FLUORINATION EFFECT ON HYDROGEN BOND TOPOLOGIES IN WATER ADDUCTS OF FLUOROPYRIDINES

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The rotational spectra of a series of 1:1 adducts of water-fluoropyridines have been investigated by using pulsed jet Fourier transform microwave spectroscopy. Depending on the fluorination sites, the hydrogen bond topologies are quite different from each other. The water links with the N n-obital of 2,3-difluoropyridine and 2,6-difluoropyridine, respectively. through an O-H...N bond. In addition, one weak C-H...O bond might be contributable to the stabilization of the complex 2,3-difluoropyridine-water, while an O-H...F bond plausibly formed in the complex 2,6-difluoropyridine-water in which water acts as a double proton donor. Additional fluorination of the third site of 2,6-difluoropyridine creates a new active site ready to interact with water: the isomer stabilized by one C-H...O and one O-H...F hydrogen bond is proved by the experimental evidences to be the global minimum. This hydrogen topology is quite different from the all former rotational studied complexes involving pyridine and fluoropyridines.