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N-[2-(4-Methylbenzoyl)ethyl]propan-2-aminium chloride

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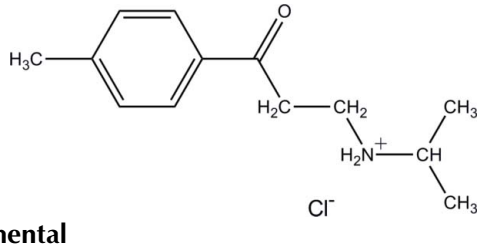
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.049; wR factor = 0.151; data-to-parameter ratio = 18.8.

In the title compound, $C_{13}H_{20}NO^+\cdot Cl^-$, the protonated amino N atom is hydrogen bonded to the chloride anion. N—H···Cl hydrogen bonds link the anions and cations into dimers, which are connected by C—H···O hydrogen bonds, forming supramolecular chains extending along [100].

Related literature

For the details of the pharmacological effects of Mannich bases and for their synthesis, see: Dimmock & Kumar (1997); Gul *et al.* (2004; 2005*a*,*b*; 2009); Gul (2005); Mete *et al.* (2011*a*,*b*); Kucukoglu *et al.* (2011); Canturk *et al.* (2008); Chen *et al.* (1991); Suleyman *et al.* (2007); Plastino *et al.* (1962, 1964). For bond-length data, see: Allen *et al.* (1987). For hydrogen-bond motifs, see: Bernstein *et al.* (1995); Etter (1990). For some related structures, see: Abonia *et al.* (2011); Tuzina *et al.* (2006).



Experimental

Crystal data

$C_{13}H_{20}NO^+\cdot Cl^-$
M_r = 241.75
Monoclinic, $P2_1/c$
a = 7.786 (5) Å
b = 7.511 (5) Å
c = 23.365 (5) Å
β = 95.362 (5)°
V = 1360.4 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 294 K
0.17 × 0.11 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.966, T_{max} = 0.974
26900 measured reflections
2800 independent reflections
2007 reflections with $I > 2\sigma(I)$
R_{int} = 0.066

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.151
S = 1.06
2800 reflections
149 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H14A···Cl1	0.90	2.26	3.148 (3)	172
N1—H14B···Cl1^{i}	0.90	2.25	3.145 (3)	173
C1—H1···O1^{ii}	0.93	2.53	3.340 (4)	146

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear* (Rigaku/MSC, 2005); 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) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: QM2078).

References

Abonia, R., Schollmeyer, D. & Arteaga, D. (2011). *Acta Cryst.* E**67**, o2969.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Canturk, P., Kucukoglu, K., Topcu, Z., Gul, M. & Gul, H. I. (2008). *Arzneim. Forsch.* **58**, 686–691.
Chen, H. T., Jing, Y. K., Ji, Z. Z. & Zhang, B. F. (1991). *YaoXueXueBao*, **26**, 183–192.
Dimmock, J. R. & Kumar, P. (1997). *Curr. Med. Chem.* **4**, 1–22.
Etter, M. C. (1990). *Acc. Chem. Res.* **23**, 120–126.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Gul, M. (2005). PhD thesis, Kuopio University, Finland.
Gul, M., Atalay, M., Gul, H. I., Nakao, C., Lappalainen, J. & Hanninen, O. (2005*a*). *Toxicol. Vitro*, **19**, 573–580.
Gul, H. I., Calis, U. & Vepsalainen, J. (2004). *Arzneim. Forsch.* **54**, 359–364.
Gul, H. I., Sahin, F., Gul, M., Ozturk, S. & Yerdelen, K. O. (2005*b*). *Arch. Pharm.* **338**, 335–338.
Gul, H. I., Suleyman, H. & Gul, M. (2009). *Pharm. Biol.* **47**, 968–972.
Kucukoglu, K., Gul, M., Atalay, M., Mete, E., Kazaz, C., Hanninen, O. & Gul, H. I. (2011). *Arzneim. Forsch. Drug Res.* **61**, 366–371.
Mete, E., Gul, H. I., Bilginer, S., Algul, O., Topaloglu, M. E., Gulluce, M. & Kazaz, C. (2011*a*). *Molecules*, **16**, 4660–4671.

Mete, E., Gul, H. I., Cetin-Atalay, R., Das, U., Sahin, E., Gul, M., Kazaz, C. & Dimmock, J. R. (2011*b*). *Arch. Pharm. Chem. Life Sci.* **11**, 333–339.
Plastino, E., Loprieno, N., Bugian, A. & Tenerini, J. (1962). *Chem. Abstr.* **60**, 3025.
Plastino, E., Loprieno, N., Bugian, A. & Tenerini, J. (1964). Italian Patent 637371.
Rigaku/MSC (2005). *CrystalClear*. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Suleyman, H., Gul, H. I., Gul, M., Alkan, M. & Gocer, F. (2007). *Biol. Pharm. Bull.* **30**, 63–67.
Tuzina, P., Fischer, A. & Somfai, P. (2006). *Acta Cryst.* E**62**, o2971–o2972.

supplementary materials

Acta Cryst. (2012). E**68**, o2706–o2707 [doi:10.1107/S1600536812035271]

N-[2-(4-Methylbenzoyl)ethyl]propan-2-aminium chloride

Abdullah Aydın, Mehmet Akkurt, Halise Inci Gul, Ebru Mete and Ertan Sahin

Comment

Mannich bases are generally formed by the reaction between formaldehyde, a secondary amine and a compound containing reactive hydrogen atoms. On occasion, aldehydes other than formaldehyde may be employed and the secondary amine may be replaced by ammonia and primary amines. This process is known as the Mannich reaction (Dimmock & Kumar, 1997).

Mannich bases display varied biological activities such as antimicrobial (Gul *et al.*, 2005; Mete *et al.*, 2011*a*), cytotoxic (Gul *et al.*, 2005; Mete *et al.*, 2011*b*; Kucukoglu *et al.*, 2011; Canturk *et al.*, 2008), anticancer (Dimmock & Kumar, 1997; Chen *et al.*, 1991; Gul, 2005), antiinflammatory (Suleyman *et al.*, 2007; Gul *et al.*, 2009), anticonvulsant (Gul *et al.*, 2004) and DNA topoisomeraseI inhibiting properties (Canturk *et al.*, 2008).

In the title compound (I), (Fig. 1), bond lengths and bond angles are within the range of expected values for this type of compound (Allen *et al.*, 1987; Abonia *et al.*, 2011; Tuzina *et al.*, 2006). The protonated N1 atom forms a hydrogen bond to Cl1 (Table 1).

Intra- and intermolecular N—H···Cl hydrogen-bonding interactions between the free chloride anion and the organic cation link the molecules into hydrogen-bond dimers, forming a $R^2_2(6)$ motif (Bernstein *et al.*, 1995; Etter, 1990). The dimers are connected by C—H···O hydrogen bonds into chains extended along the *a* axis (Table 1, Fig. 2).

Experimental

A mixture of the appropriate ketone (50 mmol), paraformaldehyde (50 mmol), and isopropylamine hydrochloride (27 mmol) was heated in an oil bath at 403 K. The reaction vessel was then removed from the oil bath and when the temperature of the mixture dropped to 338 K, ethyl acetate (40–80 ml) was added. The mixture was stirred at room temperature for 24 h and the resultant precipitate was then collected and were recrystallized from ether/methanol. The melting point and yield of this compound was: 443–444 K (lit. Plastino *et al.*, 1964 m.p. 444–445 K), 58% (Mete *et al.*, 2011*b*).

^{1}H-NMR δ 1.50 (d, J = 6.6 Hz, 6H, $CH(CH_3)_2$), 2.34 (s, 3H, $ArCH_3$), 3.36–3.46 (m, 3H, $CH(CH_3)_2$ and 2 *x* H-2), 3.74 (t, J = 7.3 Hz, 2H, 2 *x* H-3), 7.14 (d, J = 8.1 Hz, 2H, H-3′/5′), 7.79 (d, J = 8.1 Hz, 2H, H-2′/6′), 9.54 (brs, 2H, NH_2^+); ^{13}C-NMR δ 19.4 ($CH(CH_3)_2$), 21.9, 35.1, 40.5, 51.2, 128.5, 129.6, 133.6, 144.9, 196.6; MS (EI) m/*z* (%): 190.1 $(M–CH_3)^+$, 205.3 (M^+). IR (KBr, cm^{-1}): 2461 (NH_2^+), 1679 (CO). Calcd. for $C_{13}H_{20}ClNO$ (241.76): C, 64.59: H, 8.34; N, 5.79. Found: C, 64.39; H, 8.45; N, 5.53.

Refinement

H atoms were positioned geometrically, with N—H = 0.90 Å, C—H = 0.93(aromatic), 0.97(methylene) and 0.98 Å (methine), and refined as riding with U_{iso}(H) = 1.5U_{eq}(O) for methyl H and 1.2U_{eq}(C) for the others.

Computing details

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear* (Rigaku/MSC, 2005); data reduction: *CrystalClear* (Rigaku/MSC, 2005); 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) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

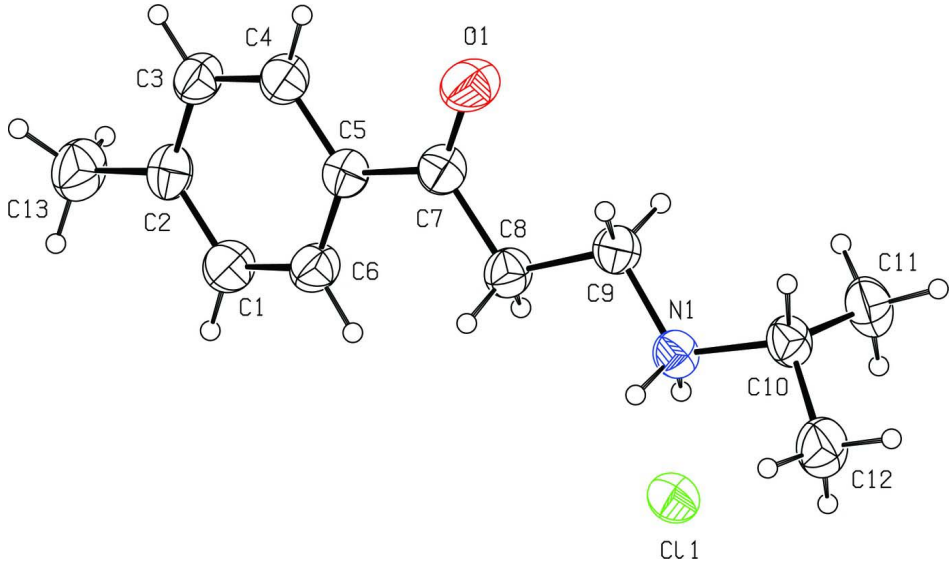

Figure 1

The title molecule with the atom numbering scheme. Displacement ellipsoids fornon-H atoms are drawn at the 30% probability level.

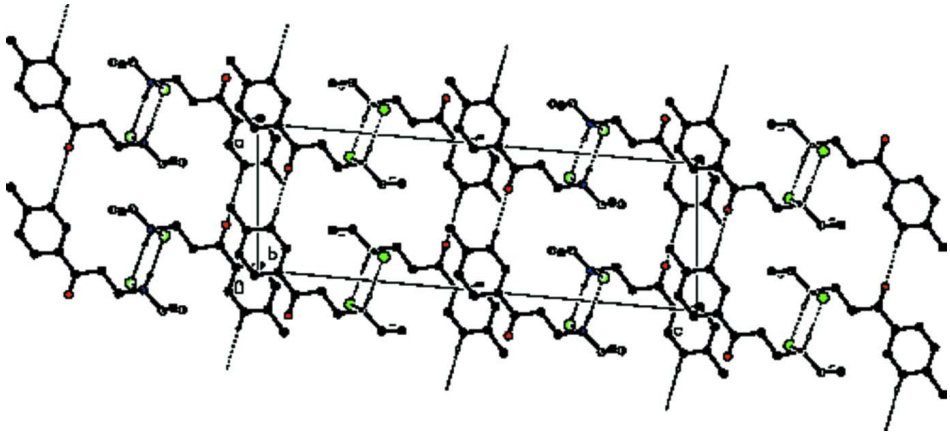

Figure 2

The packing and hydrogen bonding of the title compound viewed down the *b*axis. H atoms not involved in hydrogen bondings are omitted for clarity.

N-[2-(4-Methylbenzoyl)ethyl]propan-2-aminium chloride

Crystal data

$C_{13}H_{20}NO^{+}\cdot Cl^{-}$
$M_r = 241.75$

Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc

a = 7.786 (5) Å
b = 7.511 (5) Å
c = 23.365 (5) Å
β = 95.362 (5)°
V = 1360.4 (13) Å^3
Z = 4
F(000) = 520
D_x = 1.180 Mg m^{-3}

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4594 reflections
θ = 2.6–26.5°
μ = 0.26 mm^{-1}
T = 294 K
Block, white
0.17 × 0.11 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer
Radiation source: Sealed Tube
Graphite Monochromator monochromator
Detector resolution: 10.0000 pixels mm^{-1}
dtprofit.ref scans
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.966, T_{max} = 0.974

26900 measured reflections
2800 independent reflections
2007 reflections with $I > 2\sigma(I)$
R_{int} = 0.066
θ_{max} = 26.4°, θ_{min} = 2.6°
h = −9→9
k = −8→9
l = −29→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.151
S = 1.06
2800 reflections
149 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
$w = 1/[\sigma^2(F_o^2) + (0.0681P)^2 + 0.2172P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), FC*=KFC[1+0.001XFC$^2\Lambda^3$/SIN(2Θ)]$^{-1/4}$
Extinction coefficient: 0.010 (3)

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -R-factor-obs *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}
O1	0.7123 (2)	0.2422 (3)	0.57107 (8)	0.0903 (8)
N1	0.7916 (2)	0.0622 (2)	0.74056 (7)	0.0555 (6)
C1	1.2949 (3)	0.1740 (3)	0.53020 (10)	0.0722 (9)
C2	1.2627 (3)	0.2488 (3)	0.47633 (10)	0.0653 (8)
C3	1.0947 (3)	0.2961 (3)	0.45820 (9)	0.0680 (9)
C4	0.9644 (3)	0.2737 (3)	0.49337 (9)	0.0659 (8)
C5	0.9974 (3)	0.2024 (3)	0.54815 (9)	0.0563 (7)

C6	1.1652 (3)	0.1501 (3)	0.56544 (10)	0.0658 (8)
C7	0.8564 (3)	0.1895 (3)	0.58624 (9)	0.0616 (8)
C8	0.8956 (3)	0.1133 (3)	0.64590 (9)	0.0623 (8)
C9	0.7524 (3)	0.1489 (3)	0.68361 (9)	0.0606 (8)
C10	0.6625 (3)	0.0981 (3)	0.78362 (9)	0.0611 (8)
C11	0.6888 (4)	0.2830 (4)	0.80850 (12)	0.0807 (10)
C12	0.6811 (4)	−0.0436 (4)	0.82927 (12)	0.0864 (10)
C13	1.4074 (4)	0.2830 (5)	0.43891 (12)	0.0913 (11)
Cl1	1.17234 (7)	0.15576 (7)	0.78840 (2)	0.0665 (2)
H1	1.40660	0.13910	0.54290	0.0870*
H3	1.06950	0.34370	0.42160	0.0820*
H4	0.85250	0.30690	0.48030	0.0790*
H6	1.19010	0.09810	0.60140	0.0790*
H8A	0.91290	−0.01420	0.64310	0.0750*
H8B	1.00180	0.16520	0.66350	0.0750*
H9A	0.73980	0.27620	0.68870	0.0730*
H9B	0.64450	0.10290	0.66530	0.0730*
H10	0.54610	0.09070	0.76380	0.0730*
H11A	0.59650	0.31080	0.83150	0.1210*
H11B	0.68980	0.36790	0.77780	0.1210*
H11C	0.79670	0.28780	0.83190	0.1210*
H12A	0.66880	−0.15880	0.81160	0.1290*
H12B	0.59360	−0.02790	0.85520	0.1290*
H12C	0.79290	−0.03440	0.85020	0.1290*
H13A	1.43820	0.40670	0.44090	0.1370*
H13B	1.37010	0.25180	0.39990	0.1370*
H13C	1.50570	0.21210	0.45220	0.1370*
H14A	0.89610	0.09920	0.75560	0.0670*
H14B	0.79790	−0.05620	0.73520	0.0670*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0562 (10)	0.1386 (17)	0.0763 (11)	0.0110 (11)	0.0077 (8)	0.0214 (11)
N1	0.0530 (10)	0.0541 (10)	0.0609 (10)	−0.0019 (8)	0.0135 (8)	0.0028 (8)
C1	0.0545 (13)	0.0940 (19)	0.0683 (15)	0.0016 (12)	0.0076 (11)	0.0037 (13)
C2	0.0651 (14)	0.0730 (15)	0.0596 (13)	−0.0076 (12)	0.0152 (10)	−0.0054 (11)
C3	0.0723 (16)	0.0783 (16)	0.0541 (13)	−0.0016 (12)	0.0094 (10)	0.0048 (11)
C4	0.0618 (14)	0.0764 (15)	0.0596 (13)	−0.0001 (12)	0.0057 (10)	0.0003 (11)
C5	0.0553 (12)	0.0579 (12)	0.0555 (12)	−0.0054 (10)	0.0048 (9)	−0.0023 (9)
C6	0.0625 (14)	0.0774 (16)	0.0577 (12)	0.0004 (11)	0.0066 (10)	0.0071 (11)
C7	0.0557 (13)	0.0684 (14)	0.0609 (13)	−0.0038 (11)	0.0059 (10)	−0.0008 (10)
C8	0.0574 (13)	0.0718 (14)	0.0588 (13)	−0.0014 (11)	0.0111 (10)	0.0039 (11)
C9	0.0584 (13)	0.0630 (14)	0.0614 (13)	0.0002 (10)	0.0103 (10)	0.0041 (10)
C10	0.0535 (12)	0.0672 (14)	0.0653 (13)	0.0004 (10)	0.0195 (10)	0.0012 (10)
C11	0.0901 (19)	0.0698 (16)	0.0871 (18)	0.0072 (13)	0.0350 (14)	−0.0041 (13)
C12	0.108 (2)	0.0767 (17)	0.0808 (17)	0.0039 (15)	0.0418 (15)	0.0138 (13)
C13	0.0797 (18)	0.120 (2)	0.0775 (18)	−0.0034 (17)	0.0253 (14)	0.0074 (16)
Cl1	0.0631 (4)	0.0604 (4)	0.0756 (4)	0.0010 (3)	0.0046 (3)	−0.0014 (3)

Geometric parameters (Å, º)

O1—C7	1.211 (3)	C3—H3	0.9300
N1—C9	1.487 (3)	C4—H4	0.9300
N1—C10	1.511 (3)	C6—H6	0.9300
N1—H14B	0.9000	C8—H8A	0.9700
N1—H14A	0.9000	C8—H8B	0.9700
C1—C6	1.373 (3)	C9—H9A	0.9700
C1—C2	1.380 (3)	C9—H9B	0.9700
C2—C3	1.383 (3)	C10—H10	0.9800
C2—C13	1.511 (4)	C11—H11A	0.9600
C3—C4	1.374 (3)	C11—H11B	0.9600
C4—C5	1.389 (3)	C11—H11C	0.9600
C5—C7	1.480 (3)	C12—H12A	0.9600
C5—C6	1.388 (3)	C12—H12B	0.9600
C7—C8	1.511 (3)	C12—H12C	0.9600
C8—C9	1.508 (3)	C13—H13A	0.9600
C10—C12	1.504 (4)	C13—H13B	0.9600
C10—C11	1.512 (4)	C13—H13C	0.9600
C1—H1	0.9300		
C9—N1—C10	115.08 (16)	C7—C8—H8A	109.00
H14A—N1—H14B	107.00	C7—C8—H8B	109.00
C9—N1—H14B	109.00	C9—C8—H8A	109.00
C10—N1—H14A	109.00	C9—C8—H8B	109.00
C9—N1—H14A	108.00	H8A—C8—H8B	108.00
C10—N1—H14B	108.00	N1—C9—H9A	110.00
C2—C1—C6	121.3 (2)	N1—C9—H9B	110.00
C1—C2—C13	121.0 (2)	C8—C9—H9A	110.00
C1—C2—C3	118.0 (2)	C8—C9—H9B	110.00
C3—C2—C13	120.9 (2)	H9A—C9—H9B	108.00
C2—C3—C4	121.0 (2)	N1—C10—H10	109.00
C3—C4—C5	121.0 (2)	C11—C10—H10	109.00
C6—C5—C7	122.5 (2)	C12—C10—H10	109.00
C4—C5—C7	119.7 (2)	C10—C11—H11A	109.00
C4—C5—C6	117.7 (2)	C10—C11—H11B	109.00
C1—C6—C5	120.9 (2)	C10—C11—H11C	109.00
O1—C7—C5	121.5 (2)	H11A—C11—H11B	109.00
C5—C7—C8	118.8 (2)	H11A—C11—H11C	110.00
O1—C7—C8	119.7 (2)	H11B—C11—H11C	109.00
C7—C8—C9	112.03 (19)	C10—C12—H12A	109.00
N1—C9—C8	110.12 (18)	C10—C12—H12B	109.00
N1—C10—C12	108.65 (19)	C10—C12—H12C	109.00
C11—C10—C12	112.1 (2)	H12A—C12—H12B	110.00
N1—C10—C11	110.19 (19)	H12A—C12—H12C	109.00
C2—C1—H1	119.00	H12B—C12—H12C	109.00
C6—C1—H1	119.00	C2—C13—H13A	109.00
C2—C3—H3	119.00	C2—C13—H13B	109.00
C4—C3—H3	119.00	C2—C13—H13C	109.00
C3—C4—H4	119.00	H13A—C13—H13B	110.00

C5—C4—H4	120.00	H13A—C13—H13C	109.00
C1—C6—H6	120.00	H13B—C13—H13C	109.00
C5—C6—H6	120.00		

C9—N1—C10—C11	−76.7 (2)	C3—C4—C5—C7	176.5 (2)
C9—N1—C10—C12	160.08 (19)	C4—C5—C6—C1	2.2 (3)
C10—N1—C9—C8	176.31 (17)	C7—C5—C6—C1	−176.0 (2)
C6—C1—C2—C3	−1.3 (3)	C6—C5—C7—C8	−1.2 (3)
C6—C1—C2—C13	177.0 (2)	C4—C5—C7—O1	−1.1 (3)
C2—C1—C6—C5	−0.7 (4)	C4—C5—C7—C8	−179.4 (2)
C13—C2—C3—C4	−176.6 (2)	C6—C5—C7—O1	177.1 (2)
C1—C2—C3—C4	1.7 (3)	O1—C7—C8—C9	−11.9 (3)
C2—C3—C4—C5	−0.2 (3)	C5—C7—C8—C9	166.46 (19)
C3—C4—C5—C6	−1.8 (3)	C7—C8—C9—N1	176.54 (17)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H14*A*···Cl1	0.90	2.26	3.148 (3)	172
N1—H14*B*···Cl1^{i}	0.90	2.25	3.145 (3)	173
C1—H1···O1^{ii}	0.93	2.53	3.340 (4)	146

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