Supplementary Information

Investigating Valence Orbitals and Cationic Structure of 2,6-Difluoropyridine via High-Resolution VUV-MATI Spectroscopy and Franck–Condon Simulations

Sung Man Park, Hyojung Kim, and Chan Ho Kwon[1*]

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

* Email: chkwon@kangwon.ac.kr

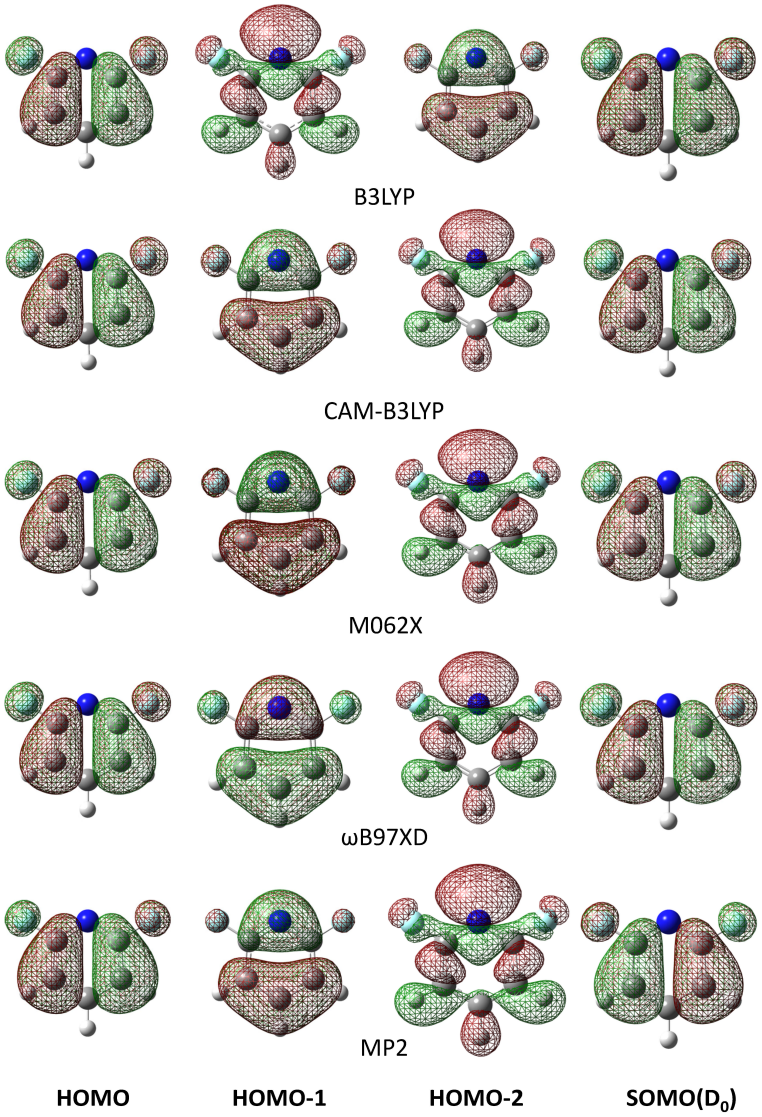

Figure S1 HOMOs and SOMOs of 2,6-DFP in the S_0 and D_0 states optimised at the B3LYP, CAM-B3LYP, M062X, ωB97XD, and MP2 levels of theory using the cc-pVTZ basis set. All HOMOs and SOMOs were analysed through the NBO calculations at each DFT level. The images on the left and right in each column show the top and side views of the molecular orbitals, respectively.