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2-Benzoylanilinium chloride monohydrate

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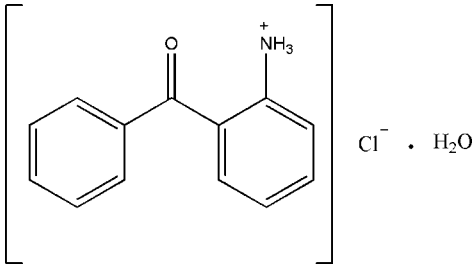
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.068; wR factor = 0.174; data-to-parameter ratio = 15.2.

In the cation of the title compound, $C_{13}H_{12}NO^+\cdot Cl^-\cdot H_2O$, the rings are oriented at a dihedral angle of 53.62 (3)°. In the crystal structure, N—H···Cl, N—H···O and O—H···Cl hydrogen bonds link the ions and water molecules, forming a three-dimensional network.

Related literature

For related literature, see: Shetty *et al.* (1999); Zhu *et al.* (2005). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{13}H_{12}NO^+\cdot Cl^-\cdot H_2O$
M_r = 251.70
Monoclinic, $P2_1/c$
a = 4.771 (1) Å
b = 17.450 (4) Å
c = 15.277 (3) Å
β = 90.50 (3)°
V = 1271.8 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 298 (2) K
0.30 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.918, T_{max} = 0.972
2786 measured reflections
2479 independent reflections
1522 reflections with $I > 2\sigma(I)$
R_{int} = 0.065
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.174
S = 1.03
2479 reflections
163 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N—H0A···Cl	0.89	2.38	3.247 (3)	165
N—H0B···Cl^{i}	0.89	2.29	3.178 (3)	175
N—H0C···OW	0.89	1.87	2.748 (5)	169
OW—HWB···Cl^{ii}	0.87 (5)	2.38 (3)	3.226 (4)	165 (5)
OW—HWA···Cl^{iii}	0.86 (4)	2.35 (4)	3.204 (4)	176 (5)

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+2, -y+1, -z+2$; (iii) $-x+1, -y+1, -z+2$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2364).

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supplementary materials

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2-Benzoylanilinium chloride monohydrate

S.-P. Deng, S. Liu, G.-L. Song and H.-J. Zhu

Comment

(2-aminophenyl)(phenyl)methanone is one of the important monomers, being utilized to synthesize oligomers containing quinoline unit (Shetty *et al.*, 1999). We report herein the crystal structure of the title compound, (I).

In the molecule of (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Rings A (C1—C6) and B (C8—C13) are, of course, planar and they are oriented at a dihedral angle of A/B = 53.62 (3)°.

In the crystal structure, N—H···Cl, N—H···O and O—H···Cl hydrogen bonds (Table 1) link the molecules to form a three dimensional network (Fig. 2), in which they may be effective in the stabilization of the structure.

Experimental

(2-aminophenyl)(phenyl)methanone was prepared by a method reported recently with a little modification (Zhu *et al.*, 2005). Crystals of (I) suitable for X-ray analysis were obtained by dissolving (2-aminophenyl)(phenyl)methanone (1.0 g, 5.1 mmol) in a solution of hydrochloride acid (5 ml, 1.0 mol/l) and evaporating the solvent slowly at room temperature for about 5 d.

Refinement

H atoms (for H_2O) were located in difference syntheses and refined isotropically [O—H = 0.86 (4) and 0.87 (5) Å, U_{iso}(H) = 0.10 (2) and 0.11 (2) Å^2]. The remaining H atoms were positioned geometrically with N—H = 0.89 Å (for NH_3) and C—H = 0.93 Å for aromatic H atoms, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C,*N*), where x = 1.2 for aromatic H and x = 1.5 for NH_3 H atoms.

Figures

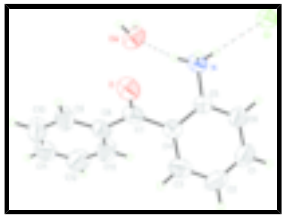

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines.

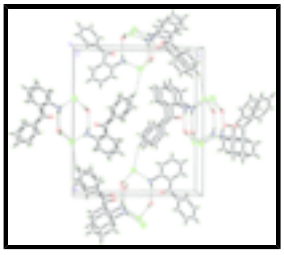

Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

2-Benzoylanilinium chloride monohydrate

Crystal data

$C_{13}H_{12}NO^{+}\cdot Cl^{-}\cdot H_2O$	$F_{000} = 528$
$M_r = 251.70$	$D_x = 1.315$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 25 reflections
$a = 4.771$ (1) Å	$\theta = 9$–12º
$b = 17.450$ (4) Å	$\mu = 0.29$ mm^{-1}
$c = 15.277$ (3) Å	$T = 298$ (2) K
$\beta = 90.50$ (3)º	Needle, colorless
$V = 1271.8$ (5) Å^3	0.30 × 0.10 × 0.10 mm
$Z = 4$	

Data collection

Nonius CAD-4 diffractometer	$R_{int} = 0.065$
Radiation source: fine-focus sealed tube	$\theta_{max} = 26.0$º
Monochromator: graphite	$\theta_{min} = 1.8$º
$T = 298(2)$ K	$h = -5\rightarrow5$
$\omega/2\theta$ scans	$k = 0\rightarrow21$
Absorption correction: ψ scan (North *et al.*, 1968)	$l = 0\rightarrow18$
$T_{min} = 0.918$, $T_{max} = 0.972$	3 standard reflections
2786 measured reflections	every 120 min
2479 independent reflections	intensity decay: none
1522 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.068$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.174$	$w = 1/[\sigma^2(F_o^2) + (0.07P)^2 + 0.6P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.03	$(\Delta/\sigma)_{max}$ = 0.001
2479 reflections	$\Delta\rho_{max}$ = 0.35 e Å^{-3}
163 parameters	$\Delta\rho_{min}$ = −0.23 e Å^{-3}
3 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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}
Cl	1.0018 (2)	0.34988 (6)	1.01031 (6)	0.0466 (3)
OW	0.4922 (7)	0.56862 (19)	0.8837 (2)	0.0602 (9)
HWA	0.366 (8)	0.591 (3)	0.914 (3)	0.10 (2)*
HWB	0.632 (7)	0.596 (3)	0.903 (4)	0.11 (2)*
O	−0.0034 (6)	0.47495 (18)	0.81909 (19)	0.0541 (8)
N	0.4887 (6)	0.41120 (18)	0.88813 (19)	0.0394 (8)
H0A	0.6493	0.3993	0.9149	0.059*
H0B	0.3457	0.3968	0.9213	0.059*
H0C	0.4809	0.4616	0.8794	0.059*
C1	0.6114 (11)	0.2658 (3)	0.7154 (3)	0.0650 (13)
H1A	0.7167	0.2215	0.7081	0.078*
C2	0.4379 (11)	0.2909 (3)	0.6492 (3)	0.0651 (14)
H2A	0.4250	0.2633	0.5973	0.078*
C3	0.2834 (10)	0.3566 (3)	0.6594 (3)	0.0585 (12)
H3A	0.1667	0.3732	0.6141	0.070*
C4	0.2994 (8)	0.3992 (2)	0.7374 (2)	0.0408 (9)
C5	0.4727 (8)	0.3716 (2)	0.8040 (2)	0.0384 (9)
C6	0.6292 (9)	0.3067 (2)	0.7928 (3)	0.0516 (11)
H6A	0.7479	0.2899	0.8375	0.062*
C7	0.1231 (8)	0.4689 (2)	0.7509 (3)	0.0432 (10)
C8	0.1051 (8)	0.5295 (3)	0.6834 (3)	0.0457 (10)
C9	−0.0827 (10)	0.5888 (3)	0.6937 (3)	0.0626 (13)
H9A	−0.2023	0.5887	0.7415	0.075*
C10	−0.0957 (12)	0.6478 (3)	0.6347 (4)	0.0761 (15)
H10A	−0.2215	0.6877	0.6437	0.091*
C11	0.0721 (12)	0.6489 (3)	0.5634 (3)	0.0679 (14)

H11A	0.0594	0.6887	0.5231	0.082*
C12	0.2563 (13)	0.5918 (3)	0.5519 (3)	0.0771 (16)
H12A	0.3717	0.5923	0.5032	0.093*
C13	0.2776 (11)	0.5322 (3)	0.6115 (3)	0.0638 (13)
H13A	0.4093	0.4937	0.6029	0.077*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.0380 (5)	0.0552 (6)	0.0465 (6)	0.0004 (5)	0.0016 (4)	0.0006 (5)
OW	0.0421 (18)	0.062 (2)	0.076 (2)	−0.0039 (17)	0.0082 (17)	−0.0183 (17)
O	0.0365 (15)	0.074 (2)	0.0516 (18)	0.0013 (14)	0.0056 (14)	0.0060 (15)
N	0.0293 (16)	0.052 (2)	0.0368 (17)	−0.0025 (15)	0.0005 (14)	0.0011 (15)
C1	0.075 (3)	0.044 (3)	0.076 (3)	0.005 (2)	0.001 (3)	−0.004 (2)
C2	0.089 (4)	0.050 (3)	0.057 (3)	−0.008 (3)	0.006 (3)	−0.014 (2)
C3	0.062 (3)	0.063 (3)	0.049 (2)	−0.009 (3)	−0.008 (2)	−0.002 (2)
C4	0.036 (2)	0.043 (2)	0.044 (2)	−0.0054 (18)	0.0012 (17)	0.0018 (18)
C5	0.035 (2)	0.041 (2)	0.039 (2)	−0.0065 (18)	0.0046 (16)	0.0012 (17)
C6	0.053 (3)	0.046 (3)	0.056 (3)	0.001 (2)	−0.003 (2)	0.000 (2)
C7	0.031 (2)	0.059 (3)	0.040 (2)	−0.0082 (19)	−0.0008 (17)	0.000 (2)
C8	0.038 (2)	0.056 (3)	0.043 (2)	−0.005 (2)	−0.0028 (18)	0.002 (2)
C9	0.054 (3)	0.069 (3)	0.065 (3)	0.016 (3)	0.006 (2)	0.006 (3)
C10	0.076 (4)	0.060 (3)	0.092 (4)	0.021 (3)	−0.010 (3)	0.003 (3)
C11	0.093 (4)	0.050 (3)	0.060 (3)	−0.006 (3)	−0.017 (3)	0.006 (3)
C12	0.109 (5)	0.066 (3)	0.056 (3)	0.001 (3)	0.017 (3)	0.008 (3)
C13	0.075 (3)	0.056 (3)	0.060 (3)	0.010 (3)	0.014 (3)	0.008 (2)

Geometric parameters (Å, °)

OW—HWA	0.86 (4)	C4—C7	1.493 (6)
OW—HWB	0.87 (5)	C5—C6	1.369 (5)
O—C7	1.213 (4)	C6—H6A	0.9300
N—C5	1.461 (5)	C7—C8	1.480 (6)
N—H0A	0.8900	C8—C13	1.379 (6)
N—H0B	0.8900	C8—C9	1.379 (6)
N—H0C	0.8900	C9—C10	1.369 (7)
C1—C2	1.372 (7)	C9—H9A	0.9300
C1—C6	1.383 (6)	C10—C11	1.358 (7)
C1—H1A	0.9300	C10—H10A	0.9300
C2—C3	1.372 (6)	C11—C12	1.341 (7)
C2—H2A	0.9300	C11—H11A	0.9300
C3—C4	1.406 (6)	C12—C13	1.385 (7)
C3—H3A	0.9300	C12—H12A	0.9300
C4—C5	1.391 (5)	C13—H13A	0.9300
HWB—OW—HWA	96 (3)	C5—C6—H6A	119.9
C5—N—H0A	109.5	C1—C6—H6A	119.9
C5—N—H0B	109.5	O—C7—C8	120.6 (4)
H0A—N—H0B	109.5	O—C7—C4	118.4 (4)

C5—N—H0C	109.5	C8—C7—C4	121.0 (3)
H0A—N—H0C	109.5	C13—C8—C9	117.3 (4)
H0B—N—H0C	109.5	C13—C8—C7	123.3 (4)
C2—C1—C6	119.8 (5)	C9—C8—C7	119.4 (4)
C2—C1—H1A	120.1	C10—C9—C8	120.9 (5)
C6—C1—H1A	120.1	C10—C9—H9A	119.5
C3—C2—C1	120.3 (4)	C8—C9—H9A	119.5
C3—C2—H2A	119.9	C11—C10—C9	121.1 (5)
C1—C2—H2A	119.9	C11—C10—H10A	119.5
C2—C3—C4	120.8 (4)	C9—C10—H10A	119.5
C2—C3—H3A	119.6	C12—C11—C10	119.0 (5)
C4—C3—H3A	119.6	C12—C11—H11A	120.5
C5—C4—C3	117.7 (4)	C10—C11—H11A	120.5
C5—C4—C7	120.8 (3)	C11—C12—C13	121.1 (5)
C3—C4—C7	121.4 (4)	C11—C12—H12A	119.5
C6—C5—C4	121.1 (4)	C13—C12—H12A	119.5
C6—C5—N	118.4 (3)	C8—C13—C12	120.6 (5)
C4—C5—N	120.4 (3)	C8—C13—H13A	119.7
C5—C6—C1	120.2 (4)	C12—C13—H13A	119.7
C6—C1—C2—C3	0.4 (8)	C3—C4—C7—C8	−48.7 (5)
C1—C2—C3—C4	−0.1 (7)	O—C7—C8—C13	169.0 (4)
C2—C3—C4—C5	−1.1 (6)	C4—C7—C8—C13	−10.3 (6)
C2—C3—C4—C7	−177.2 (4)	O—C7—C8—C9	−7.7 (6)
C3—C4—C5—C6	2.1 (6)	C4—C7—C8—C9	173.0 (4)
C7—C4—C5—C6	178.2 (4)	C13—C8—C9—C10	−0.1 (7)
C3—C4—C5—N	−177.1 (4)	C7—C8—C9—C10	176.9 (5)
C7—C4—C5—N	−1.0 (5)	C8—C9—C10—C11	1.3 (8)
C4—C5—C6—C1	−1.8 (6)	C9—C10—C11—C12	−1.2 (9)
N—C5—C6—C1	177.4 (4)	C10—C11—C12—C13	−0.1 (8)
C2—C1—C6—C5	0.5 (7)	C9—C8—C13—C12	−1.2 (7)
C5—C4—C7—O	−43.9 (5)	C7—C8—C13—C12	−178.0 (4)
C3—C4—C7—O	132.0 (4)	C11—C12—C13—C8	1.3 (8)
C5—C4—C7—C8	135.4 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N—H0A···Cl	0.89	2.38	3.247 (3)	165
N—H0B···Cl^{i}	0.89	2.29	3.178 (3)	175
N—H0C···OW	0.89	1.87	2.748 (5)	169
OW—HWB···Cl^{ii}	0.87 (5)	2.38 (3)	3.226 (4)	165 (5)
OW—HWA···Cl^{iii}	0.86 (4)	2.35 (4)	3.204 (4)	176 (5)

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

Fig. 1

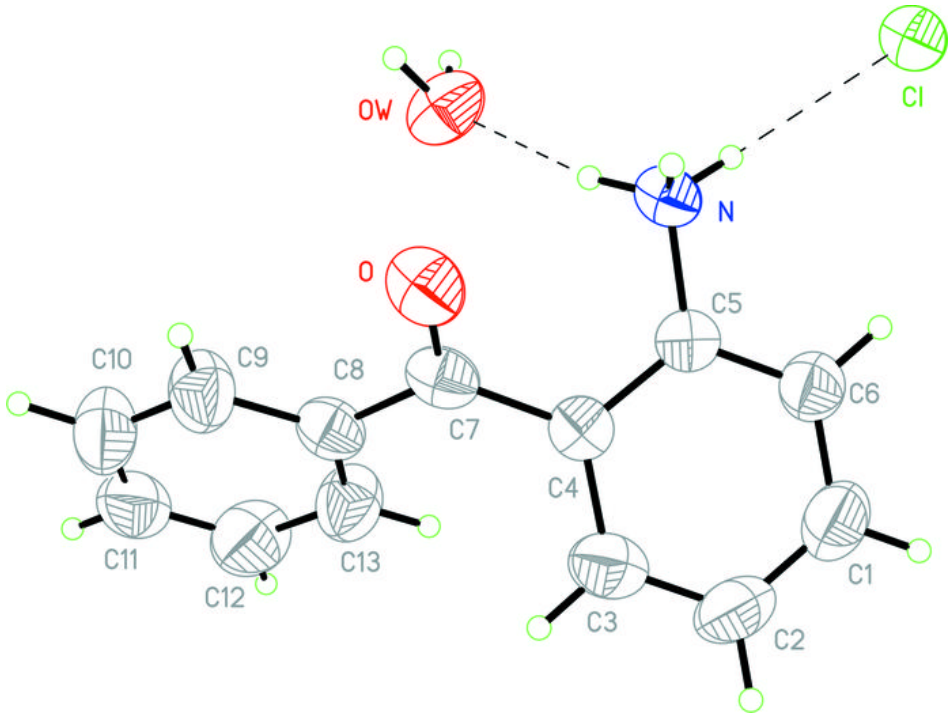

Fig. 2