Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Cocrystal of 2-(1*H*-imidazol-2-yl)-1*H*-imidazolium chloride and 4-aminobenzoic acid

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Received 20 June 2006
Accepted 4 July 2006

Key indicators

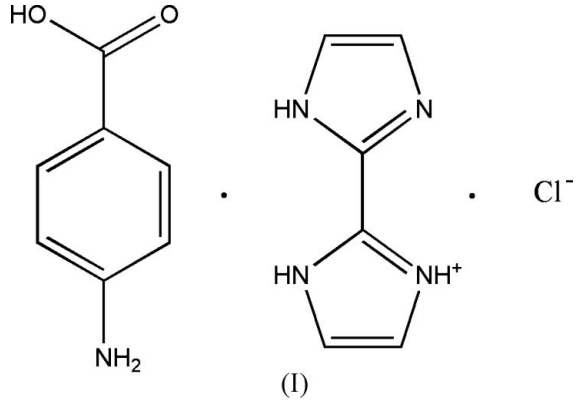
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.104
Data-to-parameter ratio = 11.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, 2-(2–1*H*-imidazolyl)-1*H*-imidazolium chloride 4-aminobenzoic acid solvate, $C_6H_7N_4^+\cdot Cl^-\cdot C_7H_7NO_2$, all three components are linked by N—H···O, O—H···N, N—H···Cl hydrogen bonds.

Comment

2,2′-Biimidazole, H_2biim, is not only a proton donor, but also a proton acceptor, so that it possesses five possible forms, *viz*. di-deprotonated (dianion, $biim^{2-}$), monodeprotonated (mono-anion, $Hbiim^-$), neutral (neutral, H_2biim), monoprotonated (monocation, H_3biim^+) and diprotonated (dication, H_4biim^{2+}). Therefore, H_2biim is an excellent candidate for the construction of supramolecular crystal structures. Homomeric hydrogen-bonded motifs $R_2^2(10)$ (Cromer *et al.*, 1987), heteromeric hydrogen-bonded motifs $R_2^2(9)$ (Ye *et al.*, 2005) and $R_1^2(7)$ (Belanger & Beauchamp, 1996) and mixed hydrogen-bonded motifs $R_2^2(10)$ and $R_1^2(7)$ (Ramirez *et al.*, 2002) have been reported. In an extension of this research, the crystal structure of the title compound, (I), is reported here.



(I)

The bond distances and angles of the monoprotonated H_3biim+ in (I) are unexceptional and compare well with the values in neutral H_2biim (Cromer *et al.*, 1987) (Fig. 1). The two rings are almost coplanar in both cases. The dihedral angle between the two five-membered rings is 4.6° in neutral H_2biim, and 1.1 (2)° in (I).

A fundamental unit of the crystal structure consists of a hydrogen-bonded (N—H···O, O—H···N and N—H···Cl) group of all three components: PABA···H_3BIM^+···Cl^- *via* $R_2^2(9)$ and $R_2^1(7)$ (Table 1; PABA is *p*-aminobenzoic acid). This unit forms a one-dimensional ribbon by hydrogen-bond interactions. This one-dimensional structure then extends into three dimensions *via* further hydrogen bonds (Table 1 and Fig. 2).

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Experimental

2,2′-Biimidazole was synthesized by a modification of the published procedure of Melloni *et al.* (1972). All other chemicals were of reagent grade and commercially available from the Beijing Chemical Reagents Company of China, and were used without further purification. 2,2′-Biimidazole (0.5 mmol, 0.067 g) was suspended in water (30 ml). A 10 ml aqueous solution of 4-aminobenzoic acid (0.5 mmol) was added to the resulting suspension. Dilute aqueous HCl was added until the suspension became clear. The resulting solution was filtered and allowed to evaporate slowly at room temperature. After two months, colorless crystals of (I) appeared.

Crystal data

$C_6H_7N_4^+\cdot Cl^-\cdot C_7H_7NO_2$
M_r = 307.74
Monoclinic, $P2_1/n$
a = 10.560 (2) Å
b = 11.408 (3) Å
c = 11.843 (3) Å
β = 91.376 (3)°
V = 1426.3 (6) Å^3
Z = 4
D_x = 1.433 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 298 (2) K
Block, colorless
0.40 × 0.30 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
5717 measured reflections
2519 independent reflections
2112 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.104
S = 1.03
2519 reflections
214 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0364P)^2 + 0.5653P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H7···Cl1^{i}	0.92 (3)	2.11 (3)	3.017 (2)	168 (2)
O2—H12···N3^{ii}	0.98 (3)	1.70 (3)	2.667 (2)	168 (3)
N5—H14···Cl1^{iii}	0.80 (2)	2.43 (3)	3.218 (2)	168 (2)
N5—H13···O1^{iv}	0.86 (3)	2.27 (3)	3.034 (3)	147 (2)
N2—H3···O1^{v}	0.85 (2)	1.87 (2)	2.713 (2)	171 (2)
N4—H6···Cl1^{i}	0.88 (2)	2.30 (2)	3.1532 (19)	165 (2)

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

H atoms involved in hydrogen-bonding interactions were located in difference maps and their positional and isotropic displacement parameters were refined. Other H atoms were included in the refinement in calculated positions (Csp^2—H = 0.93 Å) using a riding-model approximation, with U_{eq}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; 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*.

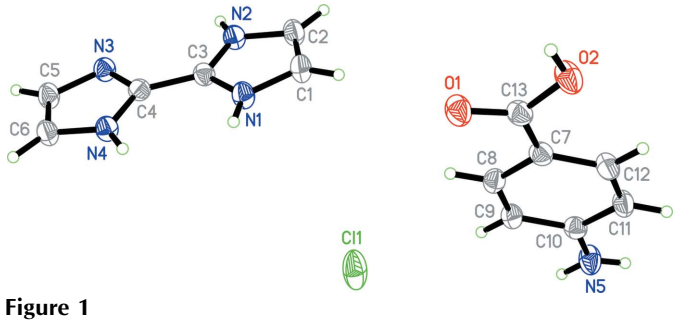

Figure 1
The asymmetric unit of the title compound, shown with 30% probability ellipsoids.

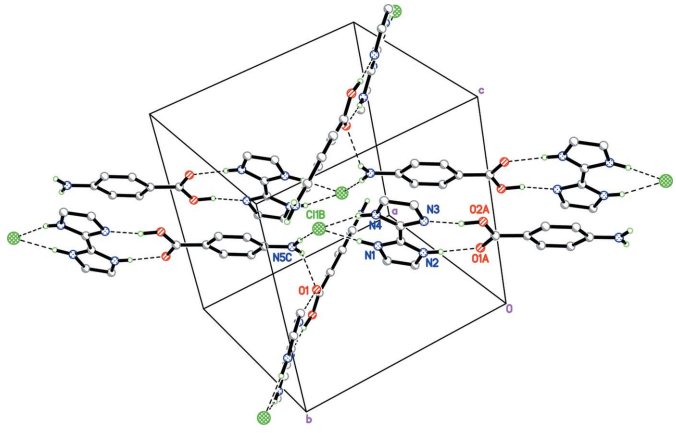

Figure 2
A view of the packing of (I), showing the hydrogen-bonding associations as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry code: (A) $-x, -y-1, -z$; (B) $-x+\frac{3}{2}, y+\frac{3}{2}, -z+\frac{3}{2}$; (C) $-x+1, -y, -z$.]

We gratefully acknowledge financial support of this work by the National Natural Science Foundation of China (No. 30470408) and the Shanxi Provincial Natural Science Foundation for Youth (No. 20041032).

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