Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Benzylammonium 3,5-dinitrobenzoate

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.040
wR factor = 0.106
Data-to-parameter ratio = 9.1

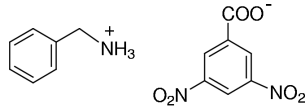
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 9 September 2004
Accepted 15 September 2004
Online 25 September 2004

In the title compound, $C_7H_{10}N^+\cdot C_7H_3N_2O_6^-$, the ammonium group of the cation and the carboxylate group of the anion are connected *via* hydrogen bonds, forming columns along the *b* axis.

Comment

Crystal structures of some charge-transfer complexes involving dopamine and its analogs as donors have been reported by us (Ohba & Ito, 2002*a*,*b*,*c*). The structure of the title compound, (I), has been determined to study the packing mode of the molecules and the hydrogen-bonding pattern.



(I)

The title compound consists of a benzylammonium cation and a dinitrobenzoate anion (Fig. 1). All three ammonium H atoms are involved in hydrogen bonds (Table 2) with the carboxylate O atoms. The ammonium and carboxylate groups are arranged around the 2_1 screw axis parallel to *b*, and connected *via* N—H···O hydrogen bonds, forming one-dimensional columns (Fig. 2).

Experimental

Benzylamine (934 mg, 8.63 mmol) and some MeOH were added to a hot solution of 3,5-dinitrobenzoic acid (1.867 g, 8.63 mmol) in EtOH (25 ml). The mixture was filtered and the filtrate was left for 4 d at

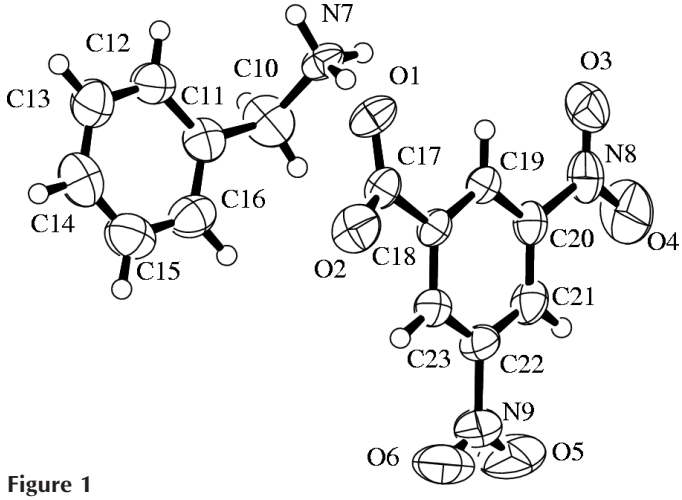


Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 50% probability level.

room temperature to obtain colourless crystals of (I) (yield 1.80 g, 65%; m.p. 459–464 K).

Crystal data

$C_7H_{10}N^+\cdot C_7H_3N_2O_6^-$
M_r = 319.27
Monoclinic, $P2_1$
a = 11.602 (3) Å
b = 6.2657 (12) Å
c = 10.898 (2) Å
β = 106.85 (2)°
V = 758.2 (3) Å^3
Z = 2
D_x = 1.398 Mg m^{-3}
Mo Kα radiation
Cell parameters from 25 reflections
θ = 10.1–12.6°
μ = 0.11 mm^{-1}
T = 298 K
Plate, colorless
0.6 × 0.5 × 0.2 mm

Data collection

Rigaku AFC-7*R* diffractometer
ω–2θ scans
Absorption correction: by integration (*ABSCOR*; Higashi, 1999)
T_{min} = 0.948, T_{max} = 0.978
2172 measured reflections
1900 independent reflections
1568 reflections with $I > 2\sigma(I)$
R_{int} = 0.014
θ_{max} = 27.5°
$h = -5 \rightarrow 15$
$k = -8 \rightarrow 3$
$l = -14 \rightarrow 14$
3 standard reflections
every 150 reflections
intensity decay: 0.5%

Refinement

Refinement on F^2
$R[F^2 > \sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.106
S = 1.08
1900 reflections
208 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0591P)^2 + 0.0545P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Table 1
Selected torsion angles (°).

O1—C17—C18—C19	17.1 (3)	O5—N9—C22—C21	−10.2 (4)
O3—N8—C20—C19	−0.4 (4)	N7—C10—C11—C12	57.8 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
N7—H7A···O1	0.95	1.83	2.774 (3)	171
N7—H7B···O2^{i}	0.95	1.81	2.715 (3)	158
N7—H7C···O1^{ii}	0.95	1.82	2.748 (2)	167

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

Friedel-pair reflections were merged before the final refinement, since anomalous scattering effects were negligible. The ammonium H atoms were located in difference syntheses and their positional parameters were recalculated geometrically (N—H = 0.95 Å). The other H atoms were positioned geometrically (C—H = 0.95 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(parent).

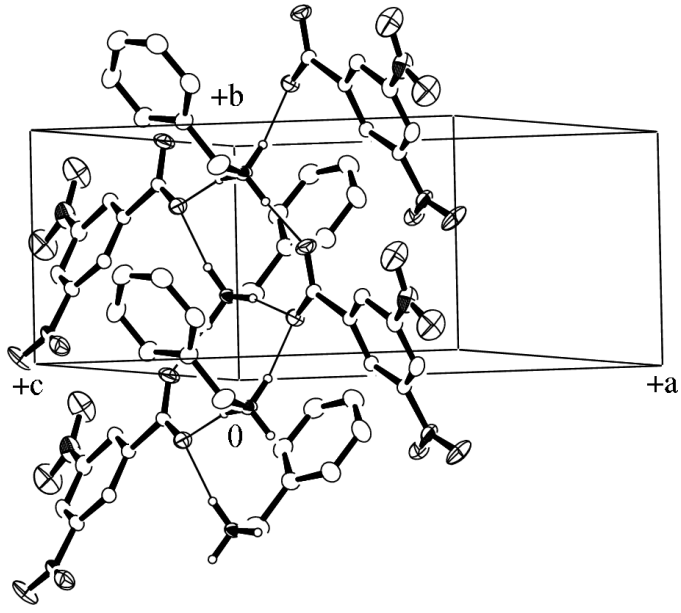


Figure 2
The hydrogen-bonded column running along the *b* axis. Thin lines indicate hydrogen bonds. H atoms bonded to C atoms have been omitted for clarity.

Data collection: *WinAFC Diffractometer Control Software* (Rigaku, 1999); cell refinement: *WinAFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 2001); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *TEXSAN*.

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