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4,4′-Bipyridinium dipicrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.035
wR factor = 0.098
Data-to-parameter ratio = 10.6

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

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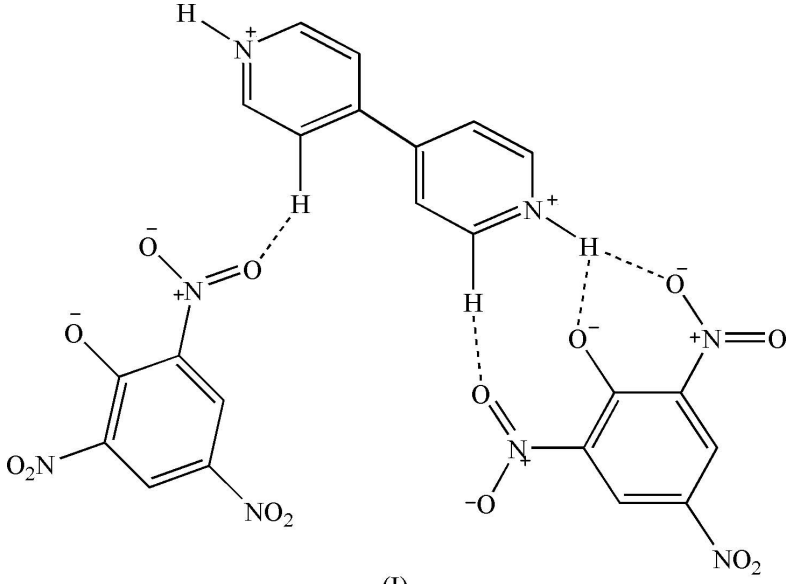
The asymmetric unit of the title compound, $C_{10}H_{10}N_2^{2+}\cdot 2C_6H_2N_3O_7^-$, comprises half of one 4,4′-bipyridinium cation and a picrate anion. The 4,4′-bipyridinium cation lies on an inversion center. The packing is governed by N—H···O and C—H···O hydrogen-bond interactions.

Comment

Intermolecular forces, such as hydrogen bonds and π–π stacking effects, play a dominant role in molecular aggregation (Hosseini & De Cian, 1998; Lehn, 1988; Tong *et al.*, 1998; Ghosh & Bharadwaj, 2004; Lu *et al.*, 2001). Of particular interest are compounds that are capable of forming very strong hydrogen bonds (Sun *et al.*, 2002*a*,*b*; Novak *et al.*, 1998). 4,4′–Bipyridine is an excellent rigid bridging ligand and liable to have some weak intermolecular interactions, such as hydrogen bonding, with other molecules (Zhu *et al.*, 2003; Liang *et al.*, 2001). Many structures involving the coordination of 4,4′-bipyridine to metals have been studied, but less studied are the non-covalent weak interactions of 4,4′-bipyridine with other molecules. In view of this, we report the molecular assembly of 4,4′-bipyridine and picric acid in order to further understand the coordination chemistry of 4,4′-bipyridine.



(I)

The asymmetric unit of 4,4′-bipyridinium dipicrate, (I), comprises half of one 4,4′-bipyridinium cation arranged around an inversion center and a picrate anion (Fig. 1). The transfer of two protons results in strong N—H···O hydrogen bonds between the cation and the anions (Fig. 1 and Table 1).

There are also weak C—H···O hydrogen-bond interactions (Table 1) which assure the cohesion of the crystal.

Cations and anions are arranged alternately in layers parallel to the *ab* plane (Fig. 2).

Experimental

An ethanol solution of 4,4′-bipyridine (0.0781 g, 0.5 mmol) was added dropwise to a stirred aqueous solution (12 ml) of picric acid (0.12 g, 0.5 mmol) at a temperature of 323 K. The reaction mixture was then filtered and the filtrate allowed to stand for about two weeks until yellow single crystals were obtained. Analysis found (%): C 43.04, H 2.23, N 18.30; calculated for $C_{22}H_{14}N_8O_{14}$ (%): C 42.97, H 2.28, N 18.23.

Crystal data

$C_{10}H_{10}N_2^{2+}\cdot 2C_6H_2N_3O_7^-$
M_r = 614.41
Triclinic, $P\overline{1}$
a = 5.369 (2) Å
b = 10.456 (4) Å
c = 11.357 (5) Å
α = 107.554 (5)°
β = 96.246 (5)°
γ = 94.581 (6)°
V = 600.0 (4) Å^3
Z = 1
D_x = 1.700 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 883 reflections
θ = 3.2–22.7°
μ = 0.15 mm^{-1}
T = 293 (2) K
Plate, yellow
0.32 × 0.22 × 0.08 mm

Data collection

Bruker SMART APEX-II CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.954, T_{max} = 0.991
3324 measured reflections
2119 independent reflections
1486 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 25.0°
$h = -5 \rightarrow 6$
$k = -12 \rightarrow 12$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.099
S = 1.06
2119 reflections
199 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.054P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.86	1.86	2.647 (2)	152
N1—H1···O7	0.86	2.49	3.097 (2)	128
C5—H5···O2	0.93	2.53	3.414 (3)	158
C1—H1A···O1^{i}	0.93	2.53	3.363 (2)	150
C2—H2···O6^{ii}	0.93	2.38	3.271 (3)	161
C5—H5···O4^{iii}	0.93	2.40	3.059 (3)	128

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

H atoms were positioned geometrically (N—H = 0.86 Å and C—H = 0.93 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *SHELXL97*.

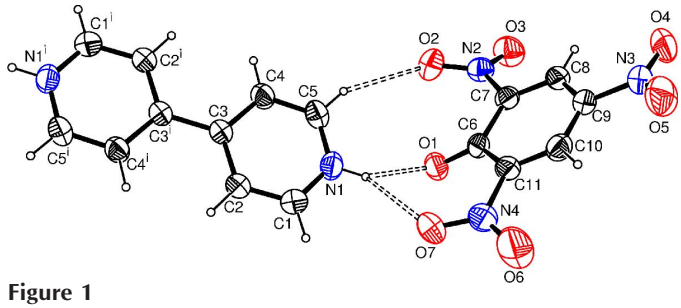


Figure 1
ORTEP-3 view (Farrugia, 1997) of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. N—H···O and C—H···O hydrogen bonds are indicated by dashed lines. [Symmetry code: (i) $-x, -y, -z$.]

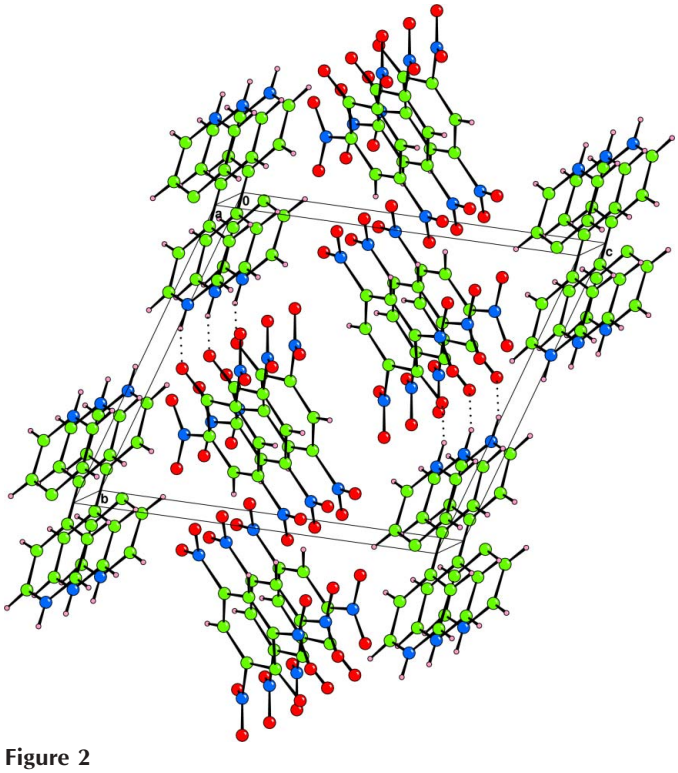


Figure 2
Packing diagram (*CAMERON*; Watkin *et al.*, 1993), showing the arrangement of cations and anions.

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