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1,1′-Methylenebis(3-methylimidazolium) dipicrate

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.002 Å
R factor = 0.050
wR factor = 0.144
Data-to-parameter ratio = 13.6

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

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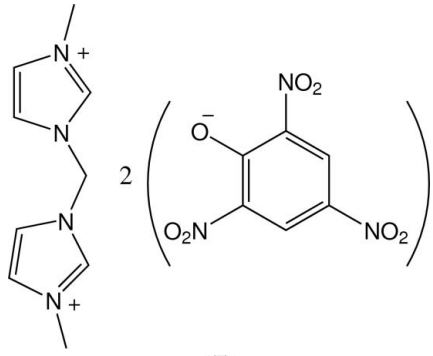
In the title compound, $C_9H_{12}N_4^{2+}\cdot 2C_6H_2N_3O_7^-$, the asymmetric unit contains two picrate anions and one 1,1′-methylene-bis(3-methylimidazolium) dication. The dihedral angle between the two imidazole rings in the dication is 74.1 (2)°, and the benzene rings of the two picrate anions are almost perpendicular, making a dihedral angle of 98.9 (1)°.

Comment

Ionic liquids have attracted considerable interest as substitutes for volatile organic solvents in synthetic chemistry (Welton, 1999). Imidazolium-based ionic liquids are well known. Ionic liquids with chelate or pincer dinuclear cations have been used extensively as reaction media due to their excellent physical and chemical properties (Jin, Twamley *et al.*, 2005). Organic picrate salts with their low melting points are a new class of energetic materials of interest because of their green chemistry properties (Singh *et al.*, 2006). Dinuclear cation picrate salts are good potential candidates for energetic ionic salts. The title organic salt, (I) (Fig. 1), was therefore prepared and its structure is reported here.



(I)

The asymmetric unit of the title compound contains two picrate anions and one 1,1′-methylenebis (3-methylimidazolium) dication. The dihedral angle between the two imidazole rings (N1,C2,N2,C4,C3 and N3,C6,N4,C8,C7) in the dication is 74.1 (2)°. The benzene rings of the two picrate anions (C10–C15 and C16–C21) are almost perpendicular, making a dihedral angle 98.9 (1)°. One imidazole ring (N3,C6,N4,C8,C7) in the dication is nearly parallel with one benzene ring (C10–C15) of a picrate anion with a dihedral angle of 0.8 (2)°, and it is perpendicular to the benzene ring in the other picrate anion (C16–C21) with a dihedral angle of 99.7 (2)°. Weak C—H···O intermolecular hydrogen bonds between the picrate anions and the zigzag dicationic chains are detailed in Table 1.

Experimental

The title molecule was synthesized by a literature method (or Jin, Ye *et al.*, 2005). It was crystallized by slow evaporation of an acetonitrile solution.

Crystal data

$C_9H_{14}N_4^{2+}\cdot 2C_6H_2N_3O_7^-$
M_r = 634.45
Triclinic, $P\overline{1}$
a = 7.8353 (7) Å
b = 12.8777 (12) Å
c = 13.2129 (12) Å
α = 83.522 (2)°
β = 79.288 (2)°
γ = 83.049 (2)°
V = 1294.7 (2) Å^3
Z = 2
D_x = 1.627 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 292 (2) K
Block, yellow
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.959, T_{max} = 0.973
11622 measured reflections
5542 independent reflections
4475 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 27.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.144
S = 1.05
5542 reflections
408 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0784P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O11^{i}	0.93	2.36	3.074 (2)	134
C2—H2···O12^{i}	0.93	2.36	2.986 (2)	124
C5—H5*B*···O12^{i}	0.97	2.27	2.997 (2)	131
C7—H7···O7^{i}	0.93	2.41	3.256 (2)	151
C7—H7···O12^{i}	0.93	2.37	3.073 (2)	132
C8—H8···O6^{i}	0.93	2.53	3.205 (2)	129
C3—H3···O9^{ii}	0.93	2.55	3.403 (2)	153
C4—H4···O1^{iii}	0.93	2.46	3.210 (3)	138
C5—H5*A*···O3^{iii}	0.97	2.45	3.252 (2)	140
C6—H6···O3^{iii}	0.93	2.16	2.9494 (19)	142
C9—H9*C*···O4^{iii}	0.96	2.50	3.334 (2)	146
C21—H21···O10^{iv}	0.93	2.57	3.189 (2)	124

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

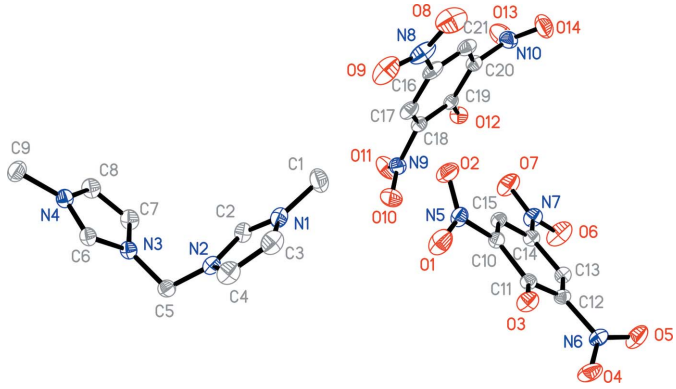


Figure 1
The asymmetric unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted.

H atoms were positioned geometrically [C—H = 0.93 (CH), 0.97 (CH_2) and 0.96 Å (CH_3)] and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl 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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