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Key indicators

Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.048
 wR factor = 0.119
Data-to-parameter ratio = 14.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

Benzimidazolium 4-carboxyphenoxyacetate

The asymmetric unit of the title compound, $\text{C}_7\text{H}_7\text{N}_2^+\text{-C}_9\text{H}_7\text{O}_5^-$, consists of one benzimidazolium cation and one 4-carboxyphenoxyacetate anion. A two-dimensional supramolecular hydrogen-bonded network structure is formed *via* intermolecular hydrogen bonds in the *bc* plane.

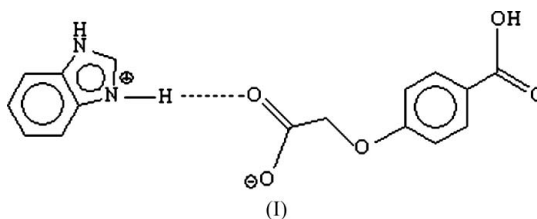
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Comment

In recent years, much interest has been focused on the design and synthesis of supramolecular complexes formed by weak intermolecular forces, especially hydrogen-bonding interactions (Iglesias *et al.*, 2003; Braga *et al.*, 2003). The rational utilization of weak intermolecular forces to build up novel supramolecular networks is still an appealing field for chemists. One of the important targets in the formation of a supramolecular assembly is the establishment of possible connections between the units involved. Fortunately, multicarboxylate ligands, such as 4-carboxyphenoxyacetic acid (4-CPOAH₂), with both rigid and flexible parts, have proved to be good candidates. They can be regarded not only as hydrogen-bond acceptors, but also as hydrogen-bond donors, depending upon the number of deprotonated carboxylic acid groups present (Gao *et al.*, 2005). Here, we describe the structure of the title new two-dimensional hydrogen-bonding organic salt, (I).



The asymmetric unit of (I) is illustrated in Fig. 1. Selected bond distances and angles are given in Table 1 and details concerning the hydrogen bonding in Table 2. Compound (I) consists of a benzimidazolium cation and a 4-carboxy-

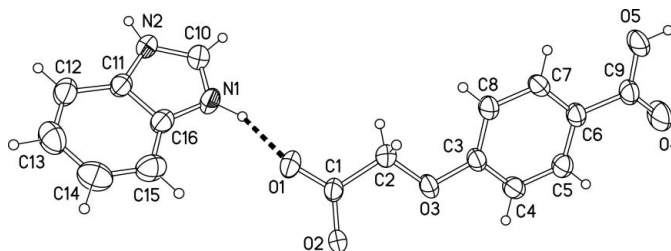


Figure 1

A plot of compound (I), with 30% probability displacement ellipsoids. The dashed line indicates a hydrogen bond.

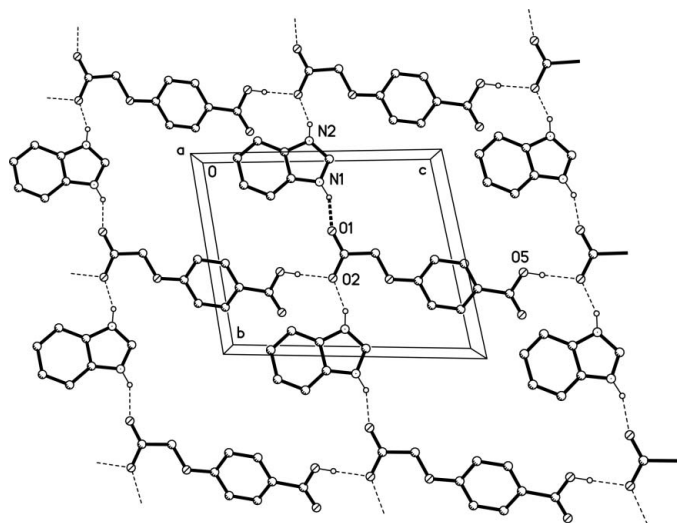


Figure 2

The crystal packing of compound (I), with hydrogen bonds denoted by dashed lines. H atoms not involved in hydrogen bonding have been omitted.

phenoxyacetate monoanion. The protonated benzimidazole atom N1 and the carboxylate atom O1 form an intermolecular hydrogen bond (Table 2). It should be noted that the C1—O2 and C9—O5 distances are longer than the C1—O1 and C9—O4 distances, agreeing with the assignment of localized single and double bonds (Table 1). The carboxylate group (O4/C9/O5) and the benzene ring are almost coplanar, with a dihedral angle of $1.70(5)^\circ$, while the oxyacetate group is twisted out of the benzene ring plane, with a dihedral angle of $22.30(5)^\circ$. The dihedral angle between the benzimidazolium cation and the benzene ring is $53.29(8)^\circ$.

In the crystal structure, ion pairs are further linked sequentially *via* O—H...O and N—H...O hydrogen bonds. The protonated atoms O5 and N2 are linked to the adjacent carboxylate atom O2, forming a two-dimensional hydrogen-bonded layer-like structure in the *bc* plane (Table 2, Fig. 2).

Experimental

Cadmium dinitrate tetrahydrate (3.08 g, 10 mmol), benzimidazole (1.18 g, 10 mmol) and 4-carboxyphenoxyacetic acid (1.96 g, 10 mmol) were dissolved in a small volume of a 1:1 ethanol–water mixture. The solution was sealed in a 50 ml Teflon-lined stainless steel bomb, which was heated at 423 K for 120 h. Colourless crystals of (I) were separated from the filtered solution after several days. Analysis calculated for $C_{16}H_{14}N_2O_5$: C 61.14, H 4.49, N 8.91%; found: C 61.11, H 4.45, N 8.94%.

Crystal data

$C_9H_7O_5^+ \cdot C_7H_7N_2^-$
 $M_r = 314.29$
 Triclinic, $P\bar{1}$
 $a = 7.2371(14) \text{ \AA}$
 $b = 9.5895(19) \text{ \AA}$
 $c = 11.633(2) \text{ \AA}$
 $\alpha = 75.80(3)^\circ$
 $\beta = 75.50(3)^\circ$
 $\gamma = 72.69(3)^\circ$
 $V = 733.4(3) \text{ \AA}^3$

$Z = 2$
 $D_x = 1.423 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 Cell parameters from 6343 reflections
 $\theta = 3.2\text{--}26.2^\circ$
 $\mu = 0.11 \text{ mm}^{-1}$
 $T = 295(2) \text{ K}$
 Prism, colourless
 $0.38 \times 0.27 \times 0.21 \text{ mm}$

Data collection

Rigaku R-Axis RAPID
 diffractometer
 ω scans
 Absorption correction: multi-scan
 (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.966$, $T_{\max} = 0.978$
 6669 measured reflections

3099 independent reflections
 2263 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.024$
 $\theta_{\max} = 26.8^\circ$
 $h = -9 \rightarrow 8$
 $k = -12 \rightarrow 12$
 $l = -14 \rightarrow 14$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.119$
 $S = 1.02$
 3099 reflections
 218 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0575P)^2 + 0.1766P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.28 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.19 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

O1—C1	1.240 (2)	C3—C8	1.401 (2)
O2—C1	1.277 (2)	C4—C5	1.391 (2)
O3—C3	1.3819 (19)	C5—C6	1.411 (2)
O3—C2	1.440 (2)	C6—C7	1.391 (2)
O4—C9	1.217 (2)	C6—C9	1.506 (2)
O5—C9	1.330 (2)	C7—C8	1.400 (2)
N1—C10	1.329 (2)	C11—C12	1.399 (3)
N1—C16	1.392 (2)	C11—C16	1.402 (2)
N2—C10	1.326 (2)	C12—C13	1.386 (3)
N2—C11	1.396 (2)	C13—C14	1.412 (3)
C1—C2	1.533 (2)	C14—C15	1.374 (3)
C3—C4	1.400 (2)	C15—C16	1.398 (3)
C3—O3—C2	116.43 (13)	C7—C8—C3	119.78 (16)
C10—N1—C16	108.70 (15)	O4—C9—O5	123.53 (16)
C10—N2—C11	108.53 (14)	O4—C9—C6	122.94 (17)
O1—C1—O2	125.38 (16)	O5—C9—C6	113.53 (15)
O1—C1—C2	116.03 (15)	N2—C10—N1	110.35 (16)
O2—C1—C2	118.49 (14)	N2—C11—C12	131.85 (16)
O3—C2—C1	110.55 (14)	N2—C11—C16	106.26 (15)
O3—C3—C4	115.41 (15)	C12—C11—C16	121.86 (17)
O3—C3—C8	124.78 (15)	C13—C12—C11	115.98 (18)
C4—C3—C8	119.80 (15)	C12—C13—C14	122.0 (2)
C5—C4—C3	119.87 (16)	C15—C14—C13	121.9 (2)
C4—C5—C6	120.89 (16)	C14—C15—C16	116.63 (18)
C7—C6—C5	118.63 (15)	N1—C16—C15	132.21 (16)
C7—C6—C9	121.59 (16)	N1—C16—C11	106.16 (15)
C5—C6—C9	119.78 (16)	C15—C16—C11	121.61 (18)
C6—C7—C8	121.01 (16)		

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O5—H19...O2 ⁱ	0.86 (2)	1.76 (3)	2.615 (3)	173 (3)
N1—H17...O1	0.90 (2)	1.92 (3)	2.718 (2)	148 (2)
N2—H18...O2 ⁱⁱ	0.90 (2)	1.83 (3)	2.691 (3)	159 (2)

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

The H atoms on the benzimidazolium N and carboxylic acid O atoms were located in difference Fourier maps and refined with distance restraints of N—H = 0.90 (1) and O—H = 0.85 (1) \AA , and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O}, \text{N})$. The remaining H atoms were placed in calculated positions and treated as riding atoms, with aromatic C—H = 0.93 and aliphatic C—H = 0.97 \AA , and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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