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

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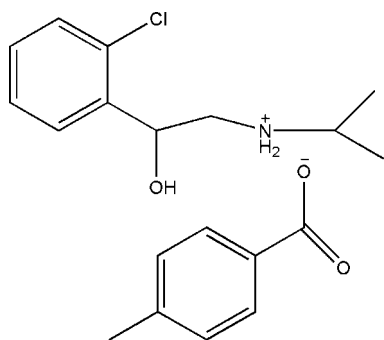
Received 2 August 2010; accepted 23 August 2010

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

The title compound,  $\text{C}_{11}\text{H}_{17}\text{ClNO}^+ \cdot \text{C}_8\text{H}_7\text{O}_2^-$ , 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.* (2009a,b).



## Experimental

## Crystal data

 $\text{C}_{11}\text{H}_{17}\text{ClNO}^+ \cdot \text{C}_8\text{H}_7\text{O}_2^-$  $M_r = 349.84$ 

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<sup>3</sup>

$Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.22$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.37 \times 0.30 \times 0.22$  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  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.036$

## 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  
 $\Delta\rho_{\text{max}} = 0.21$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.31$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
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 <sup>i</sup>	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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**supplementary materials**

*Acta Cryst.* (2010). E66, o2605 [ doi:10.1107/S1600536810033878 ]

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

H. Feng, B. T. Xing, X. Huang, Y. J. Zhou and Y. Song

### 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 hydrogen bond [2.7835 (18)Å] and the O1—H101···O3 hydrogen 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 crystal structure (Fig. 2) are essential forces in crystal formation.

### 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*-toluic acid (0.31 g, 0.0023 mol) was added. The mixture was dissolved 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.

### 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  $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5 U_{\text{eq}}(\text{parent atom})$ .

Figures

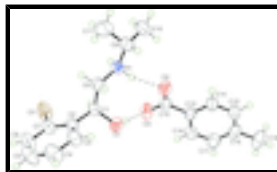


Fig. 1. The asymmetric unit of **I** with atom numbering scheme. Displacement ellipsoids are presented at 50% probability level. H atoms are presented as a small spheres of arbitrary radius.

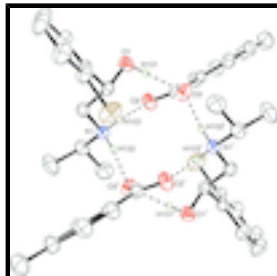


Fig. 2. The two units of **I** with atom labels. The dashed lines indicate hydrogen bonds.

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

*Crystal data*

$C_{11}H_{17}ClNO^+ \cdot C_8H_7O_2^-$

$M_r = 349.84$

Monoclinic,  $P2_1/n$

Hall symbol:  $-P\ 2_1/n$

$a = 8.5966\ (4)\ \text{\AA}$

$b = 8.1288\ (3)\ \text{\AA}$

$c = 26.8949\ (12)\ \text{\AA}$

$\beta = 91.600\ (1)^\circ$

$V = 1878.68\ (14)\ \text{\AA}^3$

$Z = 4$

$F(000) = 744$

$D_x = 1.237\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 17098 reflections

$\theta = 3.0\text{--}27.4^\circ$

$\mu = 0.22\ \text{mm}^{-1}$

$T = 296\ \text{K}$

Chunk, colourless

$0.37 \times 0.30 \times 0.22\ \text{mm}$

*Data collection*

Rigaku R-Axis RAPID/ZJUG CCD diffractometer

Radiation source: rotate anode graphite

Detector resolution:  $10.00\ \text{pixels mm}^{-1}$

$\varphi$  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  $I > 2\sigma(I)$

$R_{\text{int}} = 0.036$

$\theta_{\max} = 27.4^\circ$ ,  $\theta_{\min} = 3.0^\circ$

$h = -11 \rightarrow 11$

$k = -10 \rightarrow 9$

$l = -34 \rightarrow 34$

*Refinement*

Refinement on  $F^2$

Secondary atom site location: difference Fourier map

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

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 0.6753P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} < 0.001$$

$$\Delta\rho_{\max} = 0.21 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.31 \text{ e } \text{\AA}^{-3}$$

Extinction correction: *SHELXL97* (Sheldrick, 2008),

$$F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$$

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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	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*

## supplementary materials

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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 ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C11	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, °)*

C11—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—C11	117.75 (17)	C9—C11—H11C	109.5
C2—C7—C11	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

## supplementary materials

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)
C11—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)
C11—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)
C11—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 ( $\text{\AA}$ , $^\circ$ )

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
O1—H101 $\cdots$ O3	0.82	1.88	2.6986 (18)	173



N1—H103…O2	0.90	1.91	2.7835 (18)	164
N1—H102…O3 <sup>i</sup>	0.90	1.89	2.7824 (19)	174

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

Fig. 1

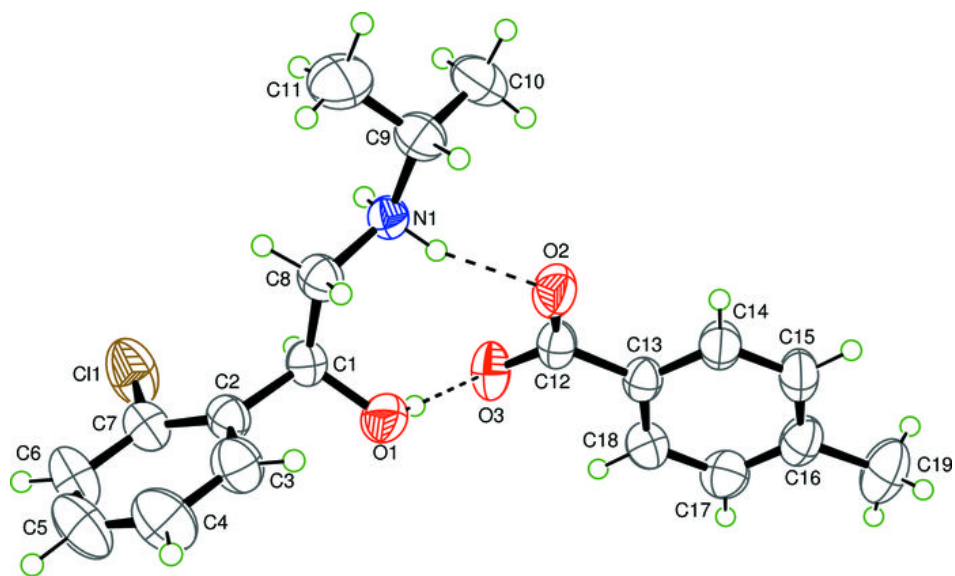


Fig. 2

