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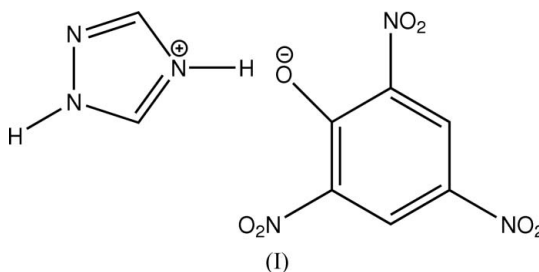
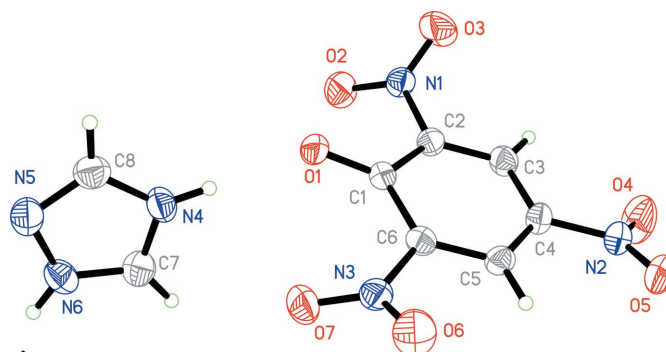
Key indicators

Single-crystal X-ray study
 $T = 292\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$
 R factor = 0.043
 wR factor = 0.110
Data-to-parameter ratio = 13.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

1,2,4-Triazolium picrate

In the title compound, $\text{C}_2\text{H}_4\text{N}_3^+\cdot\text{C}_6\text{H}_2\text{N}_3\text{O}_7^-$, the dihedral angle between the triazolium ring and the benzene ring of the picrate anion is $73.5(2)^\circ$.Received 10 September 2006
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Comment

Energetic materials are used extensively for both civilian and military applications (Sikder & Sikder, 2004). Ionic organic salts have recently emerged as a new class of energetic materials and have attracted considerable interest because of their 'green chemistry' properties (Singh *et al.*, 2006). Heterocyclic compounds such as triazoles, imidazoles and tetrazoles are readily quaternized and their salts, with a high nitrogen content, are good candidates for energetic ionic salts (Klapötke *et al.*, 2005). The title organic salt, (I) (Fig. 1), was therefore prepared by the reaction of 1,2,4-triazole with picric acid and its structure is reported here.The title compound consists of discrete picrate anions and 1,2,4-triazolium cations. Protonation of the 1,2,4-triazole ring occurred at N4. The dihedral angle between the triazolium ring and the benzene ring of the picrate anion is $73.5(2)^\circ$. In the crystal structure, intermolecular $\text{N}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds link the triazolium cations and picrate anions in a three-dimensional network (Fig. 2).

Experimental

1,2,4-Triazole (0.113 g, 1.6 mmol) and picric acid (0.373 g, 1.6 mmol) were dissolved in methanol (20 ml). The mixture was stirred for 10 h at room temperature and the solvent was removed under reduced pressure. The solid was washed with water (20 ml) and acetone (20 ml) to yield (I) as a dark-yellow solid. This was crystallized by slow evaporation of an acetonitrile solution (yield 453 mg, 95%; m.p. 442–444 K).

Crystal data

$C_2H_4N_3^+ \cdot C_6H_2N_3O_7^-$
 $M_r = 298.19$
 Monoclinic, $P2_1/n$
 $a = 7.2038$ (7) Å
 $b = 19.0535$ (19) Å
 $c = 8.2252$ (8) Å
 $\beta = 97.808$ (2)°
 $V = 1118.50$ (19) Å³
 $Z = 4$

$D_x = 1.771$ Mg m⁻³
 $D_m = 1.77$ Mg m⁻³
 D_m measured using a gas pycnometer
 Mo $K\alpha$ radiation
 $\mu = 0.16$ mm⁻¹
 $T = 292$ (2) K
 Block, yellow
 $0.30 \times 0.30 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{min} = 0.954$, $T_{max} = 0.969$

9729 measured reflections
 2556 independent reflections
 2055 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.043$
 $\theta_{max} = 27.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.110$
 $S = 1.06$
 2556 reflections
 196 parameters

H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0558P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 0.33$ e Å⁻³
 $\Delta\rho_{min} = -0.22$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$C8-H8 \cdots O2^i$	0.93	2.43	3.127 (2)	132
$C8-H8 \cdots O5^{ii}$	0.93	2.56	3.211 (2)	128
$C7-H7 \cdots O5^{iii}$	0.93	2.40	3.139 (2)	136
$C3-H3 \cdots O6^{iv}$	0.93	2.46	3.3920 (19)	175
$N6-H6 \cdots O1^v$	0.854 (9)	1.893 (10)	2.7459 (17)	177.5 (18)
$N4-H4 \cdots O1$	0.830 (9)	1.966 (10)	2.7830 (17)	168.2 (18)

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

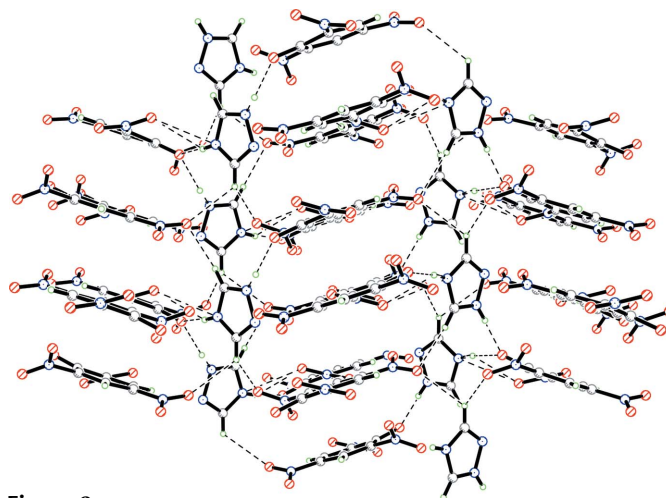


Figure 2
 A packing diagram for (I), with hydrogen bonds shown as dashed lines.

H atoms bound to N were located in a difference Fourier map and refined with $U_{iso}(H) = 1.2U_{eq}(N)$. All other H atoms were placed geometrically ($C-H = 0.93$ Å) and refined using a riding model, with $U_{iso} = 1.2U_{eq}(C)$.

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: SHELXTL (Bruker, 2001); software used to prepare material for publication: SHELXTL.

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