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# 5′,6-Dichloro-1′,3′,3′-trimethylspiro[2*H*-1-benzopyran-2,2′-indoline]

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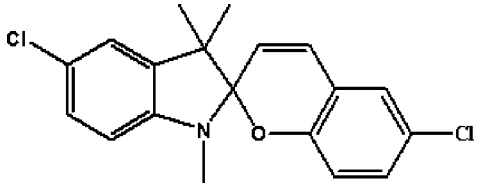
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.047; $wR$ factor = 0.123; data-to-parameter ratio = 15.6.

In the crystal structure of the title compound, $C_{19}H_{17}Cl_2NO$, the indoline and benzopyran ring systems are approximately perpendicular to each other. The indoline ring is in an envelope conformation with the spiro C atom as the flap. The N atom of the indoline ring forms a pyramidal environment, the sum of the angles at this atom being 352.46°.

## Related literature

For related literature, see: Crano & Guglielmetti (1999); Kholmanskii & Dyumanev (1987); Tamai & Miyasaka (2000); Krongauz *et al.* (2000); Minkin (2004); Crano *et al.* (1996); Dvornikov *et al.* (1994); Tamai & Miyasaka (2000); Yoshida & Morinaka (1994); Willner *et al.* (1993); Byrne *et al.* (2006*a*,*b*); Raić-Malić *et al.* (2004); Aldoshin & Atovmyan (1985); Aldoshin *et al.* (1987); Mannschreeck *et al.* (1999). For the synthesis of the title compound, see: Martin *et al.* (1998).




## Experimental

### *Crystal data*

$C_{19}H_{17}Cl_2NO$
$M_r$ = 346.24
Monoclinic, $P2_1/c$
$a$ = 8.3105 (7) Å
$b$ = 18.2576 (16) Å
$c$ = 11.1921 (10) Å
$\beta$ = 104.770 (2)°
$V$ = 1642.1 (2) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.40 mm$^{-1}$
$T$ = 100 (2) K
0.50 × 0.40 × 0.05 mm

### *Data collection*

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
$T_{min}$ = 0.740, $T_{max}$ = 0.980
16175 measured reflections
4312 independent reflections
3857 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.023

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.122
$S$ = 1.05
4312 reflections
276 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.96 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$

**Table 1**
Selected interplanar angles (°) for the title compound.

| Atoms defining plane 1 | Atoms defining plane 2 | Interplanar angle |
|---|---|---|
| C2, C6, C8, N | C11, C19, O | 85.03 (4) |
| C3, C4, C8, N | C8, C11, N | 28.9 (1) |
| C1, C2, C3, C4, C5, C6 | C3, C4, C8, N | 2.4 (1) |

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2106).

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# supporting information

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## 5′,6-Dichloro-1′,3′,3′-trimethylspiro[2*H*-1-benzopyran-2,2′-indoline]

**Nameer Alhashimy, Helge Müller-Bunz, Benjamin Schazmann and Dermot Diamond**

### S1. Comment

Spiropyrans are a family of organic photochromic compounds (Carno & Guglielmetti, 1998). This family of compounds are well studied and documented (Kholmanskii & Dyumanev, 1987; Tamai & Miyasaka, 2000; Krongauz *et al.*, 2000; Minkin, 2004) because they can be converted from a closed colourless form into a strongly coloured open form using UV irradiation. This tremendous characteristic of spiropyran compounds has been utilized by scientists for many applications such as light-sensitive eyewear (Crano *et al.*, 1996), high density optical storage (Dvornikov *et al.*,1994), molecular switches (Tamai & Miyasaka, 2000, Minkin, 2004) and molecular devices (Yoshida & Morinaka, 1994; Willner *et al.*, 1993). Our main interest was utilizing spiropyran derivatives as transducers in optical sensors, where selective binding to certain metal ions was achieved. The binding and release of such ions can be controlled by exposure to light of around 380 nm (open form) and 550 nm (close form) respectively (Byrne *et al.*, 2006*a*; Byrne *et al.*, 2006*b*). The title compound was envisaged as an intermediate in the synthesis of further spiropyran derivatives, whereby the chlorides groups can be replaced by substitution with variety of functional groups. The title compound consists of two molecular fragments: An indoline ring linked to a benzopyran ring by the spiro (C11) atom (Fig 1). The two fragments are almost perpendicular to each other (Table 2). The bond lengths of (C11—N) and (C11—O) are both approximately equal, which agrees with previous reports (Raić-Malić *et al.*, 2004; Aldoshin & Atovmyan, 1985; Aldoshin *et al.*, 1987). The spiro carbon atom (C11) is out of the plane of the other four indoline ring atoms (Table 2). The indoline ring is quite coplanar with the fused benzene ring (Table 2). The sum of the angles of the nitrogen atom at the indoline moiety is 352.46°, which indicates a pyramidal arrangement about this atom. These results are in agreement with previous reports (Raić-Malić *et al.*, 2004).

### S2. Experimental

The title compound was originally synthesized according to a method outlined in a patent (Martin *et al.*, 1998). Our procedure differs from the original synthesis, especially with regard to the purification process. Single crystals suitable for X-ray diffraction were grown by slow evaporation from ethanol solution.

To 5-chlorosalicylaldehyde (1.53 g, 9.6 mmol) in 10 ml e thanol, a solution of 5-chloro-2-methylene-1,3,3-trimethyl-indoline (1.95 ml, 9.6 mmol) in 20 ml of ethanol was added slowly, over 30 min. This reaction mixture was heated to reflux over 24 h and then cooled down to ambient temperature. The solvent was evaporated by vacuum and the resulting crude compound was purified by column chromatography from the system solvent of 1:5, ethyl acetate: hexane, yielding a white powder (2.30 g, 69.4%).

### S3. Refinement

All hydrogen atoms were located in the difference fourier map and allowed to refine isotropic without any restraints. C—H bond lenghts vary from 0.92 (2) to 1.00 (2) Å.

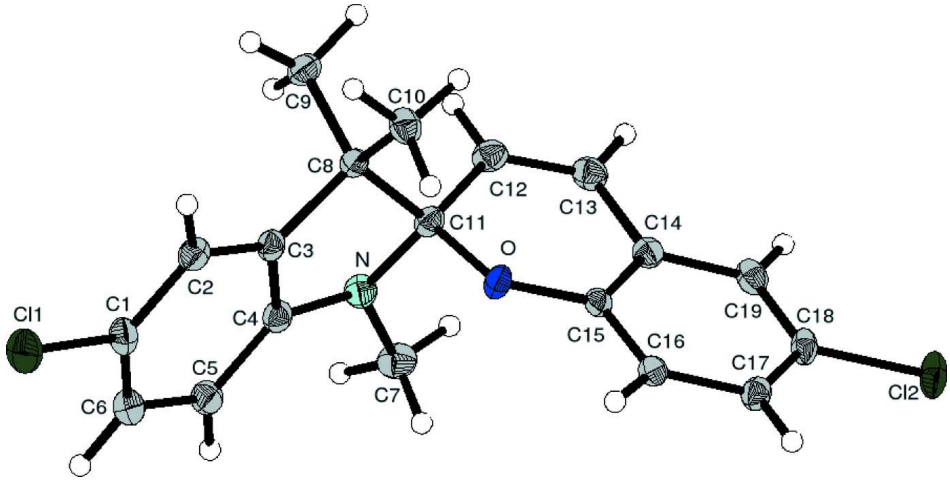


**Figure 1**

A perspective view of the asymmetric unit of title compound, showing the atom numbering and thermal ellipsoids at a 50% probability level.

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*Crystal data*

$C_{19}H_{17}Cl_2NO$
$M_r = 346.24$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.3105\ (7)$ Å
$b = 18.2576\ (16)$ Å
$c = 11.1921\ (10)$ Å
$\beta = 104.770\ (2)°$
$V = 1642.1\ (2)$ Å$^3$
$Z = 4$
$F(000) = 720$
$D_x = 1.401$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7373 reflections
$\theta = 2.2–31.7°$
$\mu = 0.40$ mm$^{-1}$
$T = 100$ K
Plate, colourless
0.50 × 0.40 × 0.05 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.366 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2000)
$T_{min} = 0.740$, $T_{max} = 0.980$
16175 measured reflections
4312 independent reflections
3857 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 29.0°$, $\theta_{min} = 2.2°$
$h = -11\rightarrow11$
$k = -24\rightarrow24$
$l = -15\rightarrow15$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.122$
$S = 1.05$
4312 reflections
276 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0653P)^2 + 1.2622P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.96 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$

*Special details*

**Experimental**. $^1$H NMR $\delta$($CDCl_3$); 1.190 (S, 3H, $CH_3$), 1.30 (S, 3H, CH~3~),2.72 (S, 3H, $CH_3$), 5.73 (d, 1H, *J*= 10.4 Hz, CH=CH), 6.46 ( d, H, *J*= 12.8 Hz, Ar-H), 6.67 (d, 1H, *J* =9.6 Hz, Ar-H), 6.83 (d, 1H, *J* = 16.4, Ar-H), 7.01-7.08 ( m, 2H, Ar-H), 7.15 ( d, 1H, *J* = 10.4 Hz, CH=CH).
$^{13}$C NMR $\delta$($CDCl_3$); 19.95, 25.68, 29.04, 51.96, 104.60, 107.78, 116.33, 119.91,120.17, 122.11, 123.93, 124.85, 126.28, 127.37, 128.80, 129.50, 138.53, 146.73,152.80.
M.S. (m/z ion) (m/z 346.2).

**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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 1.29108 (6) | 0.46363 (2) | 0.01666 (4) | 0.02892 (13) |
| C1 | 1.2126 (2) | 0.38771 (9) | 0.07835 (15) | 0.0198 (3) |
| C2 | 1.0760 (2) | 0.39650 (9) | 0.12870 (15) | 0.0187 (3) |
| H2 | 1.029 (3) | 0.4437 (13) | 0.133 (2) | 0.025 (5)* |
| C3 | 1.01780 (19) | 0.33524 (8) | 0.17644 (14) | 0.0160 (3) |
| C4 | 1.09359 (19) | 0.26690 (8) | 0.17419 (14) | 0.0169 (3) |
| C5 | 1.2295 (2) | 0.25851 (9) | 0.12441 (16) | 0.0202 (3) |
| H5 | 1.284 (3) | 0.2115 (12) | 0.120 (2) | 0.020 (5)* |
| C6 | 1.2886 (2) | 0.32043 (10) | 0.07558 (16) | 0.0223 (3) |
| H6 | 1.381 (3) | 0.3155 (12) | 0.037 (2) | 0.024 (5)* |
| N | 1.01339 (17) | 0.21423 (7) | 0.22743 (13) | 0.0186 (3) |
| C7 | 1.0459 (2) | 0.13674 (9) | 0.21878 (17) | 0.0225 (3) |
| H7A | 1.015 (3) | 0.1214 (13) | 0.136 (2) | 0.029 (6)* |
| H7B | 0.989 (3) | 0.1089 (13) | 0.271 (2) | 0.030 (6)* |
| H7C | 1.163 (3) | 0.1284 (14) | 0.256 (2) | 0.038 (7)* |
| C8 | 0.88187 (19) | 0.32673 (8) | 0.24368 (14) | 0.0150 (3) |
| C9 | 0.9546 (2) | 0.34836 (9) | 0.37930 (15) | 0.0197 (3) |
| H9A | 0.989 (3) | 0.3981 (13) | 0.383 (2) | 0.024 (5)* |
| H9B | 0.870 (3) | 0.3426 (12) | 0.427 (2) | 0.027 (6)* |
| H9C | 1.051 (3) | 0.3191 (13) | 0.419 (2) | 0.029 (6)* |
| C10 | 0.7265 (2) | 0.37244 (10) | 0.18951 (16) | 0.0204 (3) |
| H10A | 0.687 (3) | 0.3635 (12) | 0.100 (2) | 0.022 (5)* |
| H10B | 0.756 (3) | 0.4243 (13) | 0.202 (2) | 0.028 (6)* |
| H10C | 0.647 (3) | 0.3607 (12) | 0.233 (2) | 0.023 (5)* |
| C11 | 0.85232 (19) | 0.24213 (9) | 0.23280 (14) | 0.0163 (3) |
| O | 0.73274 (14) | 0.23176 (6) | 0.11246 (10) | 0.0178 (2) |
| C12 | 0.7959 (2) | 0.20568 (9) | 0.33518 (15) | 0.0194 (3) |
| H12 | 0.853 (3) | 0.2181 (12) | 0.417 (2) | 0.025 (5)* |

| | | | | |
|---|---|---|---|---|
| C13 | 0.6788 (2) | 0.15405 (9) | 0.31410 (15) | 0.0200 (3) |
| H13 | 0.651 (3) | 0.1291 (13) | 0.381 (2) | 0.028 (6)* |
| C14 | 0.5891 (2) | 0.13478 (8) | 0.18904 (15) | 0.0166 (3) |
| C15 | 0.61892 (19) | 0.17667 (8) | 0.09238 (14) | 0.0147 (3) |
| C16 | 0.52518 (19) | 0.16618 (9) | −0.02828 (14) | 0.0159 (3) |
| H16 | 0.550 (3) | 0.1972 (12) | −0.090 (2) | 0.021 (5)* |
| C17 | 0.4051 (2) | 0.11154 (9) | −0.05435 (15) | 0.0185 (3) |
| H17 | 0.345 (2) | 0.1032 (11) | −0.1356 (18) | 0.014 (5)* |
| C18 | 0.38016 (19) | 0.06811 (8) | 0.04128 (16) | 0.0183 (3) |
| Cl2 | 0.23079 (5) | −0.00073 (2) | 0.00933 (4) | 0.02523 (13) |
| C19 | 0.4695 (2) | 0.07902 (9) | 0.16192 (16) | 0.0188 (3) |
| H19 | 0.452 (3) | 0.0512 (12) | 0.226 (2) | 0.022 (5)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0321 (2) | 0.0223 (2) | 0.0349 (2) | −0.00767 (16) | 0.01332 (18) | 0.00340 (17) |
| C1 | 0.0173 (7) | 0.0211 (8) | 0.0209 (7) | −0.0046 (6) | 0.0047 (6) | 0.0022 (6) |
| C2 | 0.0180 (7) | 0.0160 (7) | 0.0208 (7) | −0.0002 (6) | 0.0026 (6) | −0.0016 (6) |
| C3 | 0.0129 (7) | 0.0172 (7) | 0.0165 (7) | −0.0009 (5) | 0.0015 (5) | −0.0014 (5) |
| C4 | 0.0145 (7) | 0.0176 (7) | 0.0171 (7) | −0.0003 (5) | 0.0016 (5) | −0.0016 (5) |
| C5 | 0.0152 (7) | 0.0200 (8) | 0.0248 (8) | 0.0016 (6) | 0.0041 (6) | −0.0025 (6) |
| C6 | 0.0174 (8) | 0.0249 (8) | 0.0248 (8) | −0.0022 (6) | 0.0061 (6) | −0.0025 (6) |
| N | 0.0187 (6) | 0.0149 (6) | 0.0224 (7) | 0.0011 (5) | 0.0054 (5) | −0.0002 (5) |
| C7 | 0.0284 (9) | 0.0143 (7) | 0.0252 (8) | 0.0031 (6) | 0.0078 (7) | 0.0011 (6) |
| C8 | 0.0141 (7) | 0.0149 (7) | 0.0158 (7) | −0.0007 (5) | 0.0033 (5) | −0.0021 (5) |
| C9 | 0.0205 (8) | 0.0199 (8) | 0.0178 (7) | −0.0011 (6) | 0.0032 (6) | −0.0037 (6) |
| C10 | 0.0157 (7) | 0.0213 (8) | 0.0240 (8) | 0.0019 (6) | 0.0048 (6) | 0.0012 (6) |
| C11 | 0.0179 (7) | 0.0166 (7) | 0.0134 (7) | −0.0020 (5) | 0.0022 (5) | −0.0011 (5) |
| O | 0.0204 (5) | 0.0194 (6) | 0.0125 (5) | −0.0082 (4) | 0.0023 (4) | 0.0001 (4) |
| C12 | 0.0235 (8) | 0.0199 (7) | 0.0145 (7) | −0.0006 (6) | 0.0045 (6) | −0.0002 (6) |
| C13 | 0.0231 (8) | 0.0203 (8) | 0.0180 (7) | −0.0001 (6) | 0.0080 (6) | 0.0026 (6) |
| C14 | 0.0169 (7) | 0.0147 (7) | 0.0190 (7) | 0.0010 (5) | 0.0058 (6) | 0.0003 (5) |
| C15 | 0.0133 (6) | 0.0134 (6) | 0.0182 (7) | −0.0001 (5) | 0.0056 (5) | −0.0013 (5) |
| C16 | 0.0132 (7) | 0.0173 (7) | 0.0171 (7) | 0.0004 (5) | 0.0039 (5) | −0.0006 (5) |
| C17 | 0.0143 (7) | 0.0182 (7) | 0.0216 (8) | 0.0001 (6) | 0.0018 (6) | −0.0028 (6) |
| C18 | 0.0122 (7) | 0.0117 (6) | 0.0308 (8) | −0.0002 (5) | 0.0052 (6) | −0.0012 (6) |
| Cl2 | 0.0158 (2) | 0.01421 (19) | 0.0436 (3) | −0.00319 (13) | 0.00372 (17) | 0.00058 (15) |
| C19 | 0.0179 (7) | 0.0146 (7) | 0.0256 (8) | 0.0007 (6) | 0.0086 (6) | 0.0034 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C1 | 1.7474 (17) | C9—H9C | 0.97 (2) |
| C1—C6 | 1.385 (2) | C10—H10A | 0.98 (2) |
| C1—C2 | 1.399 (2) | C10—H10B | 0.98 (2) |
| C2—C3 | 1.379 (2) | C10—H10C | 0.94 (2) |
| C2—H2 | 0.95 (2) | C11—O | 1.4680 (18) |
| C3—C4 | 1.401 (2) | C11—C12 | 1.500 (2) |

| | | | |
|---|---|---|---|
| C3—C8 | 1.517 (2) | O—C15 | 1.3596 (18) |
| C4—N | 1.388 (2) | C12—C13 | 1.332 (2) |
| C4—C5 | 1.389 (2) | C12—H12 | 0.94 (2) |
| C5—C6 | 1.398 (2) | C13—C14 | 1.451 (2) |
| C5—H5 | 0.98 (2) | C13—H13 | 0.95 (2) |
| C6—H6 | 0.98 (2) | C14—C15 | 1.397 (2) |
| N—C11 | 1.448 (2) | C14—C19 | 1.401 (2) |
| N—C7 | 1.448 (2) | C15—C16 | 1.390 (2) |
| C7—H7A | 0.94 (2) | C16—C17 | 1.389 (2) |
| C7—H7B | 0.98 (2) | C16—H16 | 0.96 (2) |
| C7—H7C | 0.96 (3) | C17—C18 | 1.389 (2) |
| C8—C10 | 1.527 (2) | C17—H17 | 0.93 (2) |
| C8—C9 | 1.535 (2) | C18—C19 | 1.379 (2) |
| C8—C11 | 1.564 (2) | C18—Cl2 | 1.7384 (16) |
| C9—H9A | 0.95 (2) | C19—H19 | 0.92 (2) |
| C9—H9B | 1.00 (2) | | |

| | | | |
|---|---|---|---|
| C6—C1—C2 | 122.16 (15) | H9B—C9—H9C | 107.9 (19) |
| C6—C1—Cl1 | 118.44 (13) | C8—C10—H10A | 109.9 (13) |
| C2—C1—Cl1 | 119.41 (13) | C8—C10—H10B | 108.3 (14) |
| C3—C2—C1 | 117.62 (15) | H10A—C10—H10B | 108.3 (18) |
| C3—C2—H2 | 121.6 (14) | C8—C10—H10C | 107.7 (14) |
| C1—C2—H2 | 120.7 (14) | H10A—C10—H10C | 113.3 (18) |
| C2—C3—C4 | 120.77 (15) | H10B—C10—H10C | 109.2 (19) |
| C2—C3—C8 | 130.88 (14) | N—C11—O | 109.47 (12) |
| C4—C3—C8 | 108.24 (13) | N—C11—C12 | 110.36 (13) |
| N—C4—C5 | 128.63 (15) | O—C11—C12 | 111.93 (13) |
| N—C4—C3 | 110.00 (14) | N—C11—C8 | 102.84 (12) |
| C5—C4—C3 | 121.37 (15) | O—C11—C8 | 104.77 (12) |
| C4—C5—C6 | 118.05 (15) | C12—C11—C8 | 116.89 (13) |
| C4—C5—H5 | 123.3 (13) | C15—O—C11 | 121.79 (12) |
| C6—C5—H5 | 118.6 (13) | C13—C12—C11 | 122.36 (15) |
| C1—C6—C5 | 120.02 (15) | C13—C12—H12 | 120.5 (14) |
| C1—C6—H6 | 120.4 (13) | C11—C12—H12 | 117.0 (14) |
| C5—C6—H6 | 119.5 (13) | C12—C13—C14 | 120.98 (15) |
| C4—N—C11 | 108.93 (13) | C12—C13—H13 | 120.8 (14) |
| C4—N—C7 | 122.00 (14) | C14—C13—H13 | 118.2 (14) |
| C11—N—C7 | 122.46 (14) | C15—C14—C19 | 119.07 (15) |
| N—C7—H7A | 110.4 (14) | C15—C14—C13 | 117.73 (14) |
| N—C7—H7B | 109.9 (14) | C19—C14—C13 | 123.13 (15) |
| H7A—C7—H7B | 112 (2) | O—C15—C16 | 117.17 (14) |
| N—C7—H7C | 108.0 (16) | O—C15—C14 | 122.00 (14) |
| H7A—C7—H7C | 112 (2) | C16—C15—C14 | 120.72 (14) |
| H7B—C7—H7C | 104 (2) | C17—C16—C15 | 119.88 (15) |
| C3—C8—C10 | 114.10 (13) | C17—C16—H16 | 123.2 (13) |
| C3—C8—C9 | 107.98 (13) | C15—C16—H16 | 116.9 (13) |
| C10—C8—C9 | 109.39 (13) | C16—C17—C18 | 119.23 (15) |
| C3—C8—C11 | 100.63 (12) | C16—C17—H17 | 119.9 (12) |

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| C10—C8—C11 | 114.13 (13) | C18—C17—H17 | 120.8 (12) |
| C9—C8—C11 | 110.21 (13) | C19—C18—C17 | 121.53 (15) |
| C8—C9—H9A | 109.3 (13) | C19—C18—Cl2 | 118.93 (13) |
| C8—C9—H9B | 110.6 (13) | C17—C18—Cl2 | 119.53 (13) |
| H9A—C9—H9B | 108.9 (19) | C18—C19—C14 | 119.48 (15) |
| C8—C9—H9C | 112.7 (14) | C18—C19—H19 | 121.8 (14) |
| H9A—C9—H9C | 107.3 (19) | C14—C19—H19 | 118.7 (14) |

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| C6—C1—C2—C3 | 0.0 (2) | C9—C8—C11—N | −84.95 (15) |
| Cl1—C1—C2—C3 | 179.99 (12) | C3—C8—C11—O | −85.57 (13) |
| C1—C2—C3—C4 | 0.0 (2) | C10—C8—C11—O | 37.07 (17) |
| C1—C2—C3—C8 | 175.66 (15) | C9—C8—C11—O | 160.62 (12) |
| C2—C3—C4—N | 179.88 (14) | C3—C8—C11—C12 | 149.91 (14) |
| C8—C3—C4—N | 3.35 (17) | C10—C8—C11—C12 | −87.45 (17) |
| C2—C3—C4—C5 | 0.2 (2) | C9—C8—C11—C12 | 36.10 (19) |
| C8—C3—C4—C5 | −176.36 (14) | N—C11—O—C15 | 102.17 (16) |
| N—C4—C5—C6 | 179.99 (16) | C12—C11—O—C15 | −20.53 (19) |
| C3—C4—C5—C6 | −0.4 (2) | C8—C11—O—C15 | −148.14 (13) |
| C2—C1—C6—C5 | −0.2 (3) | N—C11—C12—C13 | −104.55 (18) |
| Cl1—C1—C6—C5 | 179.82 (13) | O—C11—C12—C13 | 17.6 (2) |
| C4—C5—C6—C1 | 0.4 (3) | C8—C11—C12—C13 | 138.45 (16) |
| C5—C4—N—C11 | −163.27 (16) | C11—C12—C13—C14 | −5.4 (3) |
| C3—C4—N—C11 | 17.04 (17) | C12—C13—C14—C15 | −5.7 (2) |
| C5—C4—N—C7 | −11.2 (3) | C12—C13—C14—C19 | 177.48 (16) |
| C3—C4—N—C7 | 169.10 (15) | C11—O—C15—C16 | −172.39 (13) |
| C2—C3—C8—C10 | 41.2 (2) | C11—O—C15—C14 | 11.3 (2) |
| C4—C3—C8—C10 | −142.78 (14) | C19—C14—C15—O | 179.72 (14) |
| C2—C3—C8—C9 | −80.7 (2) | C13—C14—C15—O | 2.8 (2) |
| C4—C3—C8—C9 | 95.37 (15) | C19—C14—C15—C16 | 3.6 (2) |
| C2—C3—C8—C11 | 163.81 (16) | C13—C14—C15—C16 | −173.34 (14) |
| C4—C3—C8—C11 | −20.12 (15) | O—C15—C16—C17 | −178.97 (14) |
| C4—N—C11—O | 81.89 (15) | C14—C15—C16—C17 | −2.7 (2) |
| C7—N—C11—O | −70.01 (18) | C15—C16—C17—C18 | 0.2 (2) |
| C4—N—C11—C12 | −154.49 (13) | C16—C17—C18—C19 | 1.4 (2) |
| C7—N—C11—C12 | 53.62 (19) | C16—C17—C18—Cl2 | −179.66 (12) |
| C4—N—C11—C8 | −29.08 (16) | C17—C18—C19—C14 | −0.4 (2) |
| C7—N—C11—C8 | 179.02 (14) | Cl2—C18—C19—C14 | −179.39 (12) |
| C3—C8—C11—N | 28.87 (14) | C15—C14—C19—C18 | −2.0 (2) |
| C10—C8—C11—N | 151.51 (13) | C13—C14—C19—C18 | 174.72 (15) |