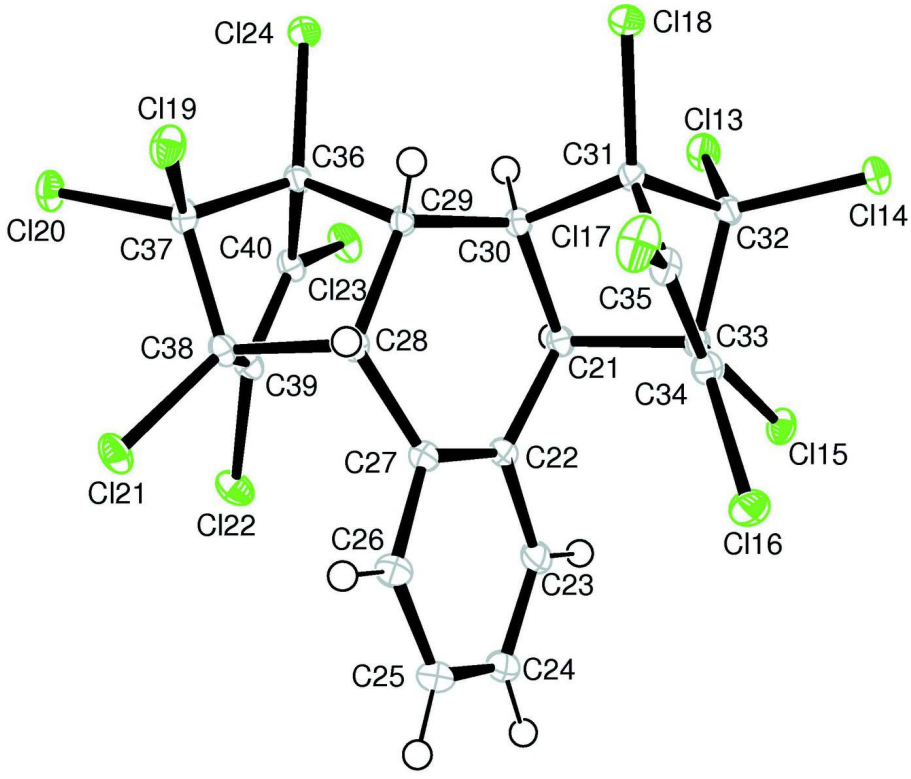


**Figure 2**

View of **Ib** (Λ, 50% probability displacement ellipsoids)

**1,2,3,4,5,6,7,8,13,13,14,14-Dodecachloro-1,4,4a,4b,5,8,8a,12b- octahydro-1,4:5,8-dimethanotriphenylene**

*Crystal data*

$C_{20}H_8Cl_{12}$
$M_r = 673.66$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 9.6434$ (1) Å
$b = 15.4287$ (2) Å
$c = 16.4161$ (2) Å
$\alpha = 92.1948$ (6)°
$\beta = 98.2331$ (7)°
$\gamma = 91.3097$ (6)°
$V = 2414.53$ (5) Å$^3$
$Z = 4$
$F(000) = 1328$
$D_x = 1.853$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 27797 reflections
$\theta = 2.6$–$40.3°$
$\mu = 1.39$ mm$^{-1}$
$T = 90$ K
Prism, colourless
0.40 × 0.35 × 0.15 mm

*Data collection*

Nonius KappaCCD diffractometer
Radiation source: sealed tube
Horizonally mounted graphite crystal monochromator
Detector resolution: 9 pixels mm$^{-1}$
CCD rotation images, thick slices scans
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
$T_{min} = 0.607$, $T_{max} = 0.819$
111692 measured reflections
30125 independent reflections
24699 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 40.3°$, $\theta_{min} = 2.6°$
$h = -17 \rightarrow 17$
$k = -28 \rightarrow 28$
$l = -29 \rightarrow 29$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.086$
$S = 1.03$
30125 reflections
578 parameters
0 restraints
0 constraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0362P)^2 + 1.2577P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.87$ e Å$^{-3}$
$\Delta\rho_{min} = -0.63$ e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0013 (2)

*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 | 0.78302 (10) | 0.24744 (6) | 0.36584 (6) | 0.01060 (13) |
| H1 | 0.718 | 0.2785 | 0.3984 | 0.013* |
| C2 | 0.76826 (10) | 0.15090 (6) | 0.37568 (6) | 0.01118 (14) |
| C3 | 0.77164 (12) | 0.12163 (7) | 0.45581 (6) | 0.01484 (16) |
| H3 | 0.7646 | 0.1622 | 0.4999 | 0.018* |
| C4 | 0.78510 (13) | 0.03398 (7) | 0.47153 (7) | 0.01839 (18) |
| H4 | 0.7853 | 0.0148 | 0.5258 | 0.022* |
| C5 | 0.79834 (13) | −0.02536 (7) | 0.40736 (7) | 0.01770 (18) |
| H5 | 0.8149 | −0.0845 | 0.4183 | 0.021* |
| C6 | 0.78719 (12) | 0.00244 (7) | 0.32715 (7) | 0.01483 (16) |
| H6 | 0.7938 | −0.0386 | 0.2833 | 0.018* |
| C7 | 0.76641 (10) | 0.08995 (6) | 0.30980 (6) | 0.01141 (14) |
| C8 | 0.72700 (10) | 0.11372 (6) | 0.22086 (6) | 0.01102 (13) |
| H8 | 0.7957 | 0.0893 | 0.1866 | 0.013* |
| C9 | 0.70962 (10) | 0.21274 (6) | 0.20593 (6) | 0.01055 (13) |
| H9 | 0.7587 | 0.2264 | 0.1581 | 0.013* |
| C10 | 0.76252 (10) | 0.27912 (6) | 0.27577 (6) | 0.01032 (13) |
| H10 | 0.6952 | 0.3276 | 0.273 | 0.012* |
| C11 | 0.91010 (10) | 0.31842 (6) | 0.26664 (6) | 0.01082 (13) |
| C12 | 0.95297 (10) | 0.36467 (6) | 0.35265 (6) | 0.01182 (14) |
| C13 | 0.94026 (10) | 0.27907 (6) | 0.39788 (6) | 0.01102 (13) |
| C14 | 1.03221 (10) | 0.22190 (6) | 0.35207 (6) | 0.01196 (14) |
| C15 | 1.01323 (10) | 0.24454 (7) | 0.27332 (6) | 0.01183 (14) |
| C16 | 0.54883 (10) | 0.21886 (6) | 0.17658 (6) | 0.01145 (14) |
| C17 | 0.52148 (10) | 0.13722 (6) | 0.11775 (6) | 0.01270 (14) |
| C18 | 0.57301 (10) | 0.07562 (6) | 0.18742 (6) | 0.01136 (14) |

| | | | | |
|---|---|---|---|---|
| C19 | 0.48189 (10) | 0.10455 (6) | 0.25116 (6) | 0.01187 (14) |
| C20 | 0.47091 (10) | 0.19063 (6) | 0.24619 (6) | 0.01197 (14) |
| Cl1 | 0.83666 (3) | 0.444688 (16) | 0.378408 (16) | 0.01515 (4) |
| Cl2 | 1.12467 (3) | 0.411451 (17) | 0.367166 (16) | 0.01537 (4) |
| Cl3 | 0.98690 (3) | 0.288372 (18) | 0.504965 (14) | 0.01546 (4) |
| Cl4 | 1.12522 (3) | 0.138821 (18) | 0.394002 (17) | 0.01819 (5) |
| Cl5 | 1.07638 (3) | 0.195595 (19) | 0.192404 (16) | 0.01775 (4) |
| Cl6 | 0.91267 (3) | 0.383648 (17) | 0.181692 (15) | 0.01553 (4) |
| Cl7 | 0.62374 (3) | 0.132935 (18) | 0.036646 (15) | 0.01693 (4) |
| Cl8 | 0.34348 (3) | 0.119848 (18) | 0.074104 (16) | 0.01669 (4) |
| Cl9 | 0.56086 (3) | −0.034447 (16) | 0.156692 (16) | 0.01555 (4) |
| Cl10 | 0.42601 (3) | 0.039085 (17) | 0.321116 (17) | 0.01683 (4) |
| Cl11 | 0.40182 (3) | 0.259640 (17) | 0.311679 (18) | 0.01724 (4) |
| Cl12 | 0.49903 (3) | 0.317864 (16) | 0.134127 (17) | 0.01638 (4) |
| C21 | 0.70185 (10) | 0.39226 (6) | 0.72349 (6) | 0.01099 (13) |
| H21 | 0.7764 | 0.4224 | 0.6977 | 0.013* |
| C22 | 0.72147 (10) | 0.41473 (6) | 0.81506 (6) | 0.01236 (14) |
| C23 | 0.73181 (12) | 0.50254 (7) | 0.84174 (7) | 0.01735 (18) |
| H23 | 0.7441 | 0.5457 | 0.8035 | 0.021* |
| C24 | 0.72439 (14) | 0.52707 (8) | 0.92324 (8) | 0.0220 (2) |
| H24 | 0.7347 | 0.5865 | 0.9408 | 0.026* |
| C25 | 0.70191 (15) | 0.46452 (9) | 0.97910 (7) | 0.0227 (2) |
| H25 | 0.6883 | 0.4814 | 1.0336 | 0.027* |
| C26 | 0.69956 (13) | 0.37723 (8) | 0.95468 (7) | 0.01833 (18) |
| H26 | 0.6872 | 0.3344 | 0.9933 | 0.022* |
| C27 | 0.71524 (11) | 0.35144 (7) | 0.87372 (6) | 0.01303 (15) |
| C28 | 0.74356 (10) | 0.25743 (6) | 0.85610 (6) | 0.01152 (14) |
| H28 | 0.6781 | 0.2197 | 0.8822 | 0.014* |
| C29 | 0.73930 (10) | 0.22747 (6) | 0.76363 (6) | 0.01075 (13) |
| H29 | 0.6754 | 0.1751 | 0.7523 | 0.013* |
| C30 | 0.69489 (10) | 0.29315 (6) | 0.69746 (6) | 0.01106 (13) |
| H30 | 0.7566 | 0.2851 | 0.6539 | 0.013* |
| C31 | 0.54023 (10) | 0.27880 (6) | 0.65463 (6) | 0.01190 (14) |
| C32 | 0.52032 (10) | 0.36220 (6) | 0.60443 (6) | 0.01211 (14) |
| C33 | 0.55125 (10) | 0.42229 (6) | 0.68299 (6) | 0.01044 (13) |
| C34 | 0.44750 (10) | 0.38391 (6) | 0.73405 (6) | 0.01182 (14) |
| C35 | 0.44278 (10) | 0.29802 (6) | 0.71796 (6) | 0.01284 (15) |
| C36 | 0.89301 (10) | 0.19842 (6) | 0.75984 (6) | 0.01145 (14) |
| C37 | 0.92908 (10) | 0.15480 (6) | 0.84375 (6) | 0.01255 (14) |
| C38 | 0.90153 (10) | 0.23844 (6) | 0.89310 (6) | 0.01190 (14) |
| C39 | 0.99247 (10) | 0.30344 (7) | 0.85577 (6) | 0.01231 (14) |
| C40 | 0.98700 (10) | 0.27995 (7) | 0.77598 (6) | 0.01191 (14) |
| Cl13 | 0.64205 (3) | 0.377793 (19) | 0.534965 (15) | 0.01720 (4) |
| Cl14 | 0.34960 (3) | 0.370694 (18) | 0.549642 (16) | 0.01676 (4) |
| Cl15 | 0.53663 (3) | 0.532852 (15) | 0.665173 (16) | 0.01426 (4) |
| Cl16 | 0.37045 (3) | 0.441131 (18) | 0.804244 (17) | 0.01757 (4) |
| Cl17 | 0.35863 (3) | 0.221032 (19) | 0.76498 (2) | 0.02185 (5) |
| Cl18 | 0.50770 (3) | 0.180207 (17) | 0.597606 (18) | 0.01900 (5) |

| | | | | |
|---|---|---|---|---|
| Cl19 | 0.81665 (3) | 0.066381 (16) | 0.857572 (17) | 0.01663 (4) |
| Cl20 | 1.10430 (3) | 0.120062 (18) | 0.864312 (16) | 0.01591 (4) |
| Cl21 | 0.93820 (3) | 0.232330 (19) | 1.000170 (15) | 0.01646 (4) |
| Cl22 | 1.06791 (3) | 0.393670 (18) | 0.906893 (16) | 0.01752 (4) |
| Cl23 | 1.05143 (3) | 0.336268 (18) | 0.701995 (15) | 0.01620 (4) |
| Cl24 | 0.91419 (3) | 0.134541 (17) | 0.672205 (15) | 0.01600 (4) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0102 (3) | 0.0109 (3) | 0.0109 (3) | 0.0006 (3) | 0.0022 (3) | 0.0009 (2) |
| C2 | 0.0118 (3) | 0.0111 (3) | 0.0109 (3) | 0.0004 (3) | 0.0023 (3) | 0.0009 (3) |
| C3 | 0.0197 (4) | 0.0137 (4) | 0.0116 (3) | −0.0007 (3) | 0.0036 (3) | 0.0020 (3) |
| C4 | 0.0258 (5) | 0.0151 (4) | 0.0146 (4) | 0.0001 (4) | 0.0030 (4) | 0.0048 (3) |
| C5 | 0.0224 (5) | 0.0122 (4) | 0.0182 (4) | 0.0020 (3) | 0.0009 (4) | 0.0033 (3) |
| C6 | 0.0169 (4) | 0.0117 (3) | 0.0154 (4) | 0.0024 (3) | 0.0005 (3) | 0.0007 (3) |
| C7 | 0.0113 (3) | 0.0111 (3) | 0.0118 (3) | 0.0014 (3) | 0.0014 (3) | 0.0011 (3) |
| C8 | 0.0102 (3) | 0.0114 (3) | 0.0113 (3) | 0.0008 (3) | 0.0013 (3) | −0.0006 (3) |
| C9 | 0.0093 (3) | 0.0116 (3) | 0.0107 (3) | −0.0004 (3) | 0.0010 (3) | 0.0012 (3) |
| C10 | 0.0092 (3) | 0.0109 (3) | 0.0107 (3) | 0.0001 (2) | 0.0012 (3) | 0.0010 (2) |
| C11 | 0.0097 (3) | 0.0124 (3) | 0.0102 (3) | −0.0006 (3) | 0.0010 (3) | 0.0018 (3) |
| C12 | 0.0107 (3) | 0.0124 (3) | 0.0120 (3) | −0.0009 (3) | 0.0008 (3) | 0.0006 (3) |
| C13 | 0.0104 (3) | 0.0132 (3) | 0.0094 (3) | −0.0001 (3) | 0.0011 (3) | 0.0009 (3) |
| C14 | 0.0100 (3) | 0.0144 (4) | 0.0118 (3) | 0.0023 (3) | 0.0017 (3) | 0.0026 (3) |
| C15 | 0.0098 (3) | 0.0157 (4) | 0.0103 (3) | 0.0012 (3) | 0.0023 (3) | 0.0009 (3) |
| C16 | 0.0106 (3) | 0.0108 (3) | 0.0125 (3) | 0.0003 (3) | −0.0001 (3) | 0.0011 (3) |
| C17 | 0.0118 (4) | 0.0140 (4) | 0.0117 (3) | −0.0009 (3) | −0.0003 (3) | 0.0002 (3) |
| C18 | 0.0111 (3) | 0.0106 (3) | 0.0123 (3) | 0.0000 (3) | 0.0016 (3) | −0.0009 (3) |
| C19 | 0.0106 (3) | 0.0115 (3) | 0.0139 (4) | −0.0002 (3) | 0.0031 (3) | 0.0004 (3) |
| C20 | 0.0099 (3) | 0.0114 (3) | 0.0147 (4) | 0.0009 (3) | 0.0023 (3) | −0.0003 (3) |
| Cl1 | 0.01452 (9) | 0.01185 (8) | 0.01893 (10) | 0.00055 (7) | 0.00233 (8) | −0.00109 (7) |
| Cl2 | 0.01118 (9) | 0.01763 (10) | 0.01655 (9) | −0.00436 (7) | −0.00006 (7) | 0.00173 (7) |
| Cl3 | 0.01539 (10) | 0.02149 (10) | 0.00901 (8) | −0.00196 (8) | 0.00049 (7) | 0.00051 (7) |
| Cl4 | 0.01609 (10) | 0.02054 (11) | 0.01883 (10) | 0.00766 (8) | 0.00282 (8) | 0.00687 (8) |
| Cl5 | 0.01531 (10) | 0.02630 (12) | 0.01232 (9) | 0.00480 (8) | 0.00425 (7) | −0.00134 (8) |
| Cl6 | 0.01548 (10) | 0.01764 (10) | 0.01337 (9) | −0.00241 (7) | 0.00075 (7) | 0.00634 (7) |
| Cl7 | 0.01755 (10) | 0.02238 (11) | 0.01071 (9) | −0.00275 (8) | 0.00244 (7) | −0.00091 (7) |
| Cl8 | 0.01222 (9) | 0.01876 (10) | 0.01734 (10) | −0.00185 (7) | −0.00323 (7) | −0.00030 (8) |
| Cl9 | 0.01529 (10) | 0.01106 (8) | 0.01946 (10) | 0.00016 (7) | 0.00067 (8) | −0.00321 (7) |
| Cl10 | 0.01749 (10) | 0.01530 (9) | 0.01925 (10) | −0.00123 (8) | 0.00744 (8) | 0.00352 (8) |
| Cl11 | 0.01515 (10) | 0.01373 (9) | 0.02399 (11) | 0.00053 (7) | 0.00797 (8) | −0.00388 (8) |
| Cl12 | 0.01552 (10) | 0.01303 (9) | 0.01943 (10) | 0.00099 (7) | −0.00262 (8) | 0.00466 (7) |
| C21 | 0.0096 (3) | 0.0118 (3) | 0.0114 (3) | −0.0004 (3) | 0.0008 (3) | 0.0013 (3) |
| C22 | 0.0120 (4) | 0.0123 (3) | 0.0120 (3) | 0.0003 (3) | −0.0007 (3) | −0.0008 (3) |
| C23 | 0.0193 (4) | 0.0132 (4) | 0.0171 (4) | 0.0014 (3) | −0.0051 (3) | −0.0015 (3) |
| C24 | 0.0272 (6) | 0.0168 (4) | 0.0187 (5) | 0.0065 (4) | −0.0075 (4) | −0.0061 (3) |
| C25 | 0.0280 (6) | 0.0235 (5) | 0.0151 (4) | 0.0084 (4) | −0.0015 (4) | −0.0061 (4) |
| C26 | 0.0215 (5) | 0.0212 (5) | 0.0122 (4) | 0.0045 (4) | 0.0021 (3) | −0.0012 (3) |

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|---|---|---|---|---|---|---|
| C27 | 0.0133 (4) | 0.0143 (4) | 0.0112 (3) | 0.0016 (3) | 0.0010 (3) | −0.0004 (3) |
| C28 | 0.0106 (3) | 0.0135 (3) | 0.0109 (3) | 0.0004 (3) | 0.0023 (3) | 0.0022 (3) |
| C29 | 0.0093 (3) | 0.0118 (3) | 0.0110 (3) | 0.0011 (3) | 0.0008 (3) | 0.0008 (3) |
| C30 | 0.0099 (3) | 0.0120 (3) | 0.0110 (3) | 0.0008 (3) | 0.0007 (3) | −0.0001 (3) |
| C31 | 0.0107 (3) | 0.0109 (3) | 0.0132 (3) | 0.0005 (3) | −0.0010 (3) | −0.0005 (3) |
| C32 | 0.0116 (3) | 0.0140 (3) | 0.0103 (3) | 0.0013 (3) | 0.0001 (3) | 0.0006 (3) |
| C33 | 0.0093 (3) | 0.0107 (3) | 0.0114 (3) | 0.0002 (2) | 0.0014 (3) | 0.0012 (3) |
| C34 | 0.0098 (3) | 0.0135 (3) | 0.0124 (3) | 0.0001 (3) | 0.0025 (3) | 0.0012 (3) |
| C35 | 0.0098 (3) | 0.0123 (3) | 0.0167 (4) | −0.0009 (3) | 0.0023 (3) | 0.0032 (3) |
| C36 | 0.0101 (3) | 0.0137 (3) | 0.0102 (3) | 0.0017 (3) | 0.0005 (3) | 0.0002 (3) |
| C37 | 0.0104 (3) | 0.0143 (4) | 0.0129 (3) | 0.0014 (3) | 0.0010 (3) | 0.0028 (3) |
| C38 | 0.0113 (3) | 0.0152 (4) | 0.0092 (3) | 0.0000 (3) | 0.0013 (3) | 0.0021 (3) |
| C39 | 0.0108 (3) | 0.0152 (4) | 0.0106 (3) | −0.0017 (3) | 0.0008 (3) | 0.0013 (3) |
| C40 | 0.0103 (3) | 0.0160 (4) | 0.0096 (3) | −0.0006 (3) | 0.0015 (3) | 0.0023 (3) |
| Cl13 | 0.01770 (10) | 0.02354 (11) | 0.01141 (9) | 0.00470 (8) | 0.00434 (7) | 0.00335 (8) |
| Cl14 | 0.01352 (9) | 0.01905 (10) | 0.01587 (10) | 0.00283 (8) | −0.00431 (7) | 0.00008 (8) |
| Cl15 | 0.01306 (9) | 0.01089 (8) | 0.01855 (10) | 0.00068 (7) | 0.00050 (7) | 0.00358 (7) |
| Cl16 | 0.01555 (10) | 0.02152 (11) | 0.01677 (10) | 0.00244 (8) | 0.00659 (8) | −0.00163 (8) |
| Cl17 | 0.01655 (11) | 0.01744 (11) | 0.03321 (14) | −0.00172 (8) | 0.00695 (10) | 0.01084 (10) |
| Cl18 | 0.01851 (11) | 0.01363 (9) | 0.02210 (11) | 0.00153 (8) | −0.00507 (9) | −0.00519 (8) |
| Cl19 | 0.01466 (10) | 0.01355 (9) | 0.02162 (11) | −0.00028 (7) | 0.00144 (8) | 0.00481 (8) |
| Cl20 | 0.01137 (9) | 0.02036 (10) | 0.01609 (9) | 0.00441 (7) | 0.00072 (7) | 0.00441 (8) |
| Cl21 | 0.01617 (10) | 0.02432 (11) | 0.00905 (8) | 0.00128 (8) | 0.00142 (7) | 0.00381 (7) |
| Cl22 | 0.01692 (10) | 0.01942 (10) | 0.01496 (9) | −0.00570 (8) | −0.00048 (8) | −0.00125 (8) |
| Cl23 | 0.01377 (9) | 0.02338 (11) | 0.01183 (9) | −0.00289 (8) | 0.00262 (7) | 0.00475 (8) |
| Cl24 | 0.01656 (10) | 0.01830 (10) | 0.01279 (9) | 0.00548 (8) | 0.00096 (7) | −0.00253 (7) |

*Geometric parameters (Å, º)*

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| C1—C2 | 1.5099 (13) | C21—C22 | 1.5136 (14) |
| C1—C10 | 1.5623 (13) | C21—C30 | 1.5694 (13) |
| C1—C13 | 1.5913 (13) | C21—C33 | 1.5949 (13) |
| C1—H1 | 1 | C21—H21 | 1 |
| C2—C3 | 1.4033 (14) | C22—C27 | 1.4037 (14) |
| C2—C7 | 1.4036 (14) | C22—C23 | 1.4046 (14) |
| C3—C4 | 1.3919 (15) | C23—C24 | 1.3885 (17) |
| C3—H3 | 0.95 | C23—H23 | 0.95 |
| C4—C5 | 1.3908 (17) | C24—C25 | 1.391 (2) |
| C4—H4 | 0.95 | C24—H24 | 0.95 |
| C5—C6 | 1.3907 (15) | C25—C26 | 1.3891 (17) |
| C5—H5 | 0.95 | C25—H25 | 0.95 |
| C6—C7 | 1.4035 (14) | C26—C27 | 1.4026 (15) |
| C6—H6 | 0.95 | C26—H26 | 0.95 |
| C7—C8 | 1.5163 (13) | C27—C28 | 1.5070 (14) |
| C8—C9 | 1.5655 (13) | C28—C29 | 1.5643 (13) |
| C8—C18 | 1.5980 (13) | C28—C38 | 1.5951 (14) |
| C8—H8 | 1 | C28—H28 | 1 |
| C9—C10 | 1.5305 (13) | C29—C30 | 1.5366 (13) |

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| C9—C16 | 1.5625 (13) | C29—C36 | 1.5673 (13) |
| C9—H9 | 1 | C29—H29 | 1 |
| C10—C11 | 1.5633 (13) | C30—C31 | 1.5622 (13) |
| C10—H10 | 1 | C30—H30 | 1 |
| C11—C15 | 1.5265 (14) | C31—C35 | 1.5233 (15) |
| C11—C12 | 1.5543 (13) | C31—C32 | 1.5554 (14) |
| C11—Cl6 | 1.7535 (10) | C31—Cl18 | 1.7531 (10) |
| C12—C13 | 1.5506 (14) | C32—C33 | 1.5484 (13) |
| C12—Cl1 | 1.7664 (10) | C32—Cl13 | 1.7685 (10) |
| C12—Cl2 | 1.7716 (10) | C32—Cl14 | 1.7695 (10) |
| C13—C14 | 1.5185 (14) | C33—C34 | 1.5183 (13) |
| C13—Cl3 | 1.7505 (9) | C33—Cl15 | 1.7472 (9) |
| C14—C15 | 1.3403 (13) | C34—C35 | 1.3398 (14) |
| C14—Cl4 | 1.6926 (10) | C34—Cl16 | 1.6902 (10) |
| C15—Cl5 | 1.6976 (10) | C35—Cl17 | 1.6943 (10) |
| C16—C20 | 1.5262 (14) | C36—C40 | 1.5256 (14) |
| C16—C17 | 1.5517 (14) | C36—C37 | 1.5544 (13) |
| C16—Cl12 | 1.7518 (10) | C36—Cl24 | 1.7514 (10) |
| C17—C18 | 1.5493 (14) | C37—C38 | 1.5459 (14) |
| C17—Cl7 | 1.7668 (11) | C37—Cl19 | 1.7648 (10) |
| C17—Cl8 | 1.7730 (10) | C37—Cl20 | 1.7744 (10) |
| C18—C19 | 1.5204 (14) | C38—C39 | 1.5202 (14) |
| C18—Cl9 | 1.7495 (10) | C38—Cl21 | 1.7492 (10) |
| C19—C20 | 1.3395 (14) | C39—C40 | 1.3390 (14) |
| C19—Cl10 | 1.6943 (10) | C39—Cl22 | 1.6915 (10) |
| C20—Cl11 | 1.6980 (10) | C40—Cl23 | 1.6995 (10) |

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| C2—C1—C10 | 116.62 (8) | C22—C21—C30 | 116.46 (8) |
| C2—C1—C13 | 109.50 (8) | C22—C21—C33 | 109.13 (8) |
| C10—C1—C13 | 101.60 (7) | C30—C21—C33 | 101.61 (7) |
| C2—C1—H1 | 109.6 | C22—C21—H21 | 109.8 |
| C10—C1—H1 | 109.6 | C30—C21—H21 | 109.8 |
| C13—C1—H1 | 109.6 | C33—C21—H21 | 109.8 |
| C3—C2—C7 | 119.20 (9) | C27—C22—C23 | 118.69 (9) |
| C3—C2—C1 | 117.67 (8) | C27—C22—C21 | 122.21 (9) |
| C7—C2—C1 | 122.78 (8) | C23—C22—C21 | 118.77 (9) |
| C4—C3—C2 | 120.93 (10) | C24—C23—C22 | 120.94 (11) |
| C4—C3—H3 | 119.5 | C24—C23—H23 | 119.5 |
| C2—C3—H3 | 119.5 | C22—C23—H23 | 119.5 |
| C5—C4—C3 | 119.68 (10) | C23—C24—C25 | 119.96 (11) |
| C5—C4—H4 | 120.2 | C23—C24—H24 | 120 |
| C3—C4—H4 | 120.2 | C25—C24—H24 | 120 |
| C6—C5—C4 | 119.63 (10) | C26—C25—C24 | 119.55 (11) |
| C6—C5—H5 | 120.2 | C26—C25—H25 | 120.2 |
| C4—C5—H5 | 120.2 | C24—C25—H25 | 120.2 |
| C5—C6—C7 | 121.21 (10) | C25—C26—C27 | 120.86 (11) |
| C5—C6—H6 | 119.4 | C25—C26—H26 | 119.6 |
| C7—C6—H6 | 119.4 | C27—C26—H26 | 119.6 |

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| C6—C7—C2 | 118.77 (9) | C26—C27—C22 | 119.35 (10) |
| C6—C7—C8 | 118.72 (9) | C26—C27—C28 | 117.94 (9) |
| C2—C7—C8 | 122.16 (8) | C22—C27—C28 | 122.23 (9) |
| C7—C8—C9 | 115.90 (8) | C27—C28—C29 | 116.94 (8) |
| C7—C8—C18 | 109.08 (8) | C27—C28—C38 | 109.12 (8) |
| C9—C8—C18 | 101.61 (7) | C29—C28—C38 | 101.68 (7) |
| C7—C8—H8 | 110 | C27—C28—H28 | 109.6 |
| C9—C8—H8 | 110 | C29—C28—H28 | 109.6 |
| C18—C8—H8 | 110 | C38—C28—H28 | 109.6 |
| C10—C9—C16 | 112.28 (8) | C30—C29—C28 | 118.17 (8) |
| C10—C9—C8 | 119.29 (8) | C30—C29—C36 | 110.65 (8) |
| C16—C9—C8 | 102.75 (7) | C28—C29—C36 | 102.98 (7) |
| C10—C9—H9 | 107.3 | C30—C29—H29 | 108.2 |
| C16—C9—H9 | 107.3 | C28—C29—H29 | 108.2 |
| C8—C9—H9 | 107.3 | C36—C29—H29 | 108.2 |
| C9—C10—C1 | 117.92 (8) | C29—C30—C31 | 113.40 (8) |
| C9—C10—C11 | 111.87 (8) | C29—C30—C21 | 118.58 (8) |
| C1—C10—C11 | 103.20 (7) | C31—C30—C21 | 102.81 (7) |
| C9—C10—H10 | 107.8 | C29—C30—H30 | 107.1 |
| C1—C10—H10 | 107.8 | C31—C30—H30 | 107.1 |
| C11—C10—H10 | 107.8 | C21—C30—H30 | 107.1 |
| C15—C11—C12 | 99.75 (7) | C35—C31—C32 | 99.48 (8) |
| C15—C11—C10 | 107.59 (8) | C35—C31—C30 | 108.49 (8) |
| C12—C11—C10 | 101.23 (7) | C32—C31—C30 | 100.82 (7) |
| C15—C11—Cl6 | 115.79 (7) | C35—C31—Cl18 | 115.94 (7) |
| C12—C11—Cl6 | 115.87 (7) | C32—C31—Cl18 | 115.82 (7) |
| C10—C11—Cl6 | 114.67 (6) | C30—C31—Cl18 | 114.34 (7) |
| C13—C12—C11 | 92.42 (7) | C33—C32—C31 | 92.48 (7) |
| C13—C12—Cl1 | 113.60 (7) | C33—C32—Cl13 | 112.85 (7) |
| C11—C12—Cl1 | 114.64 (7) | C31—C32—Cl13 | 114.98 (7) |
| C13—C12—Cl2 | 113.77 (7) | C33—C32—Cl14 | 114.30 (7) |
| C11—C12—Cl2 | 113.72 (7) | C31—C32—Cl14 | 113.66 (7) |
| Cl1—C12—Cl2 | 108.22 (5) | Cl13—C32—Cl14 | 108.13 (5) |
| C14—C13—C12 | 99.82 (8) | C34—C33—C32 | 99.98 (7) |
| C14—C13—C1 | 106.03 (7) | C34—C33—C21 | 105.85 (7) |
| C12—C13—C1 | 102.45 (7) | C32—C33—C21 | 102.54 (7) |
| C14—C13—Cl3 | 115.75 (7) | C34—C33—Cl15 | 116.02 (7) |
| C12—C13—Cl3 | 114.89 (7) | C32—C33—Cl15 | 114.41 (7) |
| C1—C13—Cl3 | 115.87 (7) | C21—C33—Cl15 | 116.01 (6) |
| C15—C14—C13 | 107.20 (8) | C35—C34—C33 | 106.63 (8) |
| C15—C14—Cl4 | 128.20 (8) | C35—C34—Cl16 | 128.68 (8) |
| C13—C14—Cl4 | 124.28 (7) | C33—C34—Cl16 | 124.37 (7) |
| C14—C15—C11 | 107.22 (8) | C34—C35—C31 | 107.86 (8) |
| C14—C15—Cl5 | 127.72 (8) | C34—C35—Cl17 | 127.52 (8) |
| C11—C15—Cl5 | 124.79 (7) | C31—C35—Cl17 | 124.34 (7) |
| C20—C16—C17 | 99.79 (8) | C40—C36—C37 | 100.05 (7) |
| C20—C16—C9 | 108.31 (8) | C40—C36—C29 | 106.76 (8) |
| C17—C16—C9 | 100.91 (8) | C37—C36—C29 | 101.62 (8) |

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| C20—C16—Cl12 | 115.58 (7) | C40—C36—Cl24 | 115.80 (7) |
| C17—C16—Cl12 | 116.17 (7) | C37—C36—Cl24 | 115.92 (7) |
| C9—C16—Cl12 | 114.22 (7) | C29—C36—Cl24 | 114.76 (6) |
| C18—C17—C16 | 92.43 (7) | C38—C37—C36 | 92.52 (7) |
| C18—C17—Cl7 | 112.78 (7) | C38—C37—Cl19 | 113.76 (7) |
| C16—C17—Cl7 | 114.95 (7) | C36—C37—Cl19 | 114.29 (7) |
| C18—C17—Cl8 | 114.39 (7) | C38—C37—Cl20 | 113.72 (7) |
| C16—C17—Cl8 | 114.08 (7) | C36—C37—Cl20 | 114.20 (7) |
| Cl7—C17—Cl8 | 107.83 (5) | Cl19—C37—Cl20 | 107.95 (5) |
| C19—C18—C17 | 99.77 (8) | C39—C38—C37 | 100.27 (8) |
| C19—C18—C8 | 105.71 (7) | C39—C38—C28 | 105.99 (8) |
| C17—C18—C8 | 102.71 (7) | C37—C38—C28 | 101.98 (7) |
| C19—C18—Cl9 | 116.46 (7) | C39—C38—Cl21 | 115.08 (7) |
| C17—C18—Cl9 | 114.10 (7) | C37—C38—Cl21 | 114.92 (7) |
| C8—C18—Cl9 | 116.01 (7) | C28—C38—Cl21 | 116.56 (7) |
| C20—C19—C18 | 106.61 (8) | C40—C39—C38 | 107.24 (8) |
| C20—C19—Cl10 | 128.56 (8) | C40—C39—Cl22 | 128.51 (8) |
| C18—C19—Cl10 | 124.41 (7) | C38—C39—Cl22 | 123.90 (7) |
| C19—C20—C16 | 107.69 (8) | C39—C40—C36 | 107.17 (8) |
| C19—C20—Cl11 | 127.26 (8) | C39—C40—Cl23 | 127.44 (8) |
| C16—C20—Cl11 | 124.64 (7) | C36—C40—Cl23 | 124.86 (7) |

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| C10—C1—C2—C3 | −173.50 (9) | C30—C21—C22—C27 | −8.24 (14) |
| C13—C1—C2—C3 | 71.92 (11) | C33—C21—C22—C27 | 106.00 (10) |
| C10—C1—C2—C7 | 13.41 (13) | C30—C21—C22—C23 | 178.47 (9) |
| C13—C1—C2—C7 | −101.18 (10) | C33—C21—C22—C23 | −67.29 (12) |
| C7—C2—C3—C4 | 5.48 (16) | C27—C22—C23—C24 | −5.27 (16) |
| C1—C2—C3—C4 | −167.88 (10) | C21—C22—C23—C24 | 168.26 (10) |
| C2—C3—C4—C5 | 1.35 (18) | C22—C23—C24—C25 | −2.09 (19) |
| C3—C4—C5—C6 | −4.92 (18) | C23—C24—C25—C26 | 5.7 (2) |
| C4—C5—C6—C7 | 1.69 (18) | C24—C25—C26—C27 | −1.98 (19) |
| C5—C6—C7—C2 | 5.11 (16) | C25—C26—C27—C22 | −5.41 (17) |
| C5—C6—C7—C8 | −168.25 (10) | C25—C26—C27—C28 | 166.77 (11) |
| C3—C2—C7—C6 | −8.57 (15) | C23—C22—C27—C26 | 8.92 (15) |
| C1—C2—C7—C6 | 164.42 (9) | C21—C22—C27—C26 | −164.38 (10) |
| C3—C2—C7—C8 | 164.54 (9) | C23—C22—C27—C28 | −162.92 (10) |
| C1—C2—C7—C8 | −22.46 (15) | C21—C22—C27—C28 | 23.78 (15) |
| C6—C7—C8—C9 | −178.35 (9) | C26—C27—C28—C29 | 171.49 (9) |
| C2—C7—C8—C9 | 8.53 (13) | C22—C27—C28—C29 | −16.56 (14) |
| C6—C7—C8—C18 | 67.77 (11) | C26—C27—C28—C38 | −73.90 (12) |
| C2—C7—C8—C18 | −105.35 (10) | C22—C27—C28—C38 | 98.05 (11) |
| C7—C8—C9—C10 | 13.07 (12) | C27—C28—C29—C30 | −5.02 (12) |
| C18—C8—C9—C10 | 131.16 (8) | C38—C28—C29—C30 | −123.72 (9) |
| C7—C8—C9—C16 | −111.87 (9) | C27—C28—C29—C36 | 117.26 (9) |
| C18—C8—C9—C16 | 6.21 (9) | C38—C28—C29—C36 | −1.44 (9) |
| C16—C9—C10—C1 | 99.28 (9) | C28—C29—C30—C31 | −101.76 (10) |
| C8—C9—C10—C1 | −20.94 (12) | C36—C29—C30—C31 | 139.94 (8) |
| C16—C9—C10—C11 | −141.30 (8) | C28—C29—C30—C21 | 18.97 (12) |

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| C8—C9—C10—C11 | 98.47 (10) | C36—C29—C30—C21 | −99.33 (10) |
| C2—C1—C10—C9 | 8.32 (12) | C22—C21—C30—C29 | −12.98 (12) |
| C13—C1—C10—C9 | 127.27 (8) | C33—C21—C30—C29 | −131.41 (8) |
| C2—C1—C10—C11 | −115.55 (9) | C22—C21—C30—C31 | 113.02 (9) |
| C13—C1—C10—C11 | 3.40 (9) | C33—C21—C30—C31 | −5.41 (9) |
| C9—C10—C11—C15 | −63.17 (9) | C29—C30—C31—C35 | 66.67 (10) |
| C1—C10—C11—C15 | 64.59 (9) | C21—C30—C31—C35 | −62.61 (9) |
| C9—C10—C11—C12 | −167.29 (7) | C29—C30—C31—C32 | 170.59 (8) |
| C1—C10—C11—C12 | −39.54 (9) | C21—C30—C31—C32 | 41.31 (9) |
| C9—C10—C11—Cl6 | 67.21 (9) | C29—C30—C31—Cl18 | −64.44 (10) |
| C1—C10—C11—Cl6 | −165.03 (6) | C21—C30—C31—Cl18 | 166.28 (7) |
| C15—C11—C12—C13 | −51.76 (8) | C35—C31—C32—C33 | 51.48 (8) |
| C10—C11—C12—C13 | 58.53 (8) | C30—C31—C32—C33 | −59.58 (8) |
| Cl6—C11—C12—C13 | −176.78 (7) | Cl18—C31—C32—C33 | 176.46 (7) |
| C15—C11—C12—Cl1 | −169.16 (6) | C35—C31—C32—Cl13 | 168.16 (6) |
| C10—C11—C12—Cl1 | −58.87 (8) | C30—C31—C32—Cl13 | 57.11 (9) |
| Cl6—C11—C12—Cl1 | 65.82 (9) | Cl18—C31—C32—Cl13 | −66.86 (9) |
| C15—C11—C12—Cl2 | 65.58 (8) | C35—C31—C32—Cl14 | −66.47 (8) |
| C10—C11—C12—Cl2 | 175.87 (6) | C30—C31—C32—Cl14 | −177.53 (6) |
| Cl6—C11—C12—Cl2 | −59.44 (9) | Cl18—C31—C32—Cl14 | 58.51 (9) |
| C11—C12—C13—C14 | 52.50 (8) | C31—C32—C33—C34 | −52.74 (8) |
| Cl1—C12—C13—C14 | 170.78 (6) | Cl13—C32—C33—C34 | −171.23 (6) |
| Cl2—C12—C13—C14 | −64.80 (8) | Cl14—C32—C33—C34 | 64.66 (8) |
| C11—C12—C13—C1 | −56.48 (8) | C31—C32—C33—C21 | 56.12 (8) |
| Cl1—C12—C13—C1 | 61.80 (8) | Cl13—C32—C33—C21 | −62.37 (8) |
| Cl2—C12—C13—C1 | −173.78 (6) | Cl14—C32—C33—C21 | 173.52 (6) |
| C11—C12—C13—Cl3 | 177.01 (7) | C31—C32—C33—Cl15 | −177.42 (6) |
| Cl1—C12—C13—Cl3 | −64.72 (8) | Cl13—C32—C33—Cl15 | 64.09 (8) |
| Cl2—C12—C13—Cl3 | 59.71 (9) | Cl14—C32—C33—Cl15 | −60.01 (9) |
| C2—C1—C13—C14 | 53.64 (9) | C22—C21—C33—C34 | −51.60 (10) |
| C10—C1—C13—C14 | −70.27 (8) | C30—C21—C33—C34 | 71.95 (9) |
| C2—C1—C13—C12 | 157.83 (8) | C22—C21—C33—C32 | −155.94 (8) |
| C10—C1—C13—C12 | 33.93 (9) | C30—C21—C33—C32 | −32.39 (9) |
| C2—C1—C13—Cl3 | −76.28 (9) | C22—C21—C33—Cl15 | 78.63 (9) |
| C10—C1—C13—Cl3 | 159.81 (6) | C30—C21—C33—Cl15 | −157.82 (7) |
| C12—C13—C14—C15 | −35.79 (10) | C32—C33—C34—C35 | 36.13 (10) |
| C1—C13—C14—C15 | 70.31 (10) | C21—C33—C34—C35 | −70.08 (10) |
| Cl3—C13—C14—C15 | −159.70 (7) | Cl15—C33—C34—C35 | 159.69 (7) |
| C12—C13—C14—Cl4 | 150.16 (8) | C32—C33—C34—Cl16 | −149.88 (7) |
| C1—C13—C14—Cl4 | −103.74 (9) | C21—C33—C34—Cl16 | 103.91 (9) |
| Cl3—C13—C14—Cl4 | 26.25 (11) | Cl15—C33—C34—Cl16 | −26.32 (11) |
| C13—C14—C15—C11 | 1.03 (11) | C33—C34—C35—C31 | −1.40 (11) |
| Cl4—C14—C15—C11 | 174.77 (8) | Cl16—C34—C35—C31 | −175.04 (8) |
| C13—C14—C15—Cl5 | −173.21 (8) | C33—C34—C35—Cl17 | 172.77 (8) |
| Cl4—C14—C15—Cl5 | 0.53 (15) | Cl16—C34—C35—Cl17 | −0.88 (15) |
| C12—C11—C15—C14 | 33.98 (10) | C32—C31—C35—C34 | −33.58 (10) |
| C10—C11—C15—C14 | −71.19 (10) | C30—C31—C35—C34 | 71.28 (10) |
| Cl6—C11—C15—C14 | 159.06 (7) | Cl18—C31—C35—C34 | −158.48 (7) |

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| C12—C11—C15—Cl5 | −151.57 (8) | C32—C31—C35—Cl17 | 152.03 (7) |
| C10—C11—C15—Cl5 | 103.26 (9) | C30—C31—C35—Cl17 | −103.11 (9) |
| Cl6—C11—C15—Cl5 | −26.49 (11) | Cl18—C31—C35—Cl17 | 27.12 (11) |
| C10—C9—C16—C20 | −67.18 (10) | C30—C29—C36—C40 | 60.71 (9) |
| C8—C9—C16—C20 | 62.24 (9) | C28—C29—C36—C40 | −66.49 (9) |
| C10—C9—C16—C17 | −171.43 (8) | C30—C29—C36—C37 | 165.07 (8) |
| C8—C9—C16—C17 | −42.02 (9) | C28—C29—C36—C37 | 37.87 (9) |
| C10—C9—C16—Cl12 | 63.17 (9) | C30—C29—C36—Cl24 | −69.04 (9) |
| C8—C9—C16—Cl12 | −167.41 (6) | C28—C29—C36—Cl24 | 163.76 (6) |
| C20—C16—C17—C18 | −51.30 (8) | C40—C36—C37—C38 | 51.35 (8) |
| C9—C16—C17—C18 | 59.68 (8) | C29—C36—C37—C38 | −58.25 (8) |
| Cl12—C16—C17—C18 | −176.26 (7) | Cl24—C36—C37—C38 | 176.64 (7) |
| C20—C16—C17—Cl7 | −167.86 (7) | C40—C36—C37—Cl19 | 168.89 (7) |
| C9—C16—C17—Cl7 | −56.89 (9) | C29—C36—C37—Cl19 | 59.29 (9) |
| Cl12—C16—C17—Cl7 | 67.18 (9) | Cl24—C36—C37—Cl19 | −65.83 (9) |
| C20—C16—C17—Cl8 | 66.84 (8) | C40—C36—C37—Cl20 | −66.11 (9) |
| C9—C16—C17—Cl8 | 177.82 (6) | C29—C36—C37—Cl20 | −175.71 (6) |
| Cl12—C16—C17—Cl8 | −58.12 (9) | Cl24—C36—C37—Cl20 | 59.17 (9) |
| C16—C17—C18—C19 | 53.07 (8) | C36—C37—C38—C39 | −51.74 (8) |
| Cl7—C17—C18—C19 | 171.48 (6) | Cl19—C37—C38—C39 | −169.73 (6) |
| Cl8—C17—C18—C19 | −64.80 (8) | Cl20—C37—C38—C39 | 66.13 (8) |
| C16—C17—C18—C8 | −55.62 (8) | C36—C37—C38—C28 | 57.20 (8) |
| Cl7—C17—C18—C8 | 62.79 (8) | Cl19—C37—C38—C28 | −60.78 (8) |
| Cl8—C17—C18—C8 | −173.50 (6) | Cl20—C37—C38—C28 | 175.07 (6) |
| C16—C17—C18—Cl9 | 177.98 (7) | C36—C37—C38—Cl21 | −175.75 (7) |
| Cl7—C17—C18—Cl9 | −63.61 (8) | Cl19—C37—C38—Cl21 | 66.27 (8) |
| Cl8—C17—C18—Cl9 | 60.10 (9) | Cl20—C37—C38—Cl21 | −57.87 (9) |
| C7—C8—C18—C19 | 50.31 (10) | C27—C28—C38—C39 | −55.30 (10) |
| C9—C8—C18—C19 | −72.58 (9) | C29—C28—C38—C39 | 68.84 (9) |
| C7—C8—C18—C17 | 154.44 (8) | C27—C28—C38—C37 | −159.80 (8) |
| C9—C8—C18—C17 | 31.56 (9) | C29—C28—C38—C37 | −35.66 (9) |
| C7—C8—C18—Cl9 | −80.40 (9) | C27—C28—C38—Cl21 | 74.21 (9) |
| C9—C8—C18—Cl9 | 156.71 (7) | C29—C28—C38—Cl21 | −161.65 (7) |
| C17—C18—C19—C20 | −37.05 (10) | C37—C38—C39—C40 | 35.04 (10) |
| C8—C18—C19—C20 | 69.24 (10) | C28—C38—C39—C40 | −70.71 (10) |
| Cl9—C18—C19—C20 | −160.31 (7) | Cl21—C38—C39—C40 | 158.93 (8) |
| C17—C18—C19—Cl10 | 149.88 (7) | C37—C38—C39—Cl22 | −151.30 (8) |
| C8—C18—C19—Cl10 | −103.83 (9) | C28—C38—C39—Cl22 | 102.96 (9) |
| Cl9—C18—C19—Cl10 | 26.62 (11) | Cl21—C38—C39—Cl22 | −27.41 (11) |
| C18—C19—C20—C16 | 2.56 (10) | C38—C39—C40—C36 | −0.47 (11) |
| Cl10—C19—C20—C16 | 175.25 (8) | Cl22—C39—C40—C36 | −173.75 (8) |
| C18—C19—C20—Cl11 | −170.33 (7) | C38—C39—C40—Cl23 | 171.46 (8) |
| Cl10—C19—C20—Cl11 | 2.35 (15) | Cl22—C39—C40—Cl23 | −1.82 (16) |
| C17—C16—C20—C19 | 32.74 (10) | C37—C36—C40—C39 | −34.02 (10) |
| C9—C16—C20—C19 | −72.30 (10) | C29—C36—C40—C39 | 71.46 (10) |
| Cl12—C16—C20—C19 | 158.11 (7) | Cl24—C36—C40—C39 | −159.39 (7) |
| C17—C16—C20—Cl11 | −154.13 (7) | C37—C36—C40—Cl23 | 153.79 (8) |
| C9—C16—C20—Cl11 | 100.83 (9) | C29—C36—C40—Cl23 | −100.73 (9) |

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| Cl12—C16—C20—Cl11 | −28.77 (11) | Cl24—C36—C40—Cl23 | 28.42 (11) |