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(*R*)-1-(2-Hydroxy-5-methylphenyl)-*N*-[(*S*)-1-(2-methoxy-5-methylphenyl)-2-phenylethyl]butan-1-aminium chloride

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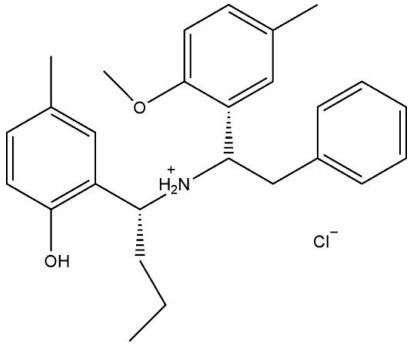
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.100; data-to-parameter ratio = 15.9.

2-{(*R*)-1-[(*S*)-1-(2-Methoxy-5-methylphenyl)-2-phenylethylamino]butyl}-4-methylphenol has been synthesized and its absolute configuration determined from the crystal structure of its hydrochloride, the title compound, $C_{27}H_{34}NO_2^+\cdot Cl^-$. The absolute configuration of the stereogenic center that carries the 2-methoxy-5-methylphenyl substituent was found to be *R*. Intermolecular N—H···Cl and O—H···Cl and intramolecular N—H···O hydrogen bonds stabilize the structure.

Related literature

For general background, see: Cimarelli *et al.* (2002); Guangyou *et al.* (2003); Joshi & Malhotra (2003); Li *et al.* (2004); Puigjaner *et al.* (1999); Soai & Niwa (1992); Tseng & Yang (2004); Watts *et al.* (2005). For related structures, see: Yang *et al.* (2005).



Experimental

Crystal data

$C_{27}H_{34}NO_2^+\cdot Cl^-$
M_r = 440.00
Orthorhombic, $P2_12_12_1$
a = 9.8553 (14) Å
b = 13.1962 (19) Å
c = 18.825 (3) Å
V = 2448.2 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 298 (2) K
0.48 × 0.40 × 0.32 mm

Data collection

Bruker SMART CCD area-detecter diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997*a*)
T_{min} = 0.919, T_{max} = 0.945
12855 measured reflections
4534 independent reflections
3992 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.100
S = 1.03
4534 reflections
285 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Absolute structure: Flack (1983), 1957 Friedel pairs
Flack parameter: −0.05 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*C*···Cl1^{i}	0.82	2.23	3.0446 (15)	171
N1—H1*A*···Cl1^{ii}	0.90	2.23	3.1193 (18)	169
N1—H1*B*···O2	0.90	2.28	2.884 (2)	125
N1—H1*B*···O1	0.90	2.26	2.864 (2)	124

Symmetry codes: (i) $x+1, y, z$; (ii) $x+\frac{1}{2}, -y+\frac{3}{2}, -z+1$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*b*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*b*); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Bruker, 1997).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2377).

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supplementary materials

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(*R*)-1-(2-Hydroxy-5-methylphenyl)-*N*-[(*S*)-1-(2-methoxy-5-methylphenyl)-2-phenylethyl]butan-1-aminium chloride

G.-Y. Zhang, M. Li, W.-H. Wang and X.-G. Gu

Comment

The search for new chiral ligands to be used in asymmetric catalysis is of great interest in the field of synthetic chemistry. (Cimarelli *et al.*, 2002; Tseng & Yang, 2004). Among them, enantiopure aminoalkyphenols have attracted wide attention as they can be used in asymmetric catalytic reactions (Puigjaner *et al.*, 1999; Guangyou *et al.*, 2003; Li *et al.*, 2004; Watts *et al.* 2005), an active area of research in organic chemistry (Joshi & Malhotra, 2003). However, most aminoalkylphenols are derived from readily available natural products (Soai & Niwa, 1992). The synthesis of new aminoalkylphenols is therefore of interest because of their potential as asymmetric catalysts.

In this paper, we report the absolute structure of the title compound (I) a hydrochloride derivative of the aminoalkylphenol 2-((*R*)-1-((*S*)-1–2-methoxy-5-methylphenyl-2-phenylethylamino)butyl)-4- methylphenol. As well as the known S configuration of C8, the structure reveals an *R* configuration for the strereogenic centre at C17. The asymmetric unit of the title compound (Fig. 1) consists of a $C_{27}H_{34}NO_2^+$ cation and a Cl^- anion. The dihedral angles between the benzene rings A (C1—C6), B (C9—C15) and C (C21—C27) are 54.51 ° for A/B, 56.51 ° for A/C and 21.17 ° for B/C respectively.

The conformation of the molecule is influenced by two intramolecular N—H···O hydrogen bonds. In the crystal structure, the Cl^- anion forms O—H···Cl and N—H···Cl hydrogen bonds to give a continuous two-dimensional framework structure Table 1, Fig. 2.

Experimental

Compound (II) was prepared according to the procedure of Yang *et al.* (2005). Compound (II) was reacted at room temperature with concentrated HCl to yield a white precipitate. The solvent was removed and the solid residue recrystallized from an ethanol/hexane (4:1, *v*/*v*) mixture to yield compound (I) (m.p. 492–494 K).

Refinement

Hydrogen atoms attached to C, N and O were placed in geometrically idealized positions and refined using a riding model. [C—H = 0.93 Å; U_{iso}(H) = 1.2U_{eq}(C) (aromatic CH); C—H = 0.98 Å; U_{iso}(H) = 1.2U_{eq}(C) (methine CH) C—H = 0.970 Å; U_{iso}(H) = 1.2U_{eq}(C) (methylene CH_2) and C—H = 0.960 Å; U_{iso}(H) = 1.5U_{eq}(C) (methyl CH_3); N—H = 0.90 Å; U_{iso}(H) = 1.2U_{eq}(N); O—H =0.82 Å; U_{iso}(H) = 1.5U_{eq}(O);]

Figures

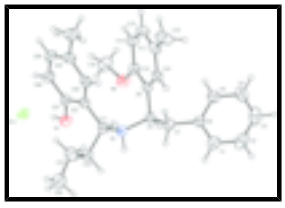

Fig. 1. The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms represented as spheres of arbitrary radii.

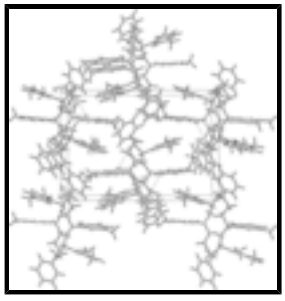

Fig. 2. Crystal packing of (I); dashed lines indicate hydrogen bonds.

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Crystal data

$C_{27}H_{34}NO_2^+ \cdot Cl^-$	F_{000} = 944
M_r = 440.00	D_x = 1.194 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 4734 reflections
a = 9.8553 (14) Å	θ = 2.3–26.9º
b = 13.1962 (19) Å	μ = 0.18 mm^{-1}
c = 18.825 (3) Å	T = 298 (2) K
V = 2448.2 (6) Å^3	Block, colourless
Z = 4	0.48 × 0.40 × 0.32 mm

Data collection

Bruker SMART CCD area-detecter diffractometer	4534 independent reflections
Radiation source: fine-focus sealed tube	3992 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.026
T = 298(2) K	θ_{max} = 25.5º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 1997a)	h = −11→11
T_{min} = 0.919, T_{max} = 0.945	k = −15→15
12855 measured reflections	l = −22→15

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.039$	$w = 1/[\sigma^2(F_o^2) + (0.0549P)^2 + 0.1969P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.100$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.03$	$\Delta\rho_{max} = 0.16$ e Å^{-3}
4534 reflections	$\Delta\rho_{min} = -0.15$ e Å^{-3}
285 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1957 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: −0.05 (6)

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 $F^2 > 2$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	0.5112 (3)	0.44927 (19)	0.38399 (13)	0.0624 (6)
H1	0.5257	0.5105	0.3608	0.075*
C2	0.4101 (3)	0.3849 (2)	0.36021 (17)	0.0802 (9)
H2	0.3591	0.4024	0.3205	0.096*
C3	0.3847 (3)	0.2961 (2)	0.39456 (19)	0.0798 (9)
H3	0.3159	0.2534	0.3790	0.096*
C4	0.4607 (3)	0.2709 (2)	0.45149 (17)	0.0766 (8)
H4	0.4437	0.2103	0.4751	0.092*
C5	0.5633 (3)	0.33371 (18)	0.47519 (14)	0.0608 (6)
H5	0.6147	0.3148	0.5144	0.073*
C6	0.5905 (2)	0.42420 (15)	0.44130 (11)	0.0465 (5)
C7	0.6996 (2)	0.49521 (16)	0.46668 (12)	0.0500 (5)
H7A	0.7391	0.5302	0.4264	0.060*
H7B	0.7709	0.4568	0.4899	0.060*
C8	0.6407 (2)	0.57302 (14)	0.51898 (11)	0.0408 (4)
H8	0.5527	0.5943	0.4999	0.049*
C9	0.6151 (2)	0.53212 (14)	0.59232 (10)	0.0388 (4)

C10	0.4840 (2)	0.52856 (15)	0.61839 (12)	0.0443 (5)
H10	0.4132	0.5502	0.5895	0.053*
C11	0.4545 (2)	0.49376 (16)	0.68641 (13)	0.0530 (5)
C12	0.5602 (2)	0.45930 (17)	0.72691 (13)	0.0573 (6)
H12	0.5424	0.4340	0.7721	0.069*
C13	0.6923 (2)	0.46093 (17)	0.70283 (12)	0.0535 (5)
H13	0.7621	0.4364	0.7313	0.064*
C14	0.72006 (19)	0.49929 (14)	0.63609 (11)	0.0444 (5)
C15	0.3097 (3)	0.4976 (2)	0.71320 (18)	0.0828 (9)
H15A	0.2549	0.4512	0.6864	0.124*
H15B	0.2748	0.5651	0.7077	0.124*
H15C	0.3076	0.4790	0.7625	0.124*
C16	0.9601 (2)	0.4959 (2)	0.65607 (15)	0.0716 (7)
H16A	0.9458	0.5351	0.6984	0.107*
H16B	1.0424	0.5175	0.6334	0.107*
H16C	0.9671	0.4254	0.6683	0.107*
C17	0.6689 (2)	0.75214 (14)	0.56655 (10)	0.0426 (5)
H17	0.5706	0.7415	0.5681	0.051*
C18	0.6927 (3)	0.85349 (15)	0.53024 (12)	0.0524 (5)
H18A	0.7893	0.8674	0.5290	0.063*
H18B	0.6606	0.8497	0.4816	0.063*
C19	0.6206 (3)	0.93971 (18)	0.56818 (15)	0.0762 (8)
H19A	0.5263	0.9212	0.5754	0.091*
H19B	0.6614	0.9491	0.6146	0.091*
C20	0.6263 (4)	1.0368 (2)	0.52876 (17)	0.0946 (10)
H20A	0.7188	1.0517	0.5166	0.142*
H20B	0.5906	1.0901	0.5579	0.142*
H20C	0.5733	1.0313	0.4861	0.142*
C21	0.71962 (19)	0.74655 (13)	0.64187 (10)	0.0413 (4)
C22	0.6296 (2)	0.73690 (15)	0.69791 (11)	0.0465 (5)
H22	0.5371	0.7343	0.6882	0.056*
C23	0.6720 (3)	0.73095 (17)	0.76779 (12)	0.0554 (6)
C24	0.5724 (3)	0.7149 (2)	0.82768 (14)	0.0807 (8)
H24A	0.4818	0.7261	0.8106	0.121*
H24B	0.5917	0.7617	0.8654	0.121*
H24C	0.5803	0.6468	0.8451	0.121*
C25	0.8098 (3)	0.73871 (18)	0.78093 (12)	0.0581 (6)
H25	0.8408	0.7364	0.8276	0.070*
C26	0.9023 (2)	0.74980 (17)	0.72650 (12)	0.0542 (5)
H26	0.9943	0.7556	0.7367	0.065*
C27	0.85830 (19)	0.75234 (15)	0.65706 (10)	0.0437 (5)
N1	0.72890 (17)	0.66615 (12)	0.52202 (8)	0.0419 (4)
H1A	0.7427	0.6888	0.4775	0.050*
H1B	0.8102	0.6490	0.5402	0.050*
O1	0.94600 (13)	0.75705 (13)	0.60056 (7)	0.0544 (4)
H1C	1.0242	0.7609	0.6152	0.082*
O2	0.84902 (14)	0.51013 (12)	0.60891 (8)	0.0544 (4)
Cl1	0.24550 (5)	0.77487 (5)	0.63820 (3)	0.05994 (17)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0754 (16)	0.0561 (13)	0.0558 (14)	0.0171 (13)	−0.0103 (13)	−0.0065 (11)
C2	0.0720 (17)	0.094 (2)	0.0746 (18)	0.0262 (16)	−0.0246 (16)	−0.0237 (18)
C3	0.0617 (16)	0.078 (2)	0.100 (2)	−0.0006 (14)	0.0007 (17)	−0.0346 (18)
C4	0.0858 (18)	0.0517 (14)	0.092 (2)	−0.0097 (14)	0.0121 (17)	−0.0063 (14)
C5	0.0716 (16)	0.0556 (14)	0.0553 (14)	0.0041 (12)	−0.0036 (13)	0.0042 (11)
C6	0.0585 (12)	0.0420 (11)	0.0389 (11)	0.0080 (9)	0.0027 (10)	−0.0065 (9)
C7	0.0540 (12)	0.0513 (12)	0.0449 (11)	0.0008 (10)	0.0058 (10)	−0.0046 (10)
C8	0.0398 (10)	0.0410 (10)	0.0416 (11)	0.0006 (8)	−0.0037 (9)	−0.0001 (8)
C9	0.0425 (10)	0.0347 (9)	0.0392 (11)	0.0006 (8)	−0.0011 (9)	0.0001 (8)
C10	0.0395 (10)	0.0404 (10)	0.0530 (12)	0.0027 (8)	−0.0014 (9)	0.0048 (9)
C11	0.0526 (12)	0.0468 (12)	0.0595 (13)	−0.0027 (10)	0.0099 (11)	0.0079 (11)
C12	0.0689 (15)	0.0530 (12)	0.0501 (13)	−0.0002 (11)	0.0064 (12)	0.0147 (11)
C13	0.0575 (13)	0.0509 (12)	0.0522 (13)	0.0078 (10)	−0.0092 (11)	0.0112 (10)
C14	0.0437 (11)	0.0409 (10)	0.0487 (11)	0.0042 (9)	−0.0026 (9)	−0.0009 (9)
C15	0.0637 (15)	0.0852 (19)	0.099 (2)	0.0069 (15)	0.0311 (16)	0.0299 (17)
C16	0.0501 (12)	0.0897 (18)	0.0751 (17)	0.0157 (13)	−0.0160 (13)	−0.0003 (15)
C17	0.0427 (10)	0.0412 (11)	0.0438 (11)	0.0015 (9)	−0.0007 (9)	−0.0031 (9)
C18	0.0666 (14)	0.0466 (12)	0.0440 (11)	−0.0007 (10)	−0.0109 (11)	0.0021 (9)
C19	0.112 (2)	0.0498 (14)	0.0672 (17)	0.0066 (14)	−0.0046 (17)	−0.0053 (12)
C20	0.141 (3)	0.0593 (15)	0.084 (2)	0.0184 (18)	−0.030 (2)	−0.0071 (15)
C21	0.0461 (10)	0.0360 (9)	0.0417 (10)	0.0006 (8)	−0.0008 (9)	−0.0002 (8)
C22	0.0512 (11)	0.0395 (10)	0.0489 (12)	0.0003 (9)	0.0073 (10)	−0.0019 (9)
C23	0.0738 (15)	0.0475 (12)	0.0449 (12)	0.0054 (11)	0.0129 (11)	0.0023 (10)
C24	0.101 (2)	0.0830 (18)	0.0579 (16)	0.0039 (16)	0.0287 (16)	0.0080 (14)
C25	0.0784 (16)	0.0618 (14)	0.0340 (10)	0.0073 (13)	−0.0051 (11)	0.0002 (10)
C26	0.0569 (12)	0.0582 (13)	0.0474 (12)	0.0036 (11)	−0.0074 (10)	0.0000 (11)
C27	0.0476 (11)	0.0459 (11)	0.0376 (10)	−0.0008 (9)	−0.0009 (9)	−0.0011 (9)
N1	0.0431 (9)	0.0456 (9)	0.0369 (8)	0.0009 (7)	−0.0019 (8)	−0.0018 (7)
O1	0.0426 (7)	0.0778 (11)	0.0429 (8)	−0.0060 (8)	−0.0001 (7)	0.0022 (8)
O2	0.0373 (7)	0.0730 (10)	0.0529 (9)	0.0089 (7)	−0.0032 (7)	0.0043 (8)
Cl1	0.0536 (3)	0.0789 (4)	0.0473 (3)	−0.0029 (3)	−0.0117 (3)	0.0066 (3)

Geometric parameters (Å, °)

C1—C6	1.372 (3)	C16—H16A	0.9600
C1—C2	1.384 (4)	C16—H16B	0.9600
C1—H1	0.9300	C16—H16C	0.9600
C2—C3	1.361 (4)	C17—C21	1.505 (3)
C2—H2	0.9300	C17—C18	1.520 (3)
C3—C4	1.349 (4)	C17—N1	1.530 (2)
C3—H3	0.9300	C17—H17	0.9800
C4—C5	1.382 (4)	C18—C19	1.520 (3)
C4—H4	0.9300	C18—H18A	0.9700
C5—C6	1.380 (3)	C18—H18B	0.9700
C5—H5	0.9300	C19—C20	1.481 (4)

C6—C7	1.504 (3)	C19—H19A	0.9700
C7—C8	1.536 (3)	C19—H19B	0.9700
C7—H7A	0.9700	C20—H20A	0.9600
C7—H7B	0.9700	C20—H20B	0.9600
C8—C9	1.504 (3)	C20—H20C	0.9600
C8—N1	1.506 (2)	C21—C22	1.385 (3)
C8—H8	0.9800	C21—C27	1.398 (3)
C9—C10	1.383 (3)	C22—C23	1.383 (3)
C9—C14	1.391 (3)	C22—H22	0.9300
C10—C11	1.391 (3)	C23—C25	1.384 (3)
C10—H10	0.9300	C23—C24	1.510 (3)
C11—C12	1.368 (3)	C24—H24A	0.9600
C11—C15	1.515 (3)	C24—H24B	0.9600
C12—C13	1.379 (3)	C24—H24C	0.9600
C12—H12	0.9300	C25—C26	1.379 (3)
C13—C14	1.382 (3)	C25—H25	0.9300
C13—H13	0.9300	C26—C27	1.378 (3)
C14—O2	1.378 (2)	C26—H26	0.9300
C15—H15A	0.9600	C27—O1	1.372 (2)
C15—H15B	0.9600	N1—H1A	0.9000
C15—H15C	0.9600	N1—H1B	0.9000
C16—O2	1.422 (3)	O1—H1C	0.8200
C6—C1—C2	121.1 (3)	H16A—C16—H16C	109.5
C6—C1—H1	119.5	H16B—C16—H16C	109.5
C2—C1—H1	119.5	C21—C17—C18	114.55 (17)
C3—C2—C1	120.5 (3)	C21—C17—N1	110.58 (15)
C3—C2—H2	119.8	C18—C17—N1	110.28 (16)
C1—C2—H2	119.8	C21—C17—H17	107.0
C4—C3—C2	119.2 (3)	C18—C17—H17	107.0
C4—C3—H3	120.4	N1—C17—H17	107.0
C2—C3—H3	120.4	C19—C18—C17	112.03 (19)
C3—C4—C5	121.0 (3)	C19—C18—H18A	109.2
C3—C4—H4	119.5	C17—C18—H18A	109.2
C5—C4—H4	119.5	C19—C18—H18B	109.2
C6—C5—C4	120.8 (3)	C17—C18—H18B	109.2
C6—C5—H5	119.6	H18A—C18—H18B	107.9
C4—C5—H5	119.6	C20—C19—C18	113.2 (2)
C1—C6—C5	117.5 (2)	C20—C19—H19A	108.9
C1—C6—C7	120.4 (2)	C18—C19—H19A	108.9
C5—C6—C7	122.1 (2)	C20—C19—H19B	108.9
C6—C7—C8	110.46 (17)	C18—C19—H19B	108.9
C6—C7—H7A	109.6	H19A—C19—H19B	107.8
C8—C7—H7A	109.6	C19—C20—H20A	109.5
C6—C7—H7B	109.6	C19—C20—H20B	109.5
C8—C7—H7B	109.6	H20A—C20—H20B	109.5
H7A—C7—H7B	108.1	C19—C20—H20C	109.5
C9—C8—N1	110.78 (15)	H20A—C20—H20C	109.5
C9—C8—C7	114.31 (16)	H20B—C20—H20C	109.5
N1—C8—C7	110.58 (16)	C22—C21—C27	118.40 (18)

C9—C8—H8	106.9	C22—C21—C17	120.64 (17)
N1—C8—H8	106.9	C27—C21—C17	120.96 (17)
C7—C8—H8	106.9	C23—C22—C21	122.4 (2)
C10—C9—C14	118.27 (18)	C23—C22—H22	118.8
C10—C9—C8	119.65 (18)	C21—C22—H22	118.8
C14—C9—C8	122.07 (18)	C22—C23—C25	117.6 (2)
C9—C10—C11	122.22 (19)	C22—C23—C24	121.4 (2)
C9—C10—H10	118.9	C25—C23—C24	121.0 (2)
C11—C10—H10	118.9	C23—C24—H24A	109.5
C12—C11—C10	117.6 (2)	C23—C24—H24B	109.5
C12—C11—C15	122.9 (2)	H24A—C24—H24B	109.5
C10—C11—C15	119.5 (2)	C23—C24—H24C	109.5
C11—C12—C13	122.0 (2)	H24A—C24—H24C	109.5
C11—C12—H12	119.0	H24B—C24—H24C	109.5
C13—C12—H12	119.0	C26—C25—C23	121.6 (2)
C12—C13—C14	119.4 (2)	C26—C25—H25	119.2
C12—C13—H13	120.3	C23—C25—H25	119.2
C14—C13—H13	120.3	C27—C26—C25	120.0 (2)
O2—C14—C13	123.95 (19)	C27—C26—H26	120.0
O2—C14—C9	115.68 (18)	C25—C26—H26	120.0
C13—C14—C9	120.36 (19)	O1—C27—C26	122.58 (18)
C11—C15—H15A	109.5	O1—C27—C21	117.36 (17)
C11—C15—H15B	109.5	C26—C27—C21	120.02 (19)
H15A—C15—H15B	109.5	C8—N1—C17	113.77 (14)
C11—C15—H15C	109.5	C8—N1—H1A	108.8
H15A—C15—H15C	109.5	C17—N1—H1A	108.8
H15B—C15—H15C	109.5	C8—N1—H1B	108.8
O2—C16—H16A	109.5	C17—N1—H1B	108.8
O2—C16—H16B	109.5	H1A—N1—H1B	107.7
H16A—C16—H16B	109.5	C27—O1—H1C	109.5
O2—C16—H16C	109.5	C14—O2—C16	117.69 (17)
C6—C1—C2—C3	1.8 (4)	C8—C9—C14—C13	−179.15 (19)
C1—C2—C3—C4	−1.0 (4)	C21—C17—C18—C19	−61.2 (3)
C2—C3—C4—C5	0.0 (4)	N1—C17—C18—C19	173.31 (19)
C3—C4—C5—C6	0.2 (4)	C17—C18—C19—C20	−172.2 (2)
C2—C1—C6—C5	−1.5 (3)	C18—C17—C21—C22	113.4 (2)
C2—C1—C6—C7	−179.8 (2)	N1—C17—C21—C22	−121.26 (19)
C4—C5—C6—C1	0.5 (3)	C18—C17—C21—C27	−65.7 (2)
C4—C5—C6—C7	178.7 (2)	N1—C17—C21—C27	59.6 (2)
C1—C6—C7—C8	86.5 (2)	C27—C21—C22—C23	−1.2 (3)
C5—C6—C7—C8	−91.7 (2)	C17—C21—C22—C23	179.64 (19)
C6—C7—C8—C9	76.7 (2)	C21—C22—C23—C25	2.3 (3)
C6—C7—C8—N1	−157.42 (17)	C21—C22—C23—C24	−176.7 (2)
N1—C8—C9—C10	117.71 (19)	C22—C23—C25—C26	−1.4 (4)
C7—C8—C9—C10	−116.6 (2)	C24—C23—C25—C26	177.7 (2)
N1—C8—C9—C14	−60.9 (2)	C23—C25—C26—C27	−0.7 (4)
C7—C8—C9—C14	64.9 (2)	C25—C26—C27—O1	−176.0 (2)
C14—C9—C10—C11	0.2 (3)	C25—C26—C27—C21	1.8 (3)
C8—C9—C10—C11	−178.45 (19)	C22—C21—C27—O1	177.00 (17)

C9—C10—C11—C12	−2.1 (3)	C17—C21—C27—O1	−3.9 (3)
C9—C10—C11—C15	176.4 (2)	C22—C21—C27—C26	−0.9 (3)
C10—C11—C12—C13	1.7 (4)	C17—C21—C27—C26	178.25 (18)
C15—C11—C12—C13	−176.8 (2)	C9—C8—N1—C17	−58.7 (2)
C11—C12—C13—C14	0.6 (4)	C7—C8—N1—C17	173.50 (16)
C12—C13—C14—O2	175.8 (2)	C21—C17—N1—C8	93.05 (18)
C12—C13—C14—C9	−2.7 (3)	C18—C17—N1—C8	−139.22 (17)
C10—C9—C14—O2	−176.33 (17)	C13—C14—O2—C16	−10.1 (3)
C8—C9—C14—O2	2.3 (3)	C9—C14—O2—C16	168.4 (2)
C10—C9—C14—C13	2.2 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1C···Cl1^{i}	0.82	2.23	3.0446 (15)	171
N1—H1A···Cl1^{ii}	0.90	2.23	3.1193 (18)	169
N1—H1B···O2	0.90	2.28	2.884 (2)	125
N1—H1B···O1	0.90	2.26	2.864 (2)	124

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*+1/2, −*y*+3/2, −*z*+1.

Fig. 1

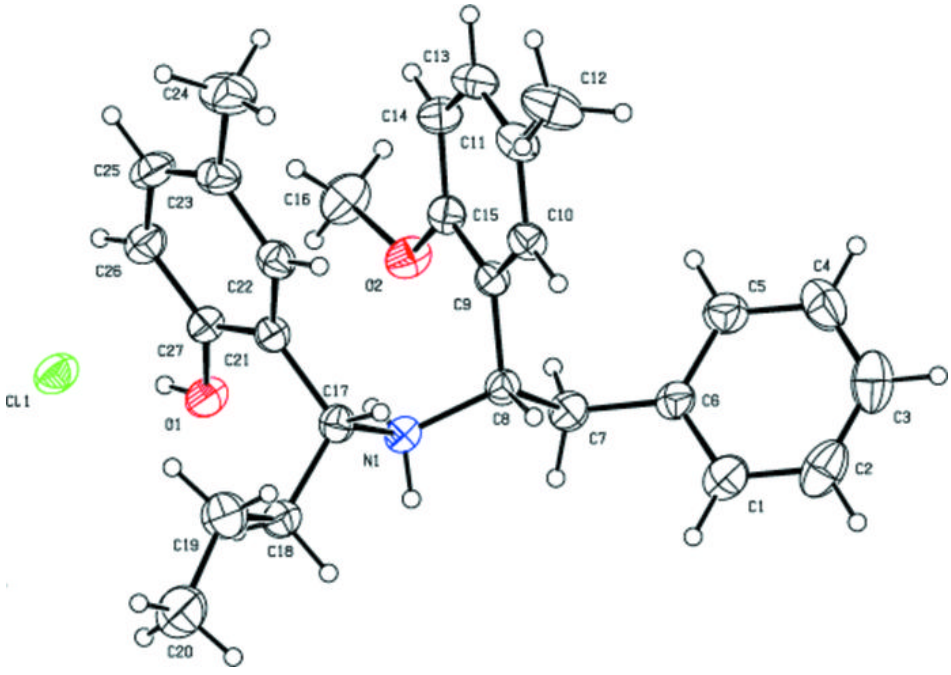
C13
C12
C24
C14
C11
C25
C23
C16
C15
C10
C26
C22
O2
C9
C4
C5
C27
C21
C17
C6
C3
Cl1
O1
C8
C7
N1
C2
C1
C19
C18
C20

Fig. 2