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Hexamethylenediammonium bis(3,5-dinitrobenzoate)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.053
wR factor = 0.146
Data-to-parameter ratio = 13.8

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

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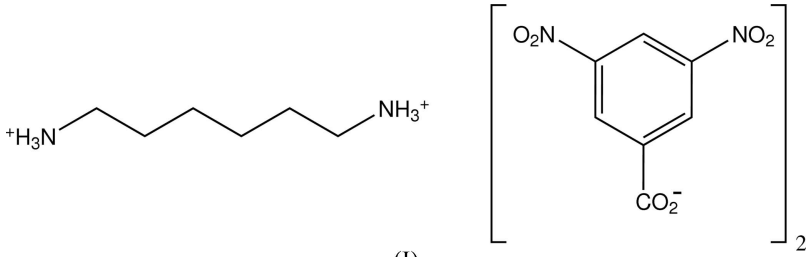
The title salt, $C_6H_{18}N_2^{2+}\cdot 2C_7H_3N_2O_6^-$, contains 3,5-dinitrobenzoate anions and hexamethylenediammonium dications, the latter lying on inversion centres. These ions interact by way of N—H···O hydrogen bonds.

Comment

We are investigating supramolecular interactions in aromatic salts and adducts. Here we have replaced saccharin (Wang *et al.*, 2006) with 3,5-dinitrobenzoic acid, resulting in the title compound, (I), in order to determine the effect of two strongly electron-withdrawing groups on the hydrogen-bond-accepting properties of the anion.



(I)

Compound (I) (Fig. 1) contains 3,5-dinitrobenzoate anions and hexamethylenediammonium dications, the latter lying on inversion centres, as in related compounds (Wang *et al.*, 2006). The carboxylate group of the anion appears to be delocalized on the basis of the C—O bond lengths (Table 1).

The component ions interact by way of N—H···O hydrogen bonds (Table 2), resulting in an infinite two-dimensional network propagating in (001) (Fig. 2).

Experimental

Hexamethylenediamine (1.0 mmol, 0.116 g) was added to an aqueous solution (25 ml) of 3,5-dinitrobenzoic acid (2.0 mmol, 0.420 g). The mixture was stirred for 10 minutes at 353 K. The solution was filtered, and the filtrate was allowed to stand at room temperature. After 5 d, colourless crystals of (I) were obtained.

Crystal data

$C_6H_{18}N_2^{2+}\cdot 2(C_7H_3N_2O_6^-)$
M_r = 540.45
Monoclinic, $P2_1/c$
a = 9.551 (3) Å
b = 6.1213 (19) Å
c = 20.847 (7) Å
β = 90.881 (6)°
V = 1218.7 (7) Å^3
Z = 2
D_x = 1.473 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 298 (2) K
Block, colourless
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.976, T_{max} = 0.988
8416 measured reflections
2394 independent reflections
1610 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.146
S = 1.05
2394 reflections
173 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0725P)^2 + 0.0778P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected bond lengths (Å).

C7—O1	1.250 (2)	C7—O2	1.254 (2)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O1^{i}	0.89	1.98	2.866 (2)	172
N3—H3*B*···O1^{ii}	0.89	1.97	2.859 (2)	174
N3—H3*C*···O2	0.89	1.84	2.724 (2)	173

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

All H atoms were positioned geometrically (C—H = 0.93–0.97 and N—H = 0.89 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(N).

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: *SHELXL97*.

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References

Bruker (2001). *SAINT-Plus* (Version 6.45) and *SMART* (Version 5.628). Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2001). *SADABS*. Version 2.10. Bruker AXS Inc., Madison, Wisconsin, USA.

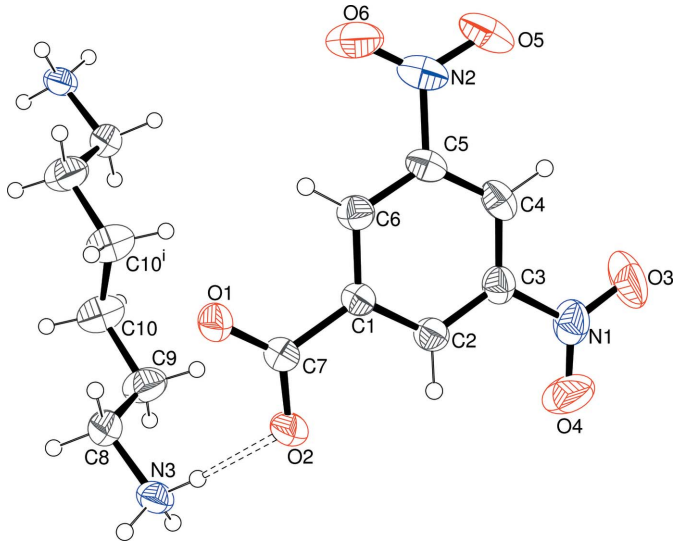

Figure 1
The molecular structure of (I), with displacement ellipsoids for non-H atoms drawn at the 40% probability level. The double dashed line indicates a hydrogen bond. [Symmetry code: (i) $1-x, 1-y, -z$.]

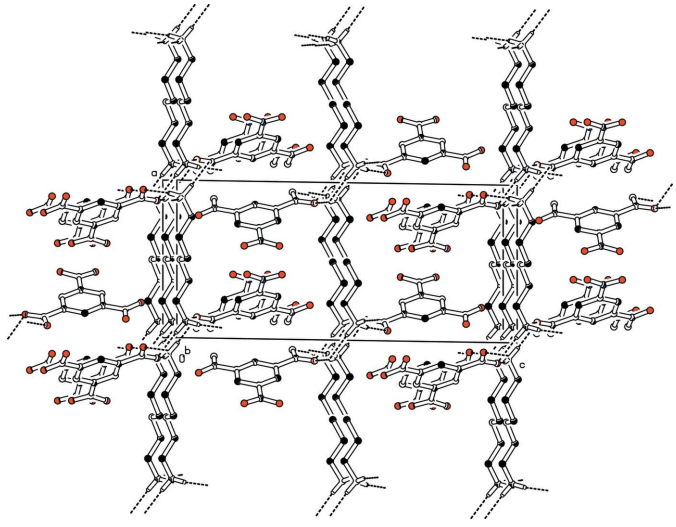

Figure 2
The crystal packing of (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines. For clarity, H atoms not involved in hydrogen bonds have been omitted.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Wang, Z.-L., Wei, L.-H., Li, M.-X. & Niu, J.-Y. (2006). *Acta Cryst.* E**62**, o1314–o1316.