

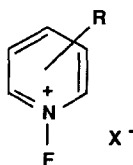
MO CALCULATION STUDY OF THE FLUORINATING REACTION OF *N*-FLUOROPYRIDINIUM SALTS

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N-fluoropyridinium salts (**I**) react with carbon nucleophiles by F transfer¹⁾. In order to investigate the mechanism of the reaction and substituent effect on the pyridine rings, the heat of formation and charge distributions of various *N*-fluoropyridinium cations and corresponding pyridine derivatives are calculated by semiempirical and *ab initio* MO methods.

The calculation results show that the cation has small negative charge on N and



(I)

positive charges on ortho C's, and well interpret the by-products of this reaction¹⁾. The fluorinating power is related to the N-F bond disassociation energies and they depend on the F charges (not N charges).

The possible reaction mechanism and intermediate will be discussed.

- 1) T. Umemoto, S. Fukami, G. Tomizawa, K. Harasawa, K. Kawada and K. Tomita, *J. Am. Chem. Soc.*, **112**, 8563 (1990).