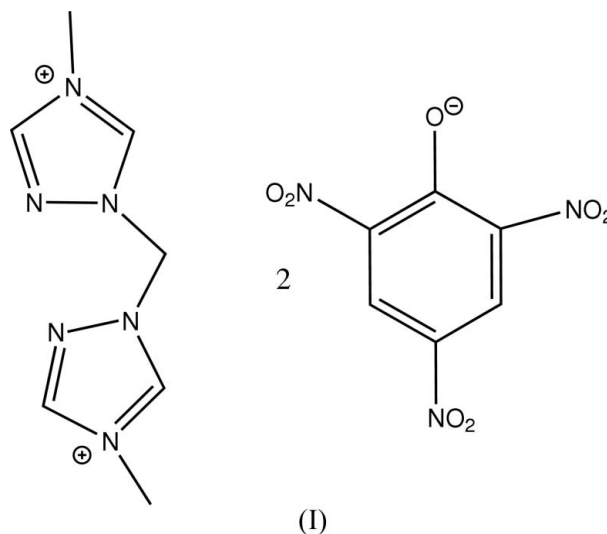# 1,1'-Methylenebis(4-methyl-1H-triazolium) dipicrate

Chuan-Ming Jin,* Cai-Yuan Chen, Wei-Dong Wang and Xin-Wan Zhou

Hubei Key Laboratory of Bioanalytic Techniques, Hubei Normal University, Huangshi 435002, People's Republic of China

Correspondence e-mail: jincm1999@yahoo.com

In the crystal structure of the title compound, $C_7H_{12}N_6^{2+} \cdot 2C_6H_2N_3O_7^-$, the asymmetric unit contains two picrate anions and one 1,1'-methylenebis(4-methyl-1H-triazolium) dication. The dihedral angle between the triazole rings of the dication is 76.1 (2)°,

Comment

Ionic liquids have attracted considerable interest as substitutes for volatile organic solvents in synthetic chemistry (Welton, 1999). Organic ionic salts with lower melting points, such as triazolium nitrate or perchlorate, are a new class of energetic materials because of their 'green chemistry' properties (Singh *et al.*, 2006). 1,2,4-Triazolium picrate has been reported as an energetic material (Jin *et al.*, 2006). In this report, we present the crystal structure of the title triazolium picrate, (I).

(I)

The asymmetric unit of (I) contains two picrate anions and one 1,1'-methylenebis(4-methyltriazolium) dication (Fig. 1). Within the dication, the dihedral angle between the triazole rings is 76.1 (2)°. Weak C—H···N hydrogen bonding occurs between dications, and weak C—H···O hydrogen bonding occurs between anions and dications (Table 1).

Experimental

Compound (I) was synthesized according to a literature method (Jin *et al.*, 2005). Single crystals were obtained by recrystallization from an acetonitrile solution.

Crystal data

$C_7H_{12}N_6{}^{2+} \cdot 2C_6H_2N_3O_7{}^-$
$M_r = 636.44$
Triclinic, $P\bar{1}$
$a = 7.0658$ (5) Å
$b = 8.8036$ (6) Å
$c = 20.5831$ (14) Å
$\alpha = 96.587$ (1)°
$\beta = 90.122$ (1)°
$\gamma = 94.255$ (1)°

$V = 1268.33$ (15) Å^3
$Z = 2$
$D_x = 1.666$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.14$ mm^{-1}
$T = 292$ (2) K
Block, yellow
$0.30 \times 0.20 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector
  diffractometer
φ and ω scans
Absorption correction: none
14366 measured reflections

5485 independent reflections
4435 reflections with $I > 2\sigma(I)$
$R_{int} = 0.046$
$\theta_{max} = 27.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.133$
$S = 1.08$
5485 reflections
408 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0674P)^2]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

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

D—H$\cdots$$A$	D—H	H$\cdots$$A$	$D$$\cdots$$A$	D—H$\cdots$$A$
C1—H1$B$$\cdots$O7^i	0.96	2.31	3.217 (3)	157
C2—H2$\cdots$O1^i	0.93	2.42	3.286 (2)	156
C3—H3$\cdots$O8	0.93	2.17	2.914 (2)	136
C3—H3$\cdots$O14	0.93	2.35	3.066 (2)	133
C4—H4$A$$\cdots$O8	0.97	2.41	3.091 (2)	127
C4—H4$A$$\cdots$O13^{ii}	0.97	2.53	3.211 (2)	127
C5—H5$\cdots$O2	0.93	2.39	2.911 (2)	115
C5—H5$\cdots$O8	0.93	2.48	3.138 (2)	127
C6—H6$\cdots$O1^{iii}	0.93	2.47	3.350 (2)	159
C6—H6$\cdots$O2^{iii}	0.93	2.41	3.042 (2)	125
C7—H7$A$$\cdots$N2^{iv}	0.96	2.62	3.467 (2)	148
C7—H7$C$$\cdots$O1	0.96	2.51	3.429 (3)	161

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

Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å, and the torsion angles were refined to fit the electron density, with $U_{iso}(H) = 1.5U_{eq}(C)$. Other H atoms were positioned geome-
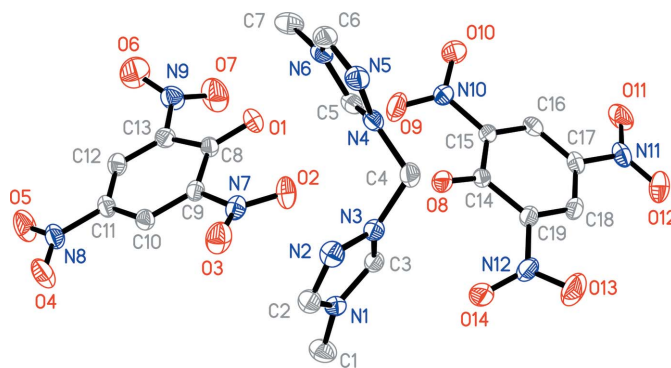

Figure 1
The asymmetric unit of (I), shown with 30% probability displacement ellipsoids. H atoms have been omitted for clarity.

trically, with C—H = 0.93 (aromatic) and 0.97 Å (methylene), and refined using a riding model with $U_{iso}(H) = 1.2U_{eq}(C)$.

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, 1997); software used to prepare material for publication: *SHELXTL*.

References

Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SAINT-Plus* (Version 6.45) and *SMART* (Version 5.628). Bruker AXS Inc., Madison, Wisconsin, USA.
Jin, C.-M., Wu, L.-Y., Chen, C.-Y. & Hu, S.-L. (2006). *Acta Cryst.* E**62**, o4515–o4516.
Jin, C.-M., Ye, C., Piekarski, C., Twamley, B. & Shreeve, J. M. (2005). *Eur. J. Inorg. Chem.* 3760–3767.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Singh, R. P., Verma, R. D., Meshri, D. T. & Shreeve, J. M. (2006). *Angew. Chem. Int. Ed.* **45**, 3584–3601.
Welton, T. (1999). *Chem. Rev.* **99**, 2071–2083.