SUPPORTING INFORMATION

Uncovering the Role of Fluorine Positioning on Cationic Properties of 2,4-

Difluoropyridine

Hyojung Kim,^{\dagger} Sung Man Park,^{\dagger} and Chan Ho Kwon^{*}

Department of Chemistry and Institute for Molecular Science and Fusion Technology, Kangwon National University, Chuncheon 24341, Republic of Korea

⁺ These authors contributed equally to this work.

^{*} Email: <a href="mailto:chamber:chamb



Fig. S1 Comparison of the (a) VUV-MATI spectrum of 2,4-DFP with the FC simulations calculated at the (b) B3LYP, (c) CAM-B3LYP, (d) M06-2X, and (e) ω B97XD levels, with scale factors of 0.985, 0.978, 0.971, and 0.975, respectively. All calculations were performed using the cc-pVTZ basis set.