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Benzimidazolium 2-chloro-4-nitrobenzoate

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Key indicators

Single-crystal X-ray study
T = 300 K
Mean σ(C–C) = 0.004 Å
R factor = 0.048
wR factor = 0.134
Data-to-parameter ratio = 15.8

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

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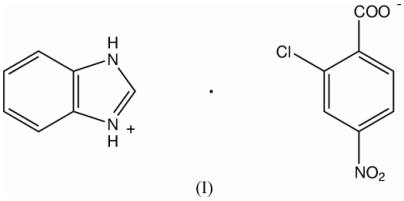
In the title compound, $C_7H_7N_2^+\cdot C_7H_3ClNO_4^-$, the cations and anions are connected by N—H···O hydrogen bonds to afford a 2_1 helical chain.

Comment

The title compound, (I), was investigated as part of a study on D—H···A hydrogen bonding (D = N, O or C; A = N, O or Cl) in chloro- and nitro-substituted benzoic acid-amine systems (Ishida *et al.*, 2001*a*,*b*,*c*,*d*,*e*). In the crystal, the cations and anions are held together by N—H···O hydrogen bonds (Table 2) and a weak C—H···π interaction [H10···*Cg* 2.93 (3) Å, C13···*Cg* 3.679 (3) Å, C13—H10···*Cg* 143.5 (19)°, where *Cg* denotes the centroid of the benzene ring C1–C6] (Fig. 1) to afford a 2_1 helical chain running along the *b* axis (Fig. 2). A similar helical chain is observed in imidazolium 2-chloro-4-nitrobenzoate, giving a chiral crystal (Ishida *et al.*, 2001*e*). The present salt, however, crystallizes in the centrosymmetric space group *C*2/*c*. Neighboring helical chains related by an inversion center are connected through C—H···O hydrogen bond (Fig. 2, Table 2), and those related by a twofold rotation axis are linked by a π–π stacking interaction between the aromatic rings C9–C14 of the benzimidazolium ion. The dihedral angle between the aromatic rings is 1.35 (11)°, and their interplanar separation and the centroid offset are 3.480 (2) and 0.769 (2) Å, respectively. The carboxyl group is twisted considerably out of the plane of the benzene ring, probably because of the strong N—H···O hydrogen bonds; the dihedral angle between them is 67.15 (13)°. This may cause a close contact of O1···N1^{iii}, 2.832 (3) Å [symmetry code: (iii) $1-x, 1-y, -z$], between two chains running in antiparallel directions. The N···O distance [2.610 (3) Å] in the N2—H4···O2 hydrogen bond is significantly shorter than the average N···O distance of 2.878 (3) Å for an N—H···O=C hydrogen bond (Taylor *et al.*, 1984).



(I)

Experimental

Crystals of (I) were obtained by slow evaporation from an aceto-nitrile solution of benzimidazole and 2-chloro-4-nitrobenzoic acid in a molar ratio of 1:1.

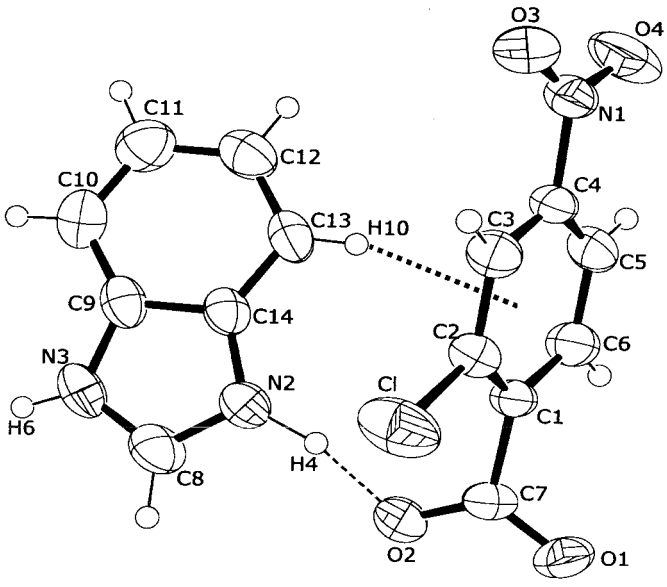


Figure 1
ORTEP-3 (Farrugia, 1997) drawing of (I), with the atom-labeling. Displacement ellipsoids of non-H atoms are drawn at the 50% probability level. The N—H···O hydrogen bond and C—H···π interaction are indicated by a dashed and a dotted line, respectively.

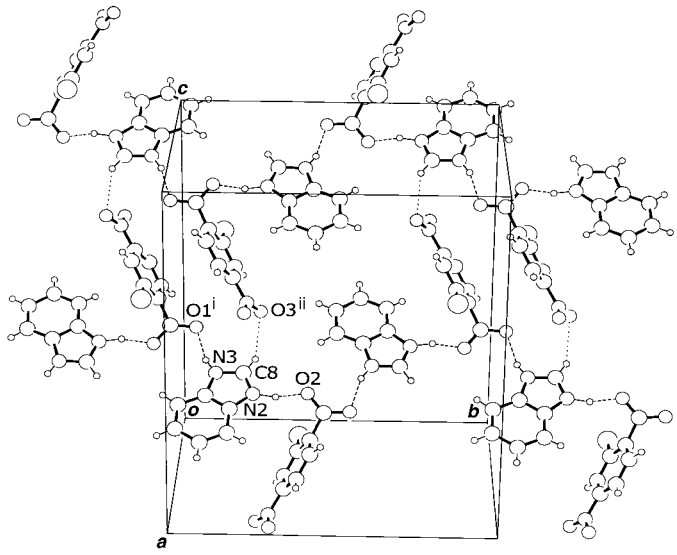


Figure 2
Packing diagram showing two 2_1 helical chains running in antiparallel directions along the *b* axis. N—H···O and C—H···O hydrogen bonds indicated by dashed and dotted lines, respectively [symmetry codes are as in Table 2].

Crystal data

$C_7H_7N_2^+\cdot C_7H_3ClNO_4^-$	D_x = 1.493 Mg m^{-3}
M_r = 319.70	Mo Kα radiation
Monoclinic, $C2/c$	Cell parameters from 25 reflections
a = 11.120 (3) Å	θ = 11.3–12.1°
b = 14.771 (3) Å	μ = 0.29 mm^{-1}
c = 17.414 (3) Å	T = 300 K
β = 95.963 (18)°	Prismatic, colorless
V = 2844.8 (11) Å^3	0.50 × 0.35 × 0.25 mm
Z = 8	

Data collection

Rigaku AFC-5*R* diffractometer	R_{int} = 0.025
ω–2θ scans	θ_{max} = 29.0°
Absorption correction: ψ scan (North *et al.*, 1968)	$h = -4 \rightarrow 14$
T_{min} = 0.876, T_{max} = 0.930	$k = -4 \rightarrow 19$
6914 measured reflections	$l = -23 \rightarrow 23$
3776 independent reflections	3 standard reflections every 97 reflections
2040 reflections with $I > 2\sigma(I)$	intensity decay: 0.8%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 1.4779P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.048	$(\Delta/\sigma)_{max}$ = 0.01
$wR(F^2)$ = 0.134	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
S = 1.00	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
3776 reflections	
239 parameters	
All H-atom parameters refined	

Table 1
Selected geometric parameters (Å).

Cl—C2	1.731 (2)	N2—C8	1.320 (3)
O1—C7	1.228 (3)	N2—C14	1.388 (3)
O2—C7	1.242 (3)	N3—C8	1.313 (4)
O3—N1	1.223 (3)	N3—C9	1.395 (3)
O4—N1	1.222 (3)	C1—C7	1.520 (3)
N1—C4	1.473 (3)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H4···O2	1.09 (3)	1.54 (3)	2.610 (3)	165 (3)
N3—H6···O1^{i}	0.85 (3)	1.84 (3)	2.654 (3)	160 (3)
C8—H5···O3^{ii}	0.98 (3)	2.54 (2)	3.395 (4)	146 (2)

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

H atoms were found in difference Fourier maps and refined isotropically. Refined distances: C—H = 0.88 (3) - 0.98 (3) Å and N—H = 0.86 (3) - 1.09 (3) Å.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1990); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *teXsan* for Windows (Molecular Structure Corporation, 1997–1999); program(s) used to solve structure: *SIR*92 (Altomare *et al.* 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *teXsan* for Windows.

X-ray measurements were made at the X-ray Laboratory of Okayama University.

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