Acta Crystallographica Section C
**Crystal Structure
Communications**
ISSN 0108-2701

4-(1*H*-Benzimidazol-3-ium-2-yl)-benzoate dihydrate

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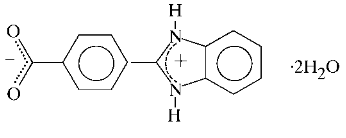
Received 13 September 2000
Accepted 30 October 2000

In the title compound, $C_{14}H_{10}N_2O_2{\cdot}2H_2O$, the water molecules are involved in hydrogen bonds and interactions. Intermolecular and intramolecular O—H···O hydrogen bonds connect the complex into chains along the *a* axis, whereas N—H···O intermolecular hydrogen bonds and C—H···O interactions interconnect these layers forming a three-dimensional network.

Comment

Benzimidazole is an interesting heterocyclic structure, because it is present in various naturally occurring drugs, such as omeprazole, astemizole and emedastine difumarate (Sakai *et al.*, 1989). The efficacy of substituted benzimidazoles in the treatment of parasitic infections is well known (Brown *et al.*, 1961; Preston, 1974; Sarkar *et al.*, 1984). Substituted benzimidazole moieties are established pharmacophores in parasitic chemotherapy. Furthermore, proton transfer accompanied by a configurational change of the π-electron structure is one of the key reactions in many proposals for molecular electronic devices (Xu *et al.*, 1994). The electrical properties depend heavily on the intermolecular interactions. Thus, the title compound, (I), may be a candidate for the construction of a novel type of conductive organic material in which the proton motion is essentially correlated to the electron conduction (Inabe, 1991).



(I)

The benzimidazole moiety is planar, with a maximum deviation of 0.008 (2) Å for the N1 atom, with protonation occurring at the other imidazole N atom. The dihedral angle between this benzimidazole moiety and the phenyl ring is 11.3 (1)°. The C—O bond lengths are comparable to those of a COO^- group (Leban & Rupnik, 1992; Aakeroy & Hitchcock, 1994). The carboxyl group makes a dihedral angle of 4.4 (2) Å with the mean plane of the phenyl ring. In the asymmetric unit, both water molecules are linked to the carboxyl group through O—H···O hydrogen bonds.

In the crystal, all the hydrogen bonds and interactions (Table 2) involve the water molecules. The water molecules are involved in O—H···O intramolecular and intermolecular hydrogen bonds with the O atoms in the COO^- group. These hydrogen bonds connect the water molecules into infinite chains in the [100] direction in which the O atoms of the COO^- group act as a bridge. This results in the molecules of the title compound being stacked along the same axis to form layers. The water molecules are also involved in N—H···O intermolecular hydrogen bonds and C—H···O interactions, which interconnect these layers. The O—H···O and N—H···O hydrogen bonds, and the C—H···O interactions form a three-dimensional network of the title compound throughout the structure.

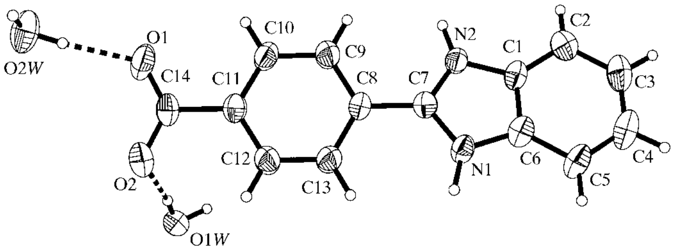


Figure 1
The structure of (I) showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Experimental

The title compound was prepared from benzene-1,4-dicarboxylic acid and 1,2-diaminobenzene in 36% yield using a modified Phillips reaction (Addison & Burke, 1981; Addison *et al.*, 1983) and was recrystallized from water. Single crystals suitable for X-ray analysis were obtained by slow evaporation at room temperature from an EtOH/H_2O solution.

Crystal data

$C_{14}H_{10}N_2O_2{\cdot}2H_2O$
$M_r = 274.27$
Monoclinic, *Cc*
$a = 4.5541$ (2) Å
$b = 16.3140$ (8) Å
$c = 17.5245$ (9) Å
$\beta = 96.234$ (2)°
$V = 1294.29$ (11) Å^3
$Z = 4$

$D_x = 1.408$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2836 reflections
$\theta = 2.34$–$29.36°$
$\mu = 0.105$ mm^{-1}
$T = 293$ (2) K
Rectangular slab, colourless
0.48 × 0.30 × 0.08 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
4352 measured reflections
1474 independent reflections
1150 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.058$
$\theta_{\max} = 27.5°$
$h = -5 \rightarrow 5$
$k = -13 \rightarrow 20$
$l = -22 \rightarrow 20$
Intensity decay: negligible

Table 1
Selected bond lengths (Å).

N2—C7	1.334 (4)	O2—C14	1.254 (5)
N2—C1	1.390 (4)	N1—C7	1.340 (4)
O1—C14	1.249 (4)	N1—C6	1.391 (4)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1W1···O2	0.91 (6)	1.92 (6)	2.825 (4)	171 (7)
O1W—H2W1···O2$^{\rm i}$	0.88 (4)	1.84 (4)	2.716 (4)	172 (3)
O2W—H2W2···O1	0.89 (5)	1.80 (5)	2.682 (4)	171 (5)
O2W—H1W2···O1$^{\rm ii}$	0.84 (6)	2.09 (6)	2.887 (4)	158 (6)
N1—H1N1···O2$W^{\rm iii}$	0.99 (5)	1.68 (5)	2.667 (4)	177 (5)
N2—H1N2···O1$W^{\rm iv}$	1.00 (5)	1.68 (5)	2.682 (4)	177 (4)
C9—H9A···O1$W^{\rm iv}$	0.93	2.57	3.433 (4)	154
C13—H13A···O2$W^{\rm iii}$	0.93	2.52	3.391 (4)	156

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

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.111$
$S = 0.97$
1474 reflections
205 parameters
H atoms: see below
$w = 1/[\sigma^2(F_o^2) + (0.0593P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.18$ e Å^{-3}
$\Delta\rho_{\min} = -0.25$ e Å^{-3}

Friedel pairs were averaged in view of an inconclusive Flack parameter value (Flack, 1983) and s.u. After checking their presence in the difference map, all H atoms were geometrically fixed and allowed to ride on their attached atoms, except for the H atoms of N1, N2, O1W and O2W, which were involved in hydrogen bonding and were refined isotropically.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 1990).

The authors would like to thank the Malaysian Government and Universiti Sains Malaysia for research grant R&D No. 305/PFIZIK/610942. SSSR thanks the Universiti Sains Malaysia for a Visiting Postdoctoral Fellowship.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: SK1423). Services for accessing these data are described at the back of the journal.

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