

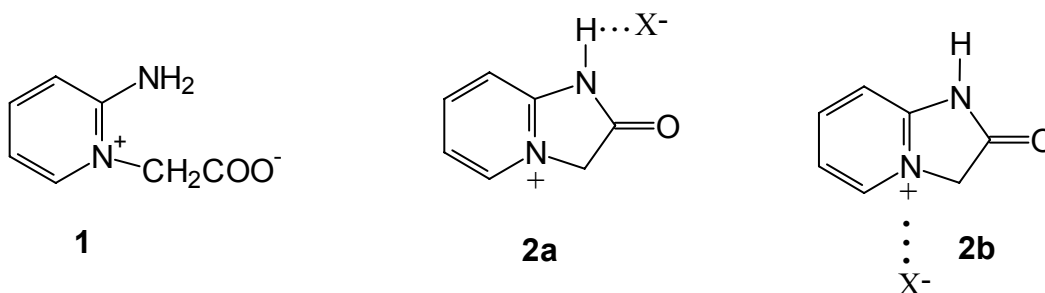
## X-Ray diffraction, FTIR and NMR Spectra, and DFT Calculations of 2-Aminopyridine Betaine and 1-*H*-2-oxo-2,3-dihydroimidazo[1,2-*a*] Pyridinium Chloride, Bromide and Perchlorate

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Betaines make a special class of zwitterions, in which net uncharged molecules have separate cationic and anionic sites [1]. The positive charge is localized on N<sup>+</sup>, S<sup>+</sup> or P<sup>+</sup> atoms which have no hydrogen atom, but the negative charge is on COO<sup>-</sup>, O<sup>-</sup>, SO<sub>2</sub>O<sup>-</sup> or R-P=OO<sup>-</sup> groups. Betaines have a variety of applications in medicine, pharmacy, biology and other scientific fields [2]. An interesting group of betaines are those containing pyridine rings, which are easily obtained by quaternization of pyridines with halogenoacetic acids as well as their salts and esters. Quaternization of 2-amino-pyridine with X-CH<sub>2</sub>-COOH (X = Cl or Br) is more complex, because it depends on reaction temperature.

This contribution reports the crystal and molecular structure and spectroscopic properties of 2-amino-pyridine betaine (1-carboxymethyl-2-amino-pyridinium inner salt) (**1**) and its complexes with HCl, HBr and HClO<sub>4</sub>. These complexes on boiling in ethanol cyclize to 1-*H*-2-oxo-imidazo[1,2-*a*]pyridinium salts (chloride, bromide and perchlorate). Two types of cyclic molecules, one with N(1)-H...X<sup>-</sup> hydrogen bonds (type **2a**) and the second with the electrostatic interactions (type **2b**) between the positively charged nitrogen atom (N<sup>+</sup>(4)) and the counter anions (X<sup>-</sup> = Cl<sup>-</sup>, Br<sup>-</sup> and ClO<sub>4</sub><sup>-</sup>) have been optimized by the B3LYP/6-31G(d,p) level of theory. Molecules of type **2b** have slightly higher energy than type **2a**. Both type of interactions are responsible for the structures of the above mentioned molecules. Structures of 2-amino-pyridine betaine complexes and 1-*H*-2-oxo-imidazo[1,2-*a*] pyridinium salts have been confirmed by the FTIR, <sup>1</sup>H and <sup>13</sup>C NMR spectra.



[1] M. Milton, R.S. Macomber, A.R. Pinhas, R.M. Wilson, *The Vocabulary and Concepts of Organic Chemistry*, J. Wiley & Sons, New Jersey, 2005, pp. 529 and 772.

[2] E.G. Lombax, X. Domingo (Eds) *Amphoteric Surfactants*, Marcel Dekker, New York, 1996, pp. 75-190.