Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

2-Aminopyridinium–succinate–succinic acid (2/1/1)

Orhan Büyükgüngör[a]* and Mustafa Odabaşoğlu[b]

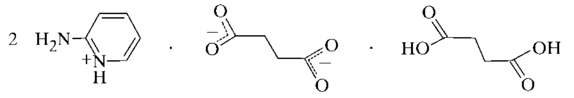
[a]Department of Physics, Ondokuz Mayıs University, TR-55139, Samsun, Turkey, and [b]Department of Chemistry, Ondokuz Mayıs University, TR-55139, Samsun, Turkey
Correspondence e-mail: orhanb@omu.edu.tr

Received 19 July 2002
Accepted 30 September 2002
Online 31 October 2002

In the title compound, $2C_5H_7N_2^{+}\cdot C_4H_4O_4^{2-}\cdot C_4H_6O_4$, cyclic eight-membered hydrogen-bonded rings exist involving 2-aminopyridinium and succinate ions. The succinic acid and succinate moieties lie on inversion centres. Succinic acid molecules and succinate ions are linked into zigzag chains by O—H···O hydrogen bonds, with O···O distances of 2.6005 (16) Å.

Comment

Hydrogen bonding plays a key role in molecular recognition (Goswami & Ghosh, 1997) and crystal engineering research (Goswami *et al.*, 1998). The design of highly specific solid-state structures is of considerable significance in organic chemistry, due to their important applications in the development of new optical, magnetic and electronic systems (Lehn, 1990). Our investigation of the title compound, (I), shows that the 2-aminopyridinium ions are linked to the succinate ions through N1—H···O3 and N2—H2N*A*···O4 hydrogen bonds, resulting in the formation of cyclic eight-membered hydrogen-bonded rings.



(I)

Each amino H atom in (I) is involved in a single hydrogen bond, one in the cyclic eight-membered hydrogen-bonded ring system and the other to another succinate ion (Fig. 1). The 2-aminopyridinium–succinate–succinic acid units are arranged so that a two-dimensional network of intermolecular N2—H2N*B*···O4 and O2—H6···O3 hydrogen bonds exists on each nearly perpendicular 2-aminopyridinium–succinate–succinic acid unit [dihedral angle = 84.34 (8)°] (Fig. 2).

2-Aminopyridine, like other organic bases, is protonated in acidic solutions. The bonding of the H atom to the ring N atom of 2-aminopyridine, but not to the amino N atom, gives an ion for which an additional resonance structure can be written. As this monocation has more resonance energy (additional ionic resonance) than 2-aminopyridine itself, 2-aminopyridine is a strong base, like amidines (Acheson, 1967).

The present investigation clearly shows that the positive charge in (I) is on the amino group in the crystal. The C1—N2 bond length is 1.3272 (19) Å, and this is approximately equal to a previously reported C═N double-bond length (Shanmuga Sundara Raj, Fun, Lu *et al.*, 2000). The location of the positive charge on the amino group is also supported by the C1—N2—H2N*A* angle of 118.4 (11)° and by the fact that atoms C1, N2, H2N*A* and H2N*B* lie in the pyridine plane, with a maximum deviation of 0.04 (2) Å for atom H2N*B*. Similar C1—N2 bond lengths have also been observed in other 2-aminopyridine-containing molecules (Yang *et al.*, 1995; Grobelny *et al.*, 1995; Shanmuga Sundara Raj, Fun, Zhao *et al.*, 2000).

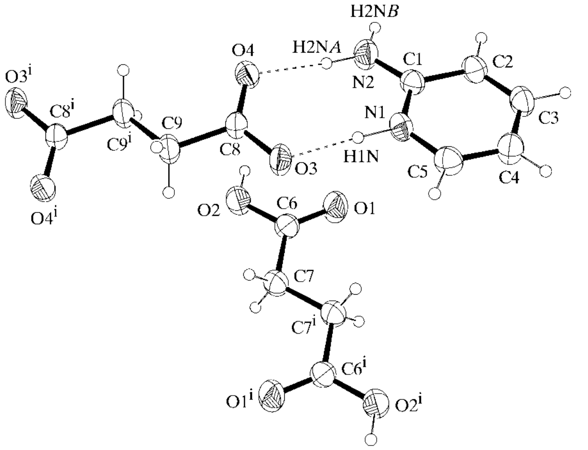


Figure 1
A view of the three moieties of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii [symmetry codes: (i) $-x, -y, -z$].

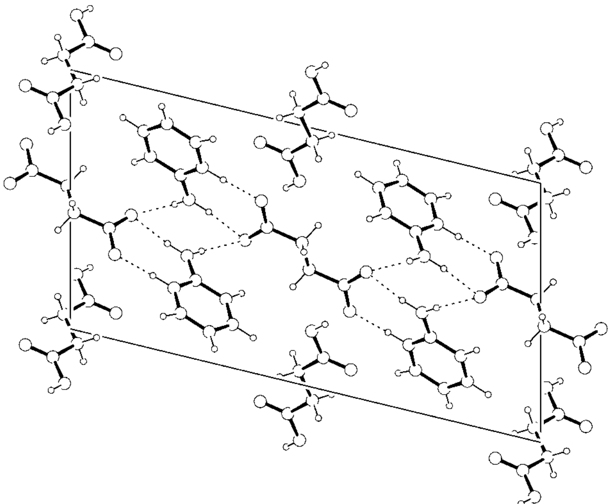


Figure 2
A packing diagram for (I), viewed along the *b* axis.

DOI: 10.1107/S0108270102017808

Experimental

The title compound was prepared by mixing 2-aminopyridine and succinic acid in a 1:1 molar ratio in water at 353 K. Crystals of (I) were obtained by slow evaporation of the solvent.

Crystal data

$2C_5H_7N_2^+\cdot C_4H_4O_4^{2-}\cdot C_4H_6O_4$
$M_r = 424.41$
Monoclinic, $P2_1/c$
$a = 10.228\ (2)$ Å
$b = 5.1840\ (10)$ Å
$c = 19.047\ (4)$ Å
$\beta = 103.60\ (3)^\circ$
$V = 981.6\ (4)$ Å^3
$Z = 2$
$D_x = 1.436$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 35 reflections
$\theta = 5$–25°
$\mu = 0.11$ mm^{-1}
$T = 153\ (2)$ K
Rectangular, light yellow
$0.3 \times 0.2 \times 0.2$ mm

Data collection

Siemens *P*4 diffractometer
ω scans
2362 measured reflections
2362 independent reflections
1690 reflections with $I > 2\sigma(I)$
$\theta_{\max} = 28^\circ$
$h = -13 \rightarrow 13$
$k = 0 \rightarrow 6$
$l = 0 \rightarrow 25$
1 standard reflection
  frequency: 120 min
  intensity decay: none

Table 1
Selected geometric parameters (Å, °).

C1—N2	1.3272 (19)	O2—C6	1.3123 (17)
C1—N1	1.3500 (18)	O3—C8	1.2747 (16)
N1—C5	1.3578 (19)	O4—C8	1.2413 (16)
O1—C6	1.2038 (17)		
O1—C6—O2	123.44 (14)	O4—C8—O3	122.95 (12)
N2—C1—N1—C5	178.53 (14)	O4—C8—C9—C9^{ii}	11.1 (3)
O1—C6—C7—C7^{i}	2.6 (3)	O3—C8—C9—C9^{ii}	−169.72 (18)
O2—C6—C7—C7^{i}	−177.09 (18)		

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1N$\cdots$O3	0.969 (18)	1.751 (18)	2.7185 (16)	176.0 (17)
N2—H2N$A\cdots$O4	0.929 (18)	1.936 (19)	2.8521 (18)	168.2 (16)
N2—H2N$B\cdots$O4^{i}	0.84 (2)	2.11 (2)	2.9447 (19)	167.7 (17)
O2—H6$\cdots$O3^{ii}	0.89 (2)	1.72 (2)	2.6005 (16)	178 (2)

Symmetry codes: (i) $1-x, y-\frac{1}{2}, \frac{3}{2}-z$; (ii) $x, y-1, z$.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.104$
$S = 1.02$
2362 reflections
185 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0496P)^2 + 0.0805P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.29$ e Å^{-3}
$\Delta\rho_{\min} = -0.19$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.015 (3)

All H-atom parameters were freely refined, with C—H distances in the range 0.92 (2)–0.982 (15) Å and $U_{\rm iso}$(H) values in the range 0.039 (4)–0.075 (6) Å^2.

Data collection: *XSCANS* (Siemens, 1991); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Bruker, 2001); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1997).

The authors wish to thank Professor Dr D. Fenske for the opportunity to use the diffractometer and computer facilities of the Institut für Anorganishe Chemie der Universität Karlsruhe, Germany, and Dr G. Helmut for his kind assistance during data handling.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: FR1391). Services for accessing these data are described at the back of the journal.

References

Acheson, R. M. (1967). *An Introduction to the Chemistry of Heterocyclic Compounds*, 2nd ed., pp. 215–218. London: Wiley.
Bruker (2001). *SHELXTL*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
Burnett, M. N. & Johnson, C. K. (1996). *ORTEP*III. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
Farrugia, L. J. (1997). *WinGX*. 16-bit Version. University of Glasgow, Scotland.
Goswami, S. P. & Ghosh, K. (1997). *Tetrahedron Lett.* **38**, 4503–4506.
Goswami, S. P., Mahapatra, A. K., Nigam, G. D., Chinnakali, K. & Fun, H.-K. (1998). *Acta Cryst.* C**54**, 1301–1302.
Grobelny, R., Glowiak, T., Mrozinski, J., Baran, W. & Tomasik, P. (1995). *Pol. J. Chem.* **69**, 559–565.
Lehn, J. M. (1990). *Angew. Chem. Int. Ed. Engl.* **29**, 1304–1311.
Shanmuga Sundara Raj, S., Fun, H.-K., Lu, Z.-L., Xiao, W., Gong, X.-Y. & Gen, C.-M. (2000). *Acta Cryst.* C**56**, 1015–1016.
Shanmuga Sundara Raj, S., Fun, H.-K., Zhao, P.-S., Jian, F.-F., Lu, L.-D., Yang, X.-J. & Wang, X. (2000). *Acta Cryst.* C**56**, 742–743.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Siemens (1991). *XSCANS User's Manual*. Version 2.10b. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Yang, R. N., Wang, D. M., Hou, Y. M., Xue, B. Y., Jin, D. M., Chen, L. R. & Luo, B. S. (1995). *Acta Chem. Scand.* **49**, 771–773.