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Imidazolium 2,4-dihydroxybenzoate

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.002 Å
R factor = 0.038
wR factor = 0.110
Data-to-parameter ratio = 16.0

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

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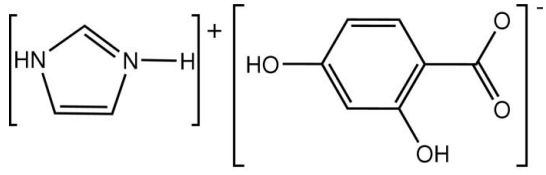
The title compound, $C_3H_5N_2^+\cdot C_7H_5O_4^-$, consists of imidazolium cations and 2,4-dihydroxybenzoate anions that link to each other *via* hydrogen bonding. Furthermore, π–π stacking is observed between parallel benzene rings and between benzene and imidazole rings.

Comment

Recently, we have been interested in π–π stacking as it is an important non-covalent intermolecular interaction and is correlated with the electron transfer process in some biological systems (Deisenhofer & Michel, 1989). As part of our ongoing investigation into the nature of π–π stacking (Li *et al.*, 2005; Xu & Xu, 2005), we present here the crystal structure of the title compound, (I).



(I)

The crystal structure of (I) consists of imidazolium cations and dihydroxybenzoate anions which link to each other *via* hydrogen bonds (Fig. 1). The imidazolium cation displays a nearly symmetric structure, the differences between N1—C8

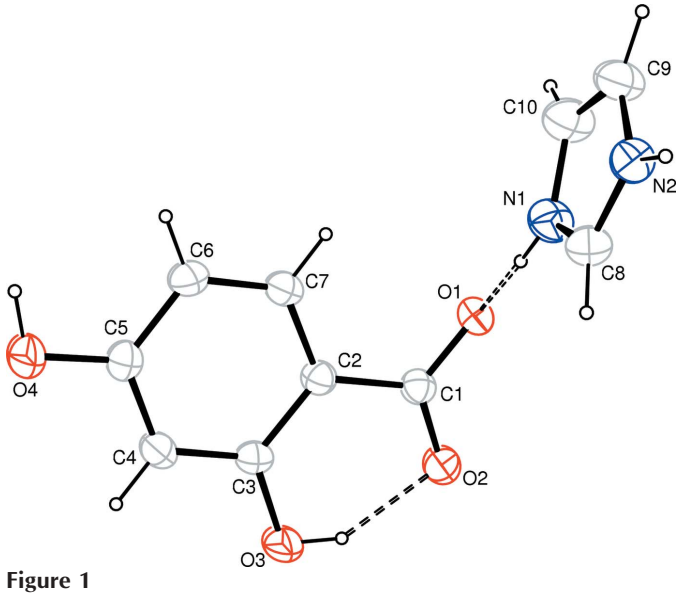


Figure 1
The molecular structure of (I) with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). Dashed lines indicate hydrogen bonds.

and N2—C8 bond distances and between N1—C10 and N2—C9 bond distances are smaller than three times the standard uncertainties (Table 1). The dihydroxybenzoate has a planar configuration, the dihedral angle between the carboxyl and benzene planes being 3.8 (3)°.

The packing is shown in Fig. 2. The face-to-face separation of 3.493 (4) Å between parallel benzene and benzene^{iv} planes [symmetry code: (iv) $-x, 1-y, -z$] clearly shows the existence of π–π stacking. The imidazole plane is approximately parallel to the benzene^{v} plane [dihedral angle = 11.25 (9)°; symmetry code: (v) $\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$]. The separation of 3.593 (3) Å from the C9 atom to the benzene^{v} plane and the centroid-to-centroid separation of 3.718 (2) Å between the imidazole and benzene rings also suggest the existence of weak π–π stacking between dihydroxybenzoate and imidazolium ions.

Extensive hydrogen bonding stabilizes the crystal structure (Table 2).

Experimental

$MnCl_2·2H_2O$ (1 mmol), 2,4-dihydroxybenzoic acid (2 mmol), imidazole (2 mmol) and Na_2CO_3 (1 mmol) were dissolved in a water/ethanol solution (20 ml, 1:1 *v*/*v*). The mixture was refluxed for 1 h and filtered after cooling to room temperature. Single crystals of (I) were obtained from the filtrate after 5 d.

Crystal data

$C_3H_5N_2^+·C_7H_5O_4^-$
M_r = 222.20
Monoclinic, $P2_1/n$
a = 10.172 (6) Å
b = 9.824 (5) Å
c = 11.433 (5) Å
β = 116.99 (2)°
V = 1018.1 (9) Å^3
Z = 4
D_x = 1.450 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8262 reflections
θ = 3.0–27.0°
μ = 0.11 mm^{-1}
T = 295 (2) K
Prism, pale-brown
0.12 × 0.10 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: none
9806 measured reflections
2335 independent reflections
1921 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 27.5°
$h = -12 \rightarrow 13$
$k = -12 \rightarrow 12$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.110
S = 1.12
2335 reflections
146 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0586P)^2 + 0.1067P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.058 (6)

Table 1
Selected bond lengths (Å).

N1—C8	1.3186 (18)	N2—C9	1.3620 (18)
N1—C10	1.3620 (19)	O1—C1	1.2643 (15)
N2—C8	1.3124 (17)	O2—C1	1.2680 (15)

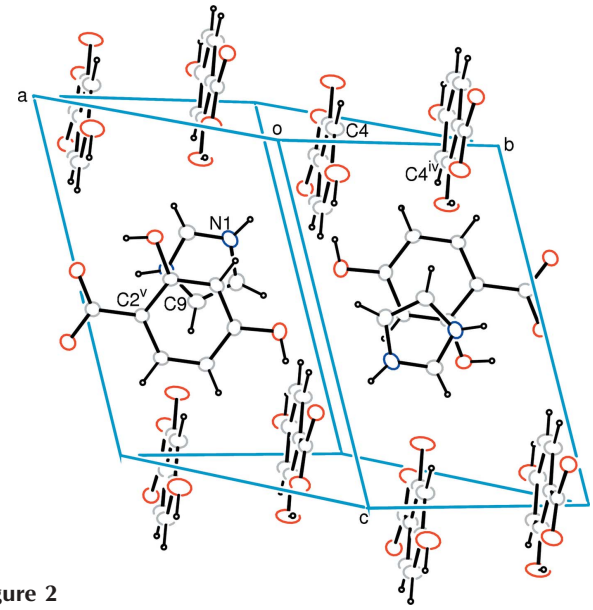


Figure 2
The packing of (I) showing π–π stacking between aromatic rings [symmetry codes: (iv) $-x, 1-y, -z$; (v) $\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$].

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.86	1.93	2.750 (2)	160
N2—H2···O2^{i}	0.86	1.88	2.736 (2)	174
O3—H3*A*···O2	0.86	1.76	2.537 (2)	149
O4—H4*A*···O1^{ii}	0.90	1.80	2.674 (2)	162
C9—H9···O3^{iii}	0.93	2.37	3.254 (3)	158

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

Hydroxy H atoms were located in a difference Fourier map and refined as riding, with O—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(O). Other H atoms were placed in calculated positions, with C—H = 0.93 Å and N—H = 0.86 Å, and included in the final cycles of refinement in riding mode, with U_{iso}(H) = 1.2U_{eq}(carrier).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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