Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Mepazinium picrate

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.036
wR factor = 0.097
Data-to-parameter ratio = 13.4

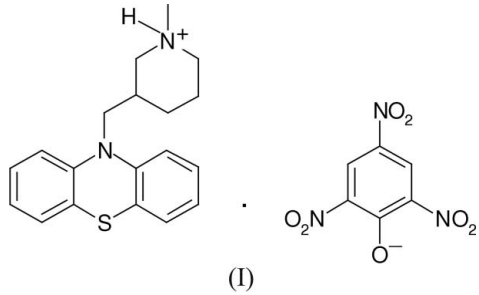
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 23 February 2007
Accepted 1 March 2007

The title compound [systematic name: 1-methyl-3-(10*H*-phenothiazin-10-ylmethyl)piperidinium 2,4,6-trinitrophenolate], $C_{19}H_{23}N_2S^+\cdot C_6H_2N_3O_7^-$, is a pharmacologically active compound. The dihedral angle between the two outer aromatic rings of the phenothiazine unit is 41.58 (7)°. The crystal packing is stabilized by N—H···O hydrogen bonds and several weak C—H···O contacts.

Comment

Mepazine, chemically 10-[(1-methyl-3-piperidyl)methyl]-10*H*-phenothiazine, is an antipsychotic drug (Tedeschi *et al.*, 1958). In continuation of our work on the crystallization of phenothiazine drugs with picrate (Yathirajan *et al.*, 2007), we present here the formation of a salt by the interaction between 10-[(1-methyl-3-piperidyl)methyl]-10*H*-phenothiazine hydrochloride and 2,4,6-trinitrophenol in an aqueous medium.



(I)

A perspective view of the structure of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.28, November 2006; Allen, 2002; *Mogul*, Version 1.1; Bruno *et al.*, 2004). The

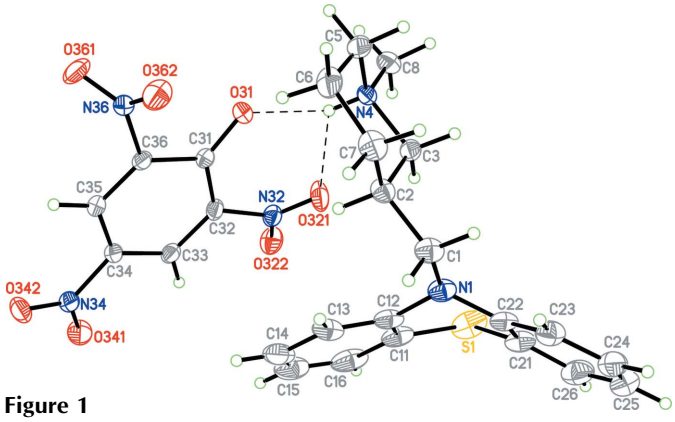


Figure 1
The molecular structure of the title compound with the atom numbering. Displacement ellipsoids are drawn at the 30% probability level. Dashed lines indicate hydrogen bonds.

dihedral angle between the two aromatic rings of the phenothiazine unit is 41.58 (7)°. The piperidyl ring adopts a chair conformation with both substituents in equatorial positions. The crystal packing is stabilized by N—H···O hydrogen bonds and several weak C—H···O contacts (Table 1).

Experimental

Mepazine hydrochloride monohydrate (0.7300 g, 0.02 *M*) and picric acid (0.4606 g, 0.02 *M*) were dissolved separately in doubly distilled water (100 ml). The solutions were mixed and stirred in a beaker. A bright-yellow salt was formed instantaneously at room temperature. The separated salt was filtered off, washed thoroughly with doubly distilled water and dried in a vacuum desiccator over phosphorus pentoxide. The compound was recrystallized from ethanol (m.p. 379 K).

Crystal data

$C_{19}H_{23}N_2S^+\cdot C_6H_2N_3O_7^-$
M_r = 539.56
Triclinic, $P\overline{1}$
a = 8.3584 (9) Å
b = 10.7782 (9) Å
c = 14.5062 (13) Å
α = 93.524 (7)°
β = 99.629 (8)°
γ = 102.419 (7)°
V = 1251.8 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 173 (2) K
0.45 × 0.45 × 0.40 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.911, T_{max} = 0.920
12751 measured reflections
4656 independent reflections
3824 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.098
S = 1.03
4656 reflections
348 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···O31	0.89 (2)	1.84 (2)	2.6879 (17)	158.2 (19)
N4—H4···O321	0.89 (2)	2.46 (2)	3.0191 (17)	121.8 (16)
C3—H3*B*···O321	0.99	2.50	3.0790 (19)	117
C5—H5*B*···O342^{i}	0.99	2.50	3.409 (2)	152
C6—H6*A*···O362	0.99	2.47	3.419 (2)	160
C6—H6*B*···O341^{ii}	0.99	2.56	3.4229 (19)	146
C35—H35···O322^{iii}	0.95	2.52	3.4568 (19)	168

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

H atoms were found in a difference map. The H atom bonded to nitrogen was refined freely and all other H atoms were refined using a riding model, with C—H = 0.95–0.99 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

MAA thanks the University of Mysore for research facilities.

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