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Benzimidazolium 2-nitrobenzoate bis(2-nitrobenzoic acid)

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.002 Å
Disorder in main residue
R factor = 0.068
wR factor = 0.175
Data-to-parameter ratio = 12.0

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

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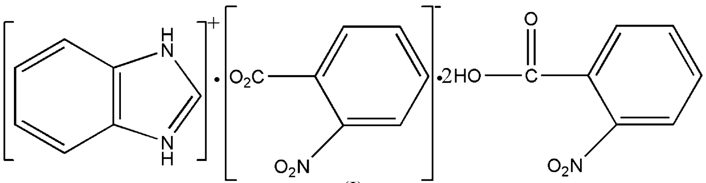
The title compound, $C_7H_7N_2^+\cdot C_7H_4NO_4^-\cdot 2C_7H_5NO_4$, consists of one benzimidazolium cation, one 2-nitrobenzoate anion and two 2-nitrobenzoic acid molecules. These ions and molecules build an infinite one-dimensional chain through hydrogen bonds.

Comment

This work continues our previous synthetic and structural studies of supramolecular interactions in aromatic molecular salts and adducts (Wang & Wei, 2007). We report here the structure of the title salt, (I).



(I)

The title salt is composed of one benzimidazolium cation, one 2-nitrobenzoate anion and two 2-nitrobenzoic acid molecules (Fig. 1). These ions and molecules give rise to an infinite one-dimensional chain along the [1$\bar{1}$0] direction through N—H···O and O—H···O hydrogen bonds (Fig. 2 and Table 1).

Experimental

All reagents were commercially available and of analytical grade. Benzimidazole (1.0 mmol, 0.118 g) was added to an aqueous solution (25 ml) of 2-nitrobenzoic acid (2.0 mmol, 0.334 g). The mixture was stirred for 10 min at 373 K. The solution was filtered and the filtrate was kept at room temperature. After 4 d, coloress crystals of the title salt were obtained.

Crystal data

$C_7H_7N_2^+\cdot C_7H_4NO_4^-\cdot 2C_7H_5NO_4$
M_r = 619.5
Triclinic, $P\bar{1}$
a = 7.6656 (13) Å
b = 13.813 (2) Å
c = 14.969 (3) Å
α = 115.085 (3)°
β = 101.372 (3)°
γ = 91.148 (3)°
V = 1397.7 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 299 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.977, T_{max} = 0.988
12065 measured reflections
5420 independent reflections
4257 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

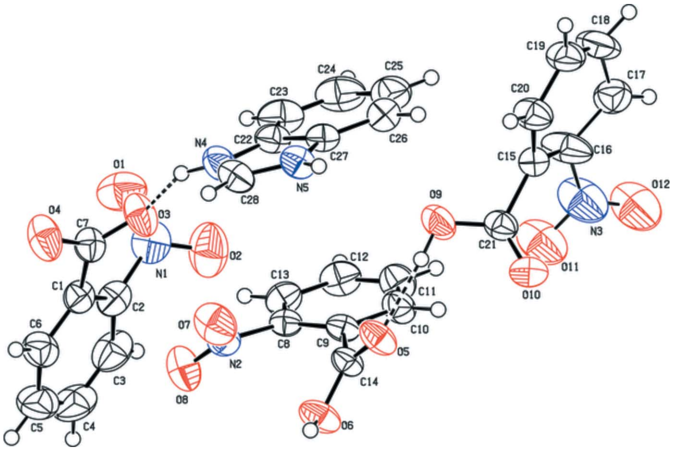


Figure 1
The asymmetric unit of (I). Displacement ellipsoids for non-H atoms are drawn at the 30% probability level. Hydrogen bonds are shown as dashed lines

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.175$
$S = 1.02$
5420 reflections
450 parameters
86 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max} = 0.76$ e Å^{-3}
$\Delta\rho_{\min} = -0.42$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···O3	0.898 (6)	1.957 (9)	2.7286 (14)	143.0 (8)
N4—H4A···O4$^{\rm i}$	0.898 (6)	2.402 (8)	2.9925 (12)	123.5 (9)
N5—H5···O5$^{\rm ii}$	0.897 (6)	2.077 (6)	2.8867 (14)	149.6 (7)
N5—H5···O6$^{\rm iii}$	0.897 (6)	2.560 (11)	3.0121 (13)	111.9 (8)
O6—H6···O6$^{\rm iv}$	0.841 (5)	1.720 (9)	2.4508 (18)	144.0 (8)
O9—H9···O5	0.849 (6)	1.849 (6)	2.6956 (12)	174.7 (13)

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

Initial refinement yielded unusually high displacement parameters for atoms C17, N3 and O12. They were treated as disordered over two positions each, with refined site occupancy factors of 0.521 (1) and 0.479 (1). In the final refinement, the anisotropic displacement parameters of atoms C17(C17′), N3(N3′) and O12(O12′) were restrained to be nearly equal. H atoms bonded to O and N were located in a difference map, and refined isotropically [O—H and N—H were restrained to 0.82 (1) and 0.90 (1) Å, respectively]. All remaining H atoms were positioned geometrically, with C—H = 0.93 Å, and were refined as riding, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

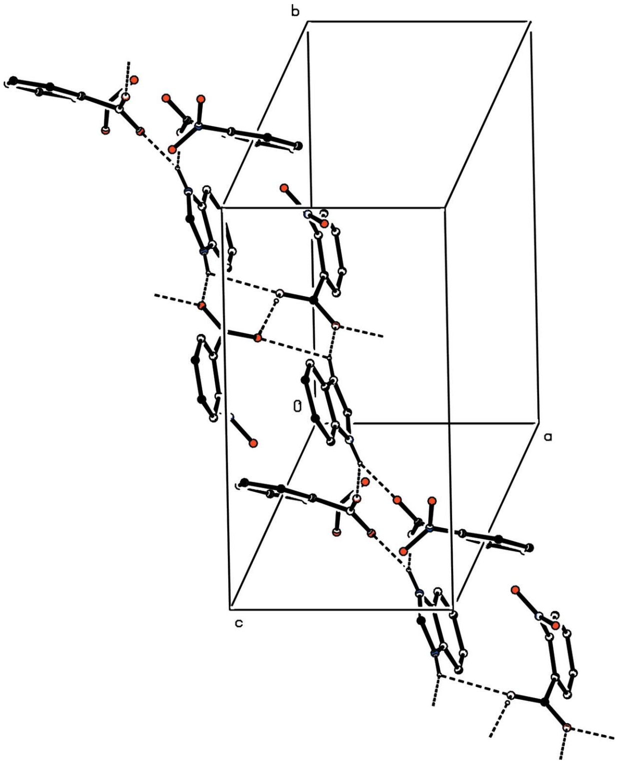


Figure 2
The packing of (I). Hydrogen bonds are shown as dashed lines. For clarity, H atoms not involved in hydrogen bonds are omitted.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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