# organic compounds

# 1-Amino-2-nitraminoethane

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The molecule of title compound, $C_2H_7N_3O_2$, has a zwitterionic structure. All non-H atoms, apart from the terminal N atom of the $NH_3$ group, lie in the same plane, with a maximum deviation of 0.056 (1) Å for the amine N atom of the nitramine group, whereas the deviation of the terminal N atom of the $NH_3$ group from the same plane is 1.222 (2) Å. Intermolecular hydrogen bonds within the crystal form a three-dimensional network.

## Comment

Aminonitramines are of interest as biologically active non-protein amino acids (Alston *et al.*, 1981; Nilssen *et al.*, 1983) and as a new class of energetic compounds (Astachov *et al.*, 2000*a*). The zwitterionic nature of aminonitramines was established on the basis of indirect physical and chemical investigations by McKay *et al.* (1954). We present here the X-ray structure determination of 1-amino-2-nitraminoethane, (I), which belongs to the same class of compounds.

$$H_3\overset{+}{N}-CH_2-CH_2-\overset{-}{N}-NO_2$$

(I)
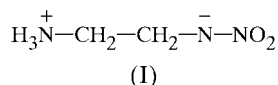
The present study unambiguously confirms the zwitterionic structure of (I). Fig. 1 provides a view of the crystal packing with the atom-numbering scheme; selected molecular bond lengths and angles are given in Table 1. The C2—N3 bond length is in accord with that of various salts of organic amines (1.474–1.480 Å; Allen & Kennard, 1993; George *et al.*, 1991; Burgess *et al.*, 1991). The N—N bond of the nitramine moiety is shorter and the N—O bonds are longer than the corresponding values in primary nitramines (N—N = 1.301 Å and N—O = 1.236 and 1.240 Å in 1,2-dinitraminoethane; Turley, 1968). Overall, the bond lengths in the nitramine fragment of (I) are close to the values characteristic of onium salts of primary nitramines (N—N = 1.273 Å and N—O 1.283 Å in the

dihydrazinium salt of 1,2-dinitraminoethane; Allen & Kennard, 1993; Bircher *et al.*, 1996).

In the structure of (I), atom O1 forms two short hydrogen bonds with atoms H6 and H7 of two neighbouring molecules. The second oxygen, O2, is not involved in any hydrogen-bonding contacts. As a consequence, there is a significant difference in the N—O bond lengths in (I) compared with
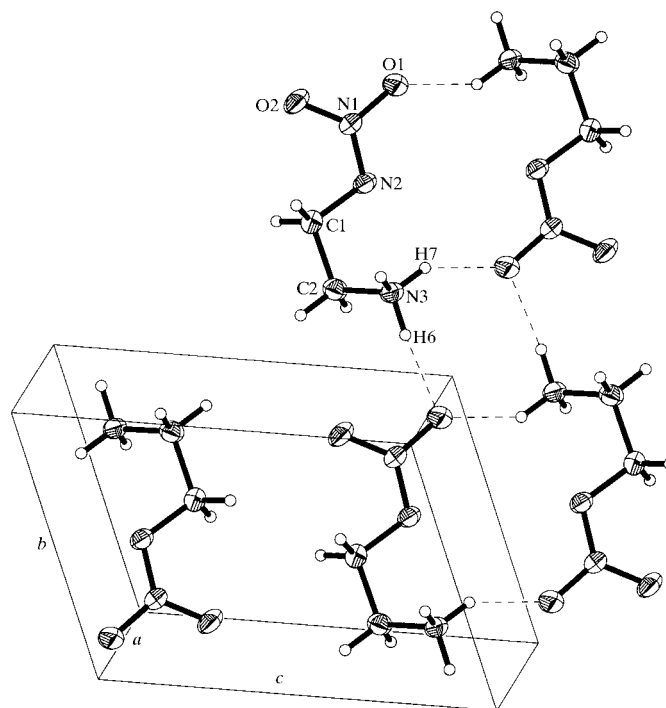


**Figure 1**
The molecular arrangement of (I) in the crystal, with the atomic numbering scheme and 50% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii and dashed lines indicate intermolecular hydrogen bonds.

both 1,2-dinitraminoethane (Turley, 1968) and its dihydrazine salt (Bircher *et al.*, 1996). An intermolecular N3—H5···N2 hydrogen bond (Table 2) completes the picture of molecular packing.

From the established bond-length values, it is difficult to fix the negative charge unambiguously on any atom of the nitramine part of the molecule. By analogy with salts of primary nitramines (Avakyan, 1971), the anion charge is rather delocalized over the whole nitramine fragment, but the electron density is distributed unevenly; the negative charge on atom O1 exceeds that on atoms N2 and O2.

In conclusion, the zwitterionic structure of aminonitramines, and of (I) in particular, leads to an increase in intermolecular interaction (crystal lattice energy) and, as a consequence, to an increase in thermal stability and the density of the compounds in comparison with the primary nitramines (Astachov *et al.*, 2000*a*; Astachov, 1999).

## Experimental

Compound (I) was synthesized as described by Astachov *et al.* (2000*b*).

### Crystal data

$C_2H_7N_3O_2$
$M_r = 105.11$
Triclinic, $P\bar{1}$
$a = 4.3449 (2)$ Å
$b = 6.2955 (3)$ Å
$c = 8.5432 (5)$ Å
$\alpha = 105.240 (5)°$
$\beta = 92.743 (4)°$
$\gamma = 96.356 (4)°$
$V = 223.36 (2)$ Å$^3$

$Z = 2$
$D_x = 1.563$ Mg m$^{-3}$
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 27–35°$
$\mu = 1.17$ mm$^{-1}$
$T = 293 (2)$ K
Lump, colourless
$0.36 \times 0.32 \times 0.27$ mm

### Data collection

Kuma KM-4 diffractometer
$\theta/2\theta$ scans
814 measured reflections
756 independent reflections
685 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 64.8°$

$h = -5 \rightarrow 5$
$k = -7 \rightarrow 7$
$l = 0 \rightarrow 9$
2 standard reflections
  every 40 reflections
  intensity variation: 0.4%

### Refinement

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.082$
$S = 1.02$
756 reflections
67 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 0.0467P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.21$ e Å$^{-3}$
$\Delta\rho_{min} = -0.14$ e Å$^{-3}$
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.135 (10)

### Table 1
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| N1—O2 | 1.2571 (14) | N2—C1 | 1.4551 (16) |
| N1—N2 | 1.2794 (15) | C1—C2 | 1.5136 (17) |
| N1—O1 | 1.2942 (14) | C2—N3 | 1.4794 (16) |
| O2—N1—N2 | 124.29 (10) | N1—N2—C1 | 112.56 (10) |
| O2—N1—O1 | 118.17 (10) | N2—C1—C2 | 108.58 (10) |
| N2—N1—O1 | 117.53 (10) | N3—C2—C1 | 112.00 (10) |
| O2—N1—N2—C1 | 2.25 (16) | N1—N2—C1—C2 | 173.66 (10) |
| O1—N1—N2—C1 | −178.19 (9) | N2—C1—C2—N3 | −55.64 (13) |

H atoms were located on a difference Fourier map and refined as riding, with a common isotropic displacement parameter of 0.032 Å$^2$ for CH$_2$ groups and 0.039 Å$^2$ for the NH$_3$ group. C—H distances were constrained to 0.97 Å and N—H distances to 0.94 Å.

### Table 2
Hydrogen-bonding geometry (Å, °).

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| N3—H5$\cdots$N2$^i$ | 0.94 | 2.09 | 2.976 (2) | 159 |
| N3—H6$\cdots$O1$^{ii}$ | 0.94 | 1.92 | 2.822 (2) | 163 |
| N3—H7$\cdots$O1$^{iii}$ | 0.94 | 2.00 | 2.832 (2) | 147 |

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

Data collection: *KM*-4 *Software* (Kuma, 1991); cell refinement: *KM*-4 *Software*; data reduction: *DATARED* in *KM*-4 *Software*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1995); software used to prepare material for publication: *SHELXL*97.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: AV1081). Services for accessing these data are described at the back of the journal.

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