

Supporting Information for

Understanding the effects of vicinal carbon substituents and configuration on organic fluorine hydrogen-bonding interaction

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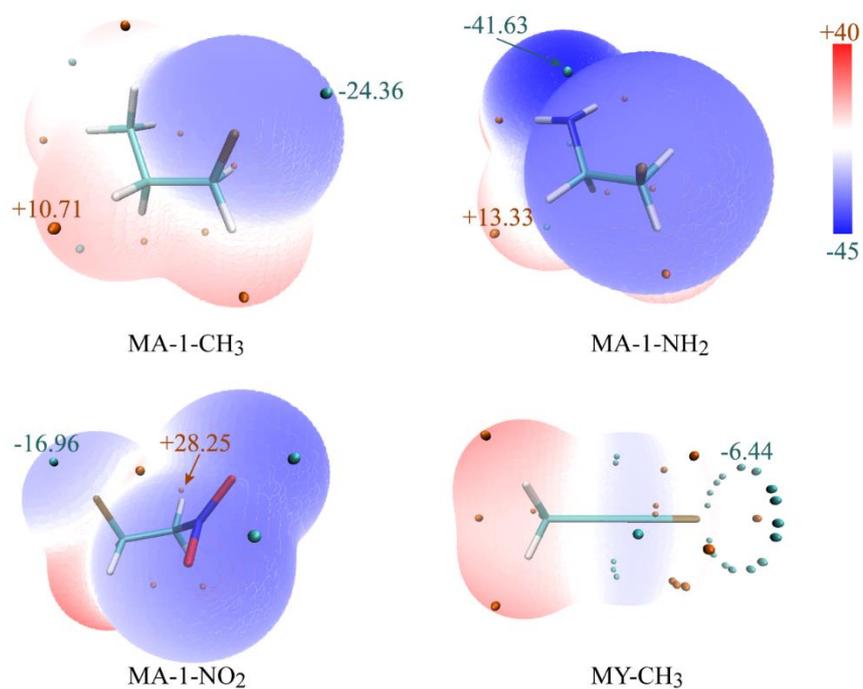


Figure S1. ESP-mapped molecular vdW surface for ortho-CH₂CH₃CH₂F, ortho-CH₂NH₂CH₂F, ortho-CH₂NO₂CH₂F and CH₃CCF, in kcal/mol. The elements of F, N, O, C and H were represented as ochre, blue, red, cyan and gray, respectively.

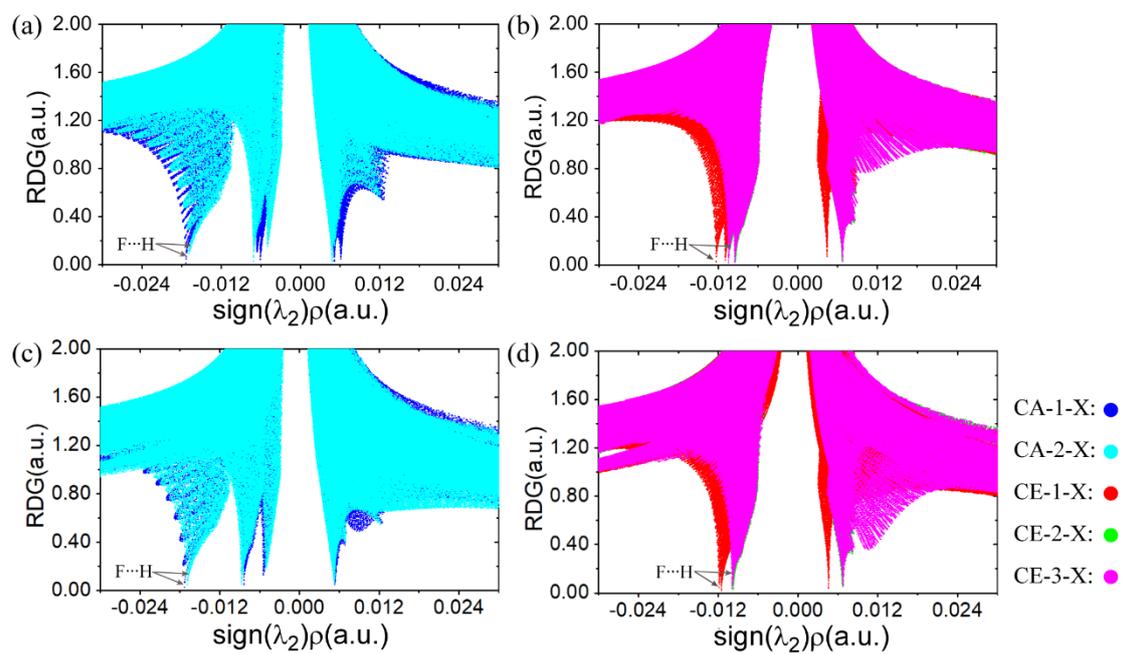


Figure S2. Scatters of the reduced density gradient, RDG, versus the electron density multiplied by the sign of the second Hessian eigenvalue, $\text{sign}(\lambda_2)\rho$ for complexes (a) CA-1-F and CA-2-F; (b) CE-1-F, CE-2-F, and CE-3-F; (c) CA-1-Br and CA-2-Br; (d) CE-1-Br, CE-2-Br, and CE-3-Br.

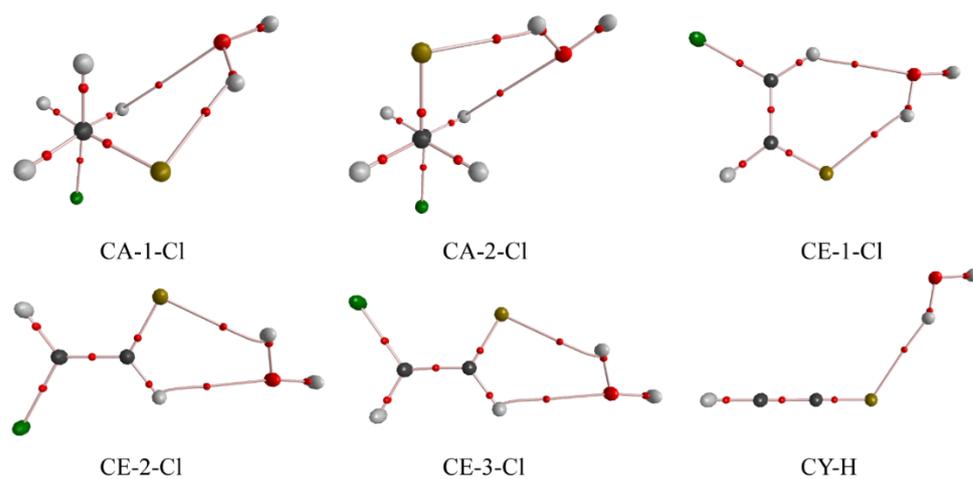


Figure S3. Molecular graphs of complex with bond critical points (BCPs) represented by red dots. The gray, red, green, black and ochre balls represent for H, O, Cl, C and F atoms, respectively. MP2/aug-cc-pVTZ level.