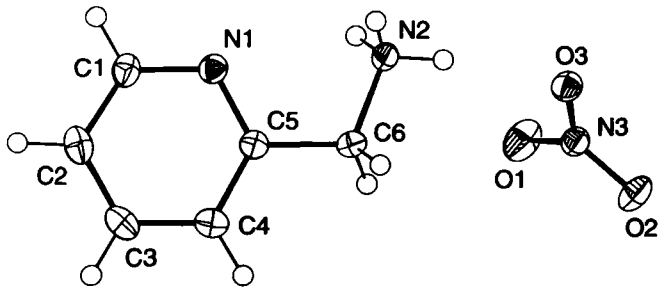
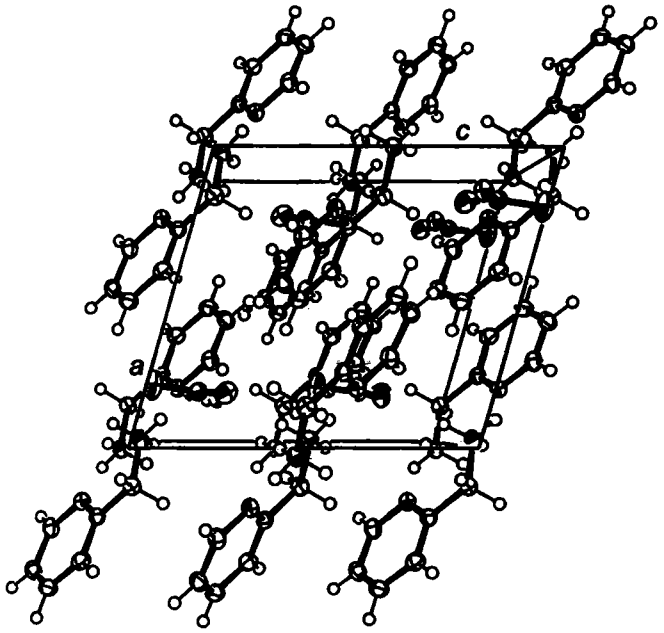
Crystal structure of pyridyl-2-methylammonium nitrate, $(C_6H_9N_2)NO_3$

A. R. Mahjoub*, A. Morsali* and S. Nouryan Aval

Tarbiat Modarres University, School of Science, Department of Chemistry, P.O. Box 14155-4838, Tehran, I. R. Iran

Received October 26, 2004, accepted and available on-line January 10, 2005; CCDC no. 1267/1420





Abstract

$C_6H_9N_3O_3$, monoclinic, $P12_1/c1$ (no. 14), $a = 8.234(2)$ Å, $b = 10.421(2)$ Å, $c = 9.395(2)$ Å, $\beta = 105.366(3)°$, $V = 777.3$ Å^3, $Z = 4$, $R_{gt}(F) = 0.044$, $wR_{ref}(F^2) = 0.097$, $T = 120$ K.

Source of material

A methanolic solution of 2-aminomethylpyridine (2 mmol) was added to an aqueous solution of the bismuth(III) nitrate (1 mmol). The resulting solution was concentrated on water bath and cooled to room temperature, when white crystals were separated. These were filtered off, washed with cold ethanol and dried over silica gel. Elemental analysis: found – C, 41.75 %; H, 5.60 %; N, 24.30 %; calc. for $C_6H_9N_3O_3$ – C, 42.10 %; H, 5.20 %; N, 24.56 %.

* Correspondence authors (e-mail: mahjouba@net1cs.modares.ac.ir; morsali_a@yahoo.com)

Discussion

For electrical conductivity, magnetic properties, or non-linear optical properties in molecular crystals, not only the electronic properties of molecules themselves, but also the molecular arrangements in the crystals are very important. Therefore, the design of crystal structures and control of molecular arrangements has attracted much attention in recent years. In this paper we show the nature of adducts formed between 2-aminomethylpyridine (AMP) and nitric acid.

The title structure consists of discrete $[AMPH]^+$ cations and NO_3^- anions (figure, top). The cation may be considered as an adduct of 2-aminopyridine and H^+. The hydrogen ion bonds to aliphatic nitrogen atom. There is aromatic-aromatic interaction [1,2] between the parallel aromatic rings belonging to adjacent chains (figure, bottom). The planar species, in which the mean molecular planes are close to parallel, are separated by a distance of about 3.5 Å, close to that of the layers in graphite.

Table 1. Data collection and handling.

Crystal:	colorless prism, size 0.22 × 0.28 × 0.30 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	1.19 cm^{-1}
Diffractometer, scan mode:	Bruker SMART 1000 CCD, φ/ω
$2\theta_{max}$:	56°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	7477, 1840
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1529
$N(param)_{refined}$:	110
Programs:	SHELXL-97 [3], SHELXTL [4]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(2A)	4e	1.0751	0.6616	0.0701	0.024
H(2B)	4e	1.0909	0.7189	–0.0705	0.024
H(2C)	4e	1.0001	0.5954	–0.0722	0.024
H(1)	4e	0.7337	0.4255	0.2173	0.029
H(2)	4e	0.4864	0.5167	0.2432	0.032
H(3)	4e	0.4022	0.7179	0.1343	0.032
H(4)	4e	0.5739	0.8208	0.0044	0.029
H(6A)	4e	0.8027	0.7513	–0.1480	0.026
H(6B)	4e	0.8890	0.8321	–0.0026	0.026

Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(1)	4*e*	0.7999(2)	0.5639(1)	0.0989(1)	0.0240(6)	0.0185(5)	0.0208(5)	–0.0010(4)	0.0070(4)	–0.0005(4)
N(2)	4*e*	1.0227(1)	0.6732(1)	–0.0273(1)	0.0232(6)	0.0173(5)	0.0211(5)	–0.0002(4)	0.0086(4)	0.0016(4)
C(1)	4*e*	0.7004(2)	0.5068(1)	0.1735(2)	0.0297(7)	0.0216(6)	0.0224(6)	–0.0041(5)	0.0092(5)	–0.0010(5)
C(2)	4*e*	0.5526(2)	0.5602(1)	0.1896(2)	0.0257(7)	0.0308(7)	0.0251(7)	–0.0084(6)	0.0112(5)	–0.0058(6)
C(3)	4*e*	0.5034(2)	0.6788(2)	0.1258(2)	0.0200(7)	0.0326(8)	0.0274(7)	–0.0002(6)	0.0064(5)	–0.0072(6)
C(4)	4*e*	0.6044(2)	0.7394(1)	0.0491(2)	0.0231(7)	0.0231(7)	0.0246(7)	0.0023(5)	0.0045(5)	–0.0023(5)
C(5)	4*e*	0.7513(2)	0.6785(1)	0.0390(1)	0.0216(6)	0.0185(6)	0.0180(6)	–0.0012(5)	0.0052(5)	–0.0026(5)
C(6)	4*e*	0.8632(2)	0.7442(1)	–0.0421(2)	0.0249(7)	0.0179(6)	0.0244(6)	0.0034(5)	0.0083(5)	0.0027(5)
N(3)	4*e*	1.1861(1)	0.9277(1)	–0.1555(1)	0.0215(6)	0.0198(5)	0.0219(5)	–0.0006(4)	0.0057(4)	0.0016(4)
O(1)	4*e*	1.2070(2)	0.9344(1)	–0.0204(1)	0.0602(8)	0.0288(6)	0.0207(5)	–0.0041(5)	0.0100(5)	–0.0022(4)
O(2)	4*e*	1.1819(1)	1.0249(1)	–0.2328(1)	0.0324(6)	0.0224(5)	0.0316(5)	–0.0041(4)	0.0035(4)	0.0088(4)
O(3)	4*e*	1.1684(1)	0.81716(9)	–0.2168(1)	0.0297(5)	0.0186(5)	0.0233(5)	–0.0002(4)	0.0091(4)	–0.0020(4)

Acknowledgment. Support of this investigation by Tarbiat Modarres University is gratefully acknowledged.

References

1. Greenwood, N. N.; Earnshaw, A.: Chemistry of the Elements. Pergamon Press, Oxford 1986.
2. Hunter, C. A.; Sanders, J. K. M.: The nature of π-π interactions, J. Am. Chem. Soc. **112** (1990) 5525-5541.
3. Sheldrick, G. M.: SHELXL-97. Program for the Refinement of Crystal Structures. University of Göttingen, Germany.
4. Sheldrick, G. M.: SHELXTL. V. 5.10. Structure Determination Software Suite. Bruker AXS, Madison, Wisconsin, USA 1998.