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# *N*-[2-(2-Chlorophenyl)-2-hydroxyethyl]-propan-2-aminium 4-methylbenzoate

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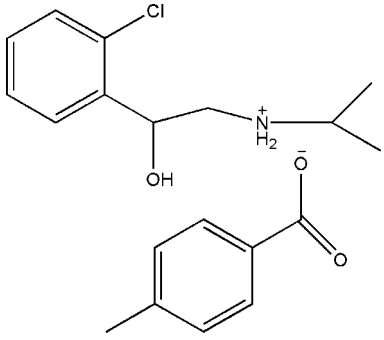
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.042; $wR$ factor = 0.125; data-to-parameter ratio = 19.2.

The title compound, $C_{11}H_{17}ClNO^+\cdot C_8H_7O_2^-$, was obtained by the reaction of chlorprenaline {or 1-(2-chlorophenyl)-2-[(1-methylethyl)amino]ethanol} and *p*-toluic acid. The chlorprenaline is twisted moderately with a C—C—C—C torsion angle of 109.6 (2)°. The two molecules are linked by classical O—H···O and N—H···O hydrogen bonds. Further N—H···O hydrogen bonds link two of these units into dimers.

## Related literature

For related structures, see: Feng *et al.* (2010); Takwale & Pant (1971); Tang *et al.* (2009*a*,*b*).




## Experimental

### Crystal data

$C_{11}H_{17}ClNO^+\cdot C_8H_7O_2^-$ $M_r$ = 349.84
Monoclinic, $P2_1/n$
$a$ = 8.5966 (4) Å
$b$ = 8.1288 (3) Å
$c$ = 26.8949 (12) Å
$\beta$ = 91.600 (1)°
$V$ = 1878.68 (14) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.22 mm$^{-1}$
$T$ = 296 K
0.37 × 0.30 × 0.22 mm

### Data collection

Rigaku R-AXIS RAPID/ZJUG CCD diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.913, $T_{max}$ = 0.953
27924 measured reflections
4271 independent reflections
2763 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.036

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.125
$S$ = 1.00
4271 reflections
222 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H101···O3 | 0.82 | 1.88 | 2.6986 (18) | 173 |
| N1—H103···O2 | 0.90 | 1.91 | 2.7835 (18) | 164 |
| N1—H102···O3$^{i}$ | 0.90 | 1.89 | 2.7824 (19) | 174 |

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Data collection: *PROCESS-AUTO* (Rigaku/MSC, 2006); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

This project was supported by the Zhejiang Provincial Natural Science Foundation of China (grant No. Y206174).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2225).

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# supporting information

*Acta Cryst.* (2010). E**66**, o2605 [doi:10.1107/S1600536810033878]

## *N*-[2-(2-Chlorophenyl)-2-hydroxyethyl]propan-2-aminium 4-methylbenzoate

**Hai Feng, Bin Tao Xing, Xin Huang, Ya Jian Zhou and Ying Song**

### S1. Comment

A recent study reports the structure of bis{*N*-[2-(2-chlorophenyl)-2-hydroxyethyl]propan-2-aminium} oxalate (Tang *et al.*, 2009*b*), which was synthesized by oxalic acid and chlorprenaline (Tang *et al.*, 2009*a*). Here using *p*-toluic acid instead of oxalic acid and following a similar synthetic procedure yields the title compound, **I**.

In **I**, the chlorprenaline molecule and the *p*-toluic molecule are linked to each other by the classical N1—H103···O2 hydogen bond [2.7835 (18)Å] and the O1—H101···O3 hydogen bond [2.6986 (18)Å] (Fig. 1 & Table 1). The chlorprenaline in **I** are twisted moderately as compared with those of other compounds. The C7—C2—C1—C8 torsion angle of 109.6 (2)° is larger than the value of the similar torsion angle of 91.9 (2)° (Tang *et al.*, 2009*a*). The C12–O2 distance of 1.248 (2)Å is much shorter than the similar distance of 1.292 (8)Å (Takwale & Pant, 1971). The C9–N1 distance of 1.507 (2)Å is longer than the value of the similar bond distance of 1.473 (4)Å (Tang *et al.*, 2009*b*), as similar as the value of the similar bond distance of 1.503 (2)Å (Feng *et al.*, 2010).

Classical O—H···O and N—H···O hydrogen bonds are found in the cystal structure (Fig. 2) are essential forces in crystal formation.

### S2. Experimental

Racemic chlorprenaline was prepared by chlorprenaline hydrochloride purchased from ShangHai Shengxin Medicine & Chemical Co., Ltd. ShangHai, China. Chlorprenaline hydrochloride and NaOH in a molar ratio of 1:1 were mixed and dissolved in a methanol–water solution (1:1 *v*/*v*). The precipitate formed was filtered off, washed with water and dried. It was used without further purification. Racemic chlorprenaline (0.5 g, 0.0023 mol) was dissolved in methanol (7 ml) and then *p*-toluylic acid (0.31 g, 0.0023 mol) was added.The mixture was dissovled by heating to 343 K where a clear solution resulted. The resulting solution was concentrated at ambient temperature. Colourless crystals of title compound separated from the solution in about 70% yield after one day.

### S3. Refinement

All of the H atoms were placed in calculated positions and allowed to ride on their parent atoms at distances of 0.93Å (aromatic), 0.98Å (methine), 0.97Å (methylene), 0.96Å (methyl) 0.82Å (hydroxyl) and 0.90Å (amine), with $U_{iso}$(H) = 1.2–1.5 $U_{eq}$(parent atom).

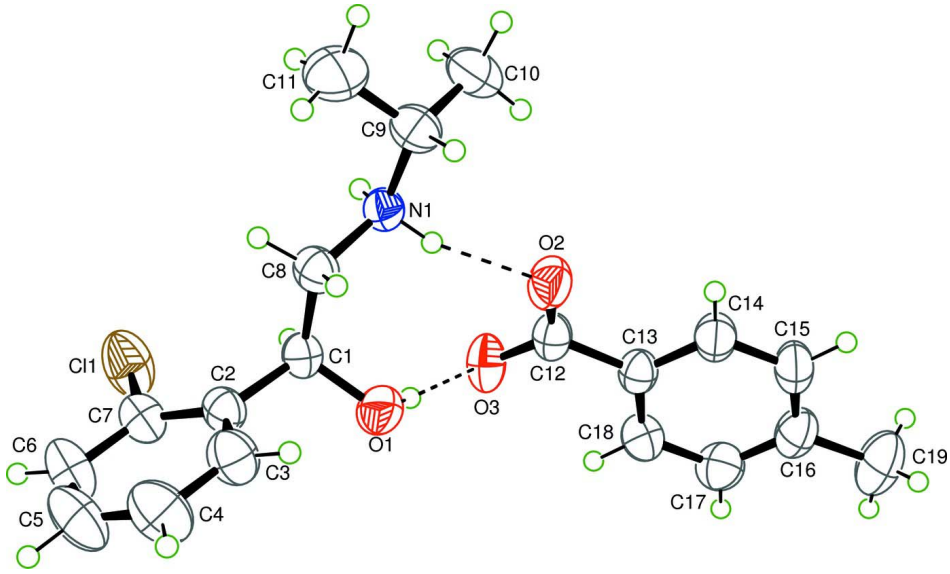


**Figure 1**

The asymmetric unit of **I** with atom numbering scheme. Displacement ellipsoids are presented at 50% probability level. H atoms are presented as a small spheres of arbitrary radius.

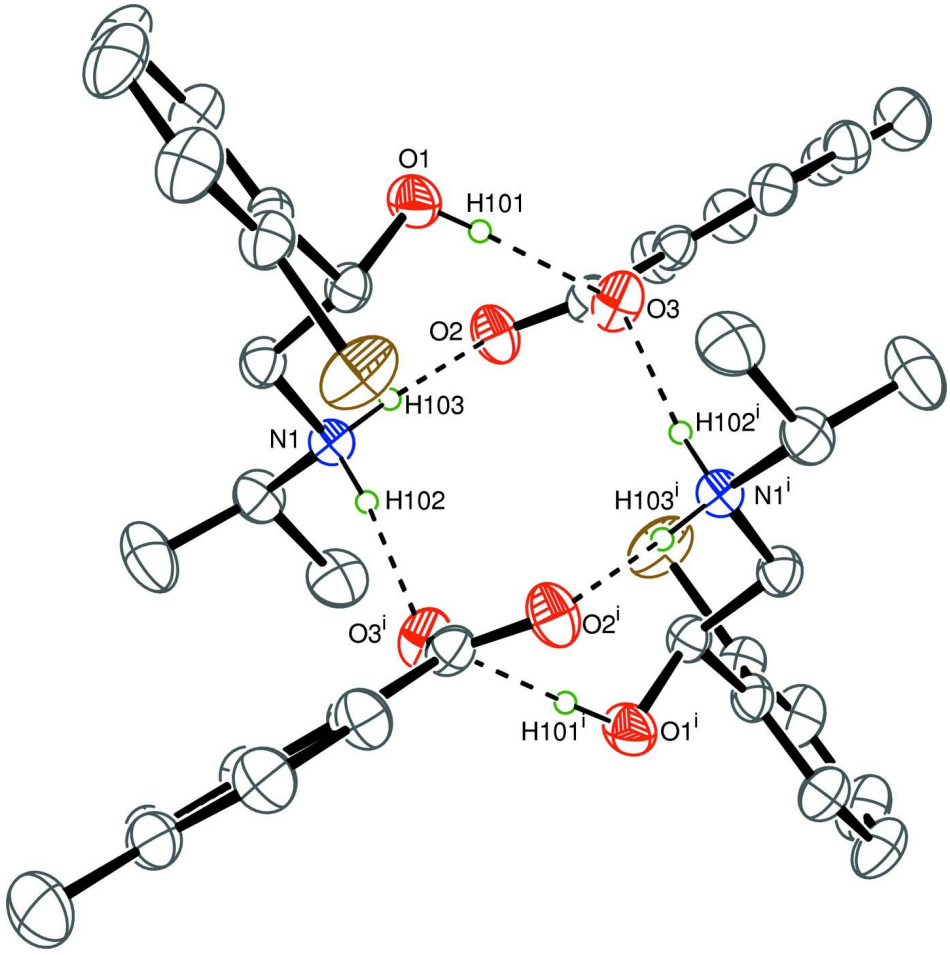


**Figure 2**

The two units of **I** with atom labels. The dashed lines indicate hydrogen bonds.

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*Crystal data*

$C_{11}H_{17}ClNO^{+}\cdot C_8H_7O_2^{-}$
$M_r = 349.84$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 8.5966\ (4)$ Å
$b = 8.1288\ (3)$ Å
$c = 26.8949\ (12)$ Å
$\beta = 91.600\ (1)°$
$V = 1878.68\ (14)$ Å$^3$
$Z = 4$
$F(000) = 744$
$D_x = 1.237$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 17098 reflections
$\theta = 3.0–27.4°$
$\mu = 0.22$ mm$^{-1}$
$T = 296$ K
Chunk, colourless
0.37 × 0.30 × 0.22 mm

*Data collection*

Rigaku R-AXIS RAPID/ZJUG CCD diffractometer
Radiation source: rotate anode
Graphite monochromator
Detector resolution: 10.00 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.913$, $T_{max} = 0.953$
27924 measured reflections

4271 independent reflections
2763 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 27.4°$, $\theta_{min} = 3.0°$
$h = -11 \rightarrow 11$
$k = -10 \rightarrow 9$
$l = -34 \rightarrow 34$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.125$
$S = 1.00$
4271 reflections
222 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
$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 0.6753P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.21$ e Å$^{-3}$
$\Delta\rho_{min} = -0.31$ e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0084 (10)

*Special details*

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.29951 (9) | 0.54161 (7) | 0.65218 (2) | 0.0833 (2) |
| O1 | 0.27619 (16) | 0.21200 (19) | 0.53119 (5) | 0.0615 (4) |
| H101 | 0.2803 | 0.2754 | 0.5076 | 0.092* |
| O2 | 0.49211 (17) | 0.21720 (18) | 0.43539 (5) | 0.0619 (4) |
| N1 | 0.62036 (16) | 0.27020 (17) | 0.53021 (5) | 0.0420 (3) |
| H102 | 0.6383 | 0.3783 | 0.5348 | 0.050* |
| H103 | 0.5619 | 0.2592 | 0.5021 | 0.050* |
| C7 | 0.2495 (2) | 0.3348 (2) | 0.65680 (7) | 0.0541 (5) |
| C1 | 0.3646 (2) | 0.2763 (2) | 0.57188 (6) | 0.0440 (4) |
| H1 | 0.3678 | 0.3966 | 0.5696 | 0.053* |
| C2 | 0.2854 (2) | 0.2261 (2) | 0.61907 (6) | 0.0459 (4) |
| C8 | 0.5294 (2) | 0.2082 (2) | 0.57268 (6) | 0.0486 (4) |
| H8A | 0.5820 | 0.2392 | 0.6037 | 0.058* |
| H8B | 0.5252 | 0.0891 | 0.5713 | 0.058* |
| C9 | 0.7739 (2) | 0.1855 (3) | 0.52294 (8) | 0.0571 (5) |
| H9 | 0.7533 | 0.0726 | 0.5118 | 0.068* |
| C4 | 0.1703 (3) | 0.0101 (3) | 0.66772 (10) | 0.0788 (7) |
| H4 | 0.1439 | −0.1001 | 0.6714 | 0.095* |
| C6 | 0.1758 (3) | 0.2841 (3) | 0.69932 (8) | 0.0749 (7) |

| | | | | |
|---|---|---|---|---|
| H6 | 0.1540 | 0.3592 | 0.7243 | 0.090* |
| C10 | 0.8567 (3) | 0.2759 (3) | 0.48204 (9) | 0.0744 (6) |
| H10A | 0.7901 | 0.2810 | 0.4528 | 0.112* |
| H10B | 0.9507 | 0.2186 | 0.4745 | 0.112* |
| H10C | 0.8817 | 0.3855 | 0.4930 | 0.112* |
| C3 | 0.2444 (2) | 0.0620 (3) | 0.62573 (8) | 0.0607 (5) |
| H3 | 0.2677 | −0.0143 | 0.6013 | 0.073* |
| C11 | 0.8699 (3) | 0.1785 (4) | 0.57050 (10) | 0.0913 (8) |
| H11A | 0.8804 | 0.2873 | 0.5841 | 0.137* |
| H11B | 0.9711 | 0.1353 | 0.5638 | 0.137* |
| H11C | 0.8196 | 0.1086 | 0.5939 | 0.137* |
| C5 | 0.1353 (3) | 0.1218 (3) | 0.70422 (9) | 0.0830 (8) |
| H5 | 0.0840 | 0.0871 | 0.7323 | 0.100* |
| O3 | 0.30804 (17) | 0.40215 (16) | 0.44986 (5) | 0.0589 (4) |
| C13 | 0.3104 (2) | 0.2771 (2) | 0.37008 (6) | 0.0439 (4) |
| C12 | 0.3761 (2) | 0.3002 (2) | 0.42202 (6) | 0.0467 (4) |
| C14 | 0.3905 (2) | 0.1855 (2) | 0.33582 (7) | 0.0547 (5) |
| H14 | 0.4842 | 0.1360 | 0.3453 | 0.066* |
| C18 | 0.1687 (2) | 0.3448 (2) | 0.35524 (7) | 0.0529 (5) |
| H18 | 0.1117 | 0.4052 | 0.3778 | 0.064* |
| C16 | 0.1925 (2) | 0.2349 (3) | 0.27234 (7) | 0.0578 (5) |
| C15 | 0.3330 (3) | 0.1666 (3) | 0.28760 (7) | 0.0609 (5) |
| H15 | 0.3901 | 0.1067 | 0.2650 | 0.073* |
| C17 | 0.1113 (2) | 0.3231 (3) | 0.30701 (7) | 0.0607 (5) |
| H17 | 0.0157 | 0.3690 | 0.2978 | 0.073* |
| C19 | 0.1321 (4) | 0.2139 (4) | 0.21933 (9) | 0.0890 (8) |
| H19A | 0.2018 | 0.2667 | 0.1971 | 0.133* |
| H19B | 0.0308 | 0.2629 | 0.2158 | 0.133* |
| H19C | 0.1254 | 0.0989 | 0.2115 | 0.133* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.1200 (5) | 0.0570 (3) | 0.0746 (4) | −0.0060 (3) | 0.0327 (3) | −0.0103 (3) |
| O1 | 0.0601 (8) | 0.0804 (10) | 0.0435 (7) | −0.0112 (7) | −0.0052 (6) | 0.0058 (7) |
| O2 | 0.0651 (9) | 0.0754 (9) | 0.0446 (7) | 0.0106 (7) | −0.0091 (6) | −0.0056 (7) |
| N1 | 0.0427 (8) | 0.0434 (8) | 0.0400 (7) | 0.0015 (6) | 0.0020 (6) | −0.0029 (6) |
| C7 | 0.0561 (11) | 0.0568 (11) | 0.0498 (10) | 0.0044 (9) | 0.0102 (8) | 0.0035 (9) |
| C1 | 0.0488 (10) | 0.0454 (9) | 0.0378 (8) | 0.0003 (7) | 0.0026 (7) | 0.0009 (7) |
| C2 | 0.0460 (10) | 0.0515 (10) | 0.0404 (9) | 0.0035 (8) | 0.0026 (7) | 0.0067 (8) |
| C8 | 0.0497 (10) | 0.0523 (10) | 0.0440 (9) | 0.0024 (8) | 0.0034 (8) | 0.0064 (8) |
| C9 | 0.0487 (11) | 0.0585 (12) | 0.0643 (12) | 0.0116 (9) | 0.0063 (9) | −0.0040 (9) |
| C4 | 0.0927 (17) | 0.0631 (14) | 0.0818 (16) | −0.0038 (12) | 0.0234 (13) | 0.0242 (12) |
| C6 | 0.0881 (17) | 0.0820 (16) | 0.0561 (12) | 0.0105 (13) | 0.0285 (12) | 0.0043 (11) |
| C10 | 0.0552 (13) | 0.0929 (17) | 0.0761 (15) | 0.0067 (12) | 0.0194 (11) | −0.0026 (13) |
| C3 | 0.0708 (13) | 0.0549 (12) | 0.0570 (12) | −0.0008 (10) | 0.0103 (10) | 0.0072 (9) |
| C11 | 0.0580 (14) | 0.131 (2) | 0.0845 (17) | 0.0235 (15) | −0.0098 (12) | 0.0098 (16) |
| C5 | 0.0928 (18) | 0.0889 (18) | 0.0691 (15) | 0.0057 (14) | 0.0357 (13) | 0.0274 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O3 | 0.0889 (10) | 0.0460 (7) | 0.0420 (7) | 0.0038 (7) | 0.0029 (6) | −0.0067 (6) |
| C13 | 0.0538 (10) | 0.0406 (9) | 0.0375 (8) | −0.0040 (7) | 0.0015 (7) | 0.0012 (7) |
| C12 | 0.0616 (11) | 0.0399 (9) | 0.0388 (9) | −0.0050 (8) | 0.0023 (8) | −0.0008 (7) |
| C14 | 0.0567 (11) | 0.0613 (12) | 0.0460 (10) | 0.0066 (9) | −0.0016 (8) | −0.0078 (9) |
| C18 | 0.0578 (12) | 0.0537 (11) | 0.0475 (10) | 0.0037 (9) | 0.0053 (8) | 0.0015 (8) |
| C16 | 0.0710 (13) | 0.0594 (12) | 0.0426 (10) | −0.0094 (10) | −0.0061 (9) | 0.0016 (9) |
| C15 | 0.0716 (14) | 0.0698 (13) | 0.0414 (10) | 0.0016 (11) | 0.0039 (9) | −0.0116 (9) |
| C17 | 0.0597 (12) | 0.0664 (13) | 0.0555 (11) | 0.0027 (10) | −0.0051 (9) | 0.0076 (10) |
| C19 | 0.114 (2) | 0.0984 (19) | 0.0531 (13) | −0.0079 (16) | −0.0230 (13) | −0.0049 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C7 | 1.741 (2) | C10—H10A | 0.9600 |
| O1—C1 | 1.415 (2) | C10—H10B | 0.9600 |
| O1—H101 | 0.8200 | C10—H10C | 0.9600 |
| O2—C12 | 1.248 (2) | C3—H3 | 0.9300 |
| N1—C8 | 1.490 (2) | C11—H11A | 0.9600 |
| N1—C9 | 1.507 (2) | C11—H11B | 0.9600 |
| N1—H102 | 0.9000 | C11—H11C | 0.9600 |
| N1—H103 | 0.9000 | C5—H5 | 0.9300 |
| C7—C6 | 1.386 (3) | O3—C12 | 1.271 (2) |
| C7—C2 | 1.387 (3) | C13—C14 | 1.383 (2) |
| C1—C2 | 1.513 (2) | C13—C18 | 1.386 (3) |
| C1—C8 | 1.521 (2) | C13—C12 | 1.504 (2) |
| C1—H1 | 0.9800 | C14—C15 | 1.384 (3) |
| C2—C3 | 1.392 (3) | C14—H14 | 0.9300 |
| C8—H8A | 0.9700 | C18—C17 | 1.386 (3) |
| C8—H8B | 0.9700 | C18—H18 | 0.9300 |
| C9—C11 | 1.504 (3) | C16—C17 | 1.381 (3) |
| C9—C10 | 1.517 (3) | C16—C15 | 1.382 (3) |
| C9—H9 | 0.9800 | C16—C19 | 1.513 (3) |
| C4—C5 | 1.376 (4) | C15—H15 | 0.9300 |
| C4—C3 | 1.379 (3) | C17—H17 | 0.9300 |
| C4—H4 | 0.9300 | C19—H19A | 0.9600 |
| C6—C5 | 1.371 (4) | C19—H19B | 0.9600 |
| C6—H6 | 0.9300 | C19—H19C | 0.9600 |
| | | | |
| C1—O1—H101 | 109.5 | H10A—C10—H10C | 109.5 |
| C8—N1—C9 | 115.19 (14) | H10B—C10—H10C | 109.5 |
| C8—N1—H102 | 108.5 | C4—C3—C2 | 121.5 (2) |
| C9—N1—H102 | 108.5 | C4—C3—H3 | 119.2 |
| C8—N1—H103 | 108.5 | C2—C3—H3 | 119.2 |
| C9—N1—H103 | 108.5 | C9—C11—H11A | 109.5 |
| H102—N1—H103 | 107.5 | C9—C11—H11B | 109.5 |
| C6—C7—C2 | 122.1 (2) | H11A—C11—H11B | 109.5 |
| C6—C7—Cl1 | 117.75 (17) | C9—C11—H11C | 109.5 |
| C2—C7—Cl1 | 120.19 (14) | H11A—C11—H11C | 109.5 |
| O1—C1—C2 | 107.74 (14) | H11B—C11—H11C | 109.5 |

| | | | |
|---|---|---|---|
| O1—C1—C8 | 110.88 (15) | C6—C5—C4 | 120.3 (2) |
| C2—C1—C8 | 109.32 (14) | C6—C5—H5 | 119.8 |
| O1—C1—H1 | 109.6 | C4—C5—H5 | 119.8 |
| C2—C1—H1 | 109.6 | C14—C13—C18 | 118.17 (16) |
| C8—C1—H1 | 109.6 | C14—C13—C12 | 120.33 (16) |
| C7—C2—C3 | 117.01 (17) | C18—C13—C12 | 121.50 (16) |
| C7—C2—C1 | 123.81 (17) | O2—C12—O3 | 124.06 (16) |
| C3—C2—C1 | 119.18 (17) | O2—C12—C13 | 118.45 (16) |
| N1—C8—C1 | 112.01 (14) | O3—C12—C13 | 117.49 (16) |
| N1—C8—H8A | 109.2 | C13—C14—C15 | 120.84 (18) |
| C1—C8—H8A | 109.2 | C13—C14—H14 | 119.6 |
| N1—C8—H8B | 109.2 | C15—C14—H14 | 119.6 |
| C1—C8—H8B | 109.2 | C13—C18—C17 | 120.41 (18) |
| H8A—C8—H8B | 107.9 | C13—C18—H18 | 119.8 |
| C11—C9—N1 | 111.64 (17) | C17—C18—H18 | 119.8 |
| C11—C9—C10 | 112.2 (2) | C17—C16—C15 | 117.54 (17) |
| N1—C9—C10 | 107.65 (16) | C17—C16—C19 | 121.9 (2) |
| C11—C9—H9 | 108.4 | C15—C16—C19 | 120.6 (2) |
| N1—C9—H9 | 108.4 | C16—C15—C14 | 121.36 (19) |
| C10—C9—H9 | 108.4 | C16—C15—H15 | 119.3 |
| C5—C4—C3 | 119.8 (2) | C14—C15—H15 | 119.3 |
| C5—C4—H4 | 120.1 | C16—C17—C18 | 121.64 (19) |
| C3—C4—H4 | 120.1 | C16—C17—H17 | 119.2 |
| C5—C6—C7 | 119.2 (2) | C18—C17—H17 | 119.2 |
| C5—C6—H6 | 120.4 | C16—C19—H19A | 109.5 |
| C7—C6—H6 | 120.4 | C16—C19—H19B | 109.5 |
| C9—C10—H10A | 109.5 | H19A—C19—H19B | 109.5 |
| C9—C10—H10B | 109.5 | C16—C19—H19C | 109.5 |
| H10A—C10—H10B | 109.5 | H19A—C19—H19C | 109.5 |
| C9—C10—H10C | 109.5 | H19B—C19—H19C | 109.5 |

| | | | |
|---|---|---|---|
| C6—C7—C2—C3 | −0.2 (3) | C1—C2—C3—C4 | −179.13 (19) |
| Cl1—C7—C2—C3 | 178.83 (15) | C7—C6—C5—C4 | 1.2 (4) |
| C6—C7—C2—C1 | 179.50 (19) | C3—C4—C5—C6 | −0.9 (4) |
| Cl1—C7—C2—C1 | −1.4 (3) | C14—C13—C12—O2 | −9.8 (3) |
| O1—C1—C2—C7 | −129.79 (18) | C18—C13—C12—O2 | 169.70 (18) |
| C8—C1—C2—C7 | 109.6 (2) | C14—C13—C12—O3 | 171.21 (17) |
| O1—C1—C2—C3 | 49.9 (2) | C18—C13—C12—O3 | −9.3 (3) |
| C8—C1—C2—C3 | −70.6 (2) | C18—C13—C14—C15 | 2.1 (3) |
| C9—N1—C8—C1 | −169.34 (15) | C12—C13—C14—C15 | −178.45 (18) |
| O1—C1—C8—N1 | 68.35 (19) | C14—C13—C18—C17 | −1.1 (3) |
| C2—C1—C8—N1 | −173.02 (14) | C12—C13—C18—C17 | 179.36 (17) |
| C8—N1—C9—C11 | −50.6 (2) | C17—C16—C15—C14 | 0.0 (3) |
| C8—N1—C9—C10 | −174.10 (16) | C19—C16—C15—C14 | 179.6 (2) |
| C2—C7—C6—C5 | −0.7 (4) | C13—C14—C15—C16 | −1.5 (3) |
| Cl1—C7—C6—C5 | −179.8 (2) | C15—C16—C17—C18 | 0.9 (3) |
| C5—C4—C3—C2 | −0.1 (4) | C19—C16—C17—C18 | −178.6 (2) |
| C7—C2—C3—C4 | 0.6 (3) | C13—C18—C17—C16 | −0.3 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H101···O3 | 0.82 | 1.88 | 2.6986 (18) | 173 |
| N1—H103···O2 | 0.90 | 1.91 | 2.7835 (18) | 164 |
| N1—H102···O3$^{i}$ | 0.90 | 1.89 | 2.7824 (19) | 174 |

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.