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Piperazinium dinitrate

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Key indicators

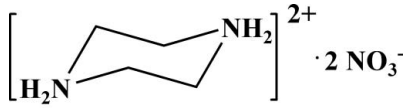
Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.003 Å
R factor = 0.034
wR factor = 0.090
Data-to-parameter ratio = 17.2

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

In the title compound, $C_4H_8N_2^{2+}\cdot 2NO_3^-$, the piperazinium dication has a centre of symmetry. The ions are linked by N—H···O hydrogen bonds into a chain.

Comment

Considerable progress has recently been made on the crystal engineering of supramolecular architectures organized and sustained by means of non-covalent supramolecular contacts (such as hydrogen bonds and π–π interactions), aurophilicity, and similar interactions (Colacio *et al.*, 2002; Roesky & Andruh, 2003; Guilera & Steed, 1999). Here, we report the crystal structure of piperazinium dinitrate, (I).



(I)

The asymmetric unit of (I) consists of one half of the piperizinium cation and one nitrate anion. As shown in Fig. 1, inversion symmetry generates the complete piperizinium cation, and the piperazinium ring in the crystal structure of (I) adopts a chair conformation.

As shown in Fig. 2, two O atoms of the nitrate anion act as hydrogen-bond acceptors and link two piperizinium cations *via* N—H···O hydrogen bonds (Table 1). The ions are thus linked into a double chain along the *b* axis.

Experimental

A mixture of $Zn(NO_3)_2\cdot 6H_2O$ (0.30 g, 1 mmol), piperazine (0.087 g, 1 mmol), succinic acid (0.18 g, 1 mmol) and water (18 ml) was sealed

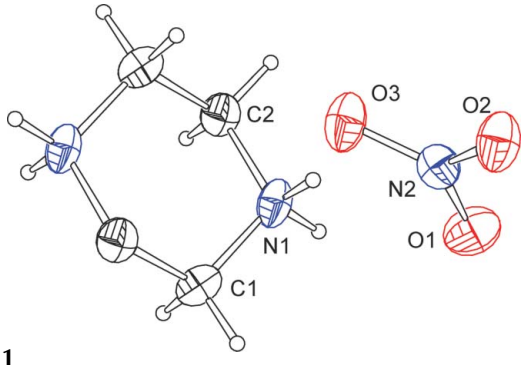


Figure 1
The cation and anion of the title compound, showing 30% probability displacement ellipsoids. [Symmetry code for unlabelled atoms: $\frac{1}{2}-x, \frac{1}{2}-y, -z$.]

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in a 25 ml Teflon-lined stainless steel reactor and heated at 433 K for 3 d. On completion of the reaction, the reactor was cooled slowly to room temperature and the mixture was filtered, giving colourless single crystals of (I) suitable for X-ray analysis.

Crystal data

$C_4H_{12}N_2^{2+}\cdot 2NO_3^-$
$M_r = 212.18$
Monoclinic, $C2/c$
$a = 14.6895\ (3)$ Å
$b = 5.9301\ (1)$ Å
$c = 12.4018\ (4)$ Å
$\beta = 120.956\ (1)^\circ$
$V = 926.44\ (4)$ Å^3
$Z = 4$
$D_x = 1.521$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.14$ mm^{-1}
$T = 273\ (2)$ K
Prism, colourless
0.30 × 0.20 × 0.06 mm

Data collection

Siemens SMART 1K CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.88$, $T_{max} = 1.00$
3535 measured reflections
1104 independent reflections
535 reflections with $I > 2\sigma(I)$
$R_{int} = 0.053$
$\theta_{max} = 28.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.090$
$S = 0.77$
1104 reflections
64 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0417P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O3	0.90	2.05	2.9025 (17)	158
N1—H1D···O2^{i}	0.90	2.01	2.8694 (17)	160

Symmetry code: (i) $x, y-1, z$.

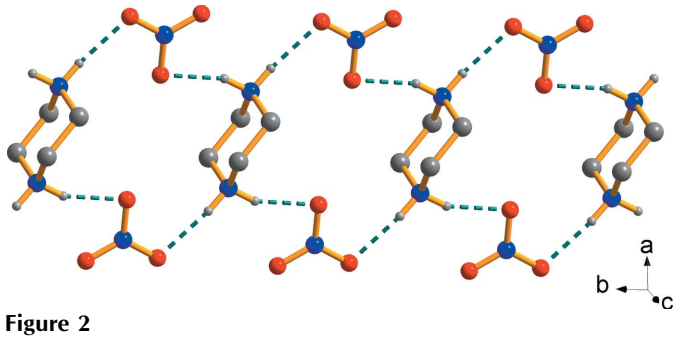

Figure 2
The double chain in the title compound. Hydrogen bonds are shown as dashed lines. C-bound H atoms have been omitted.

H atoms were placed at calculated positions and refined using a riding model, with C—H = 0.97 Å and N—H = 0.90 Å, and with $U_{iso}(H) = 1.2U_{eq}(C,N)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Bergerhoff *et al.*, 1996); software used to prepare material for publication: *SHELXL97*.

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