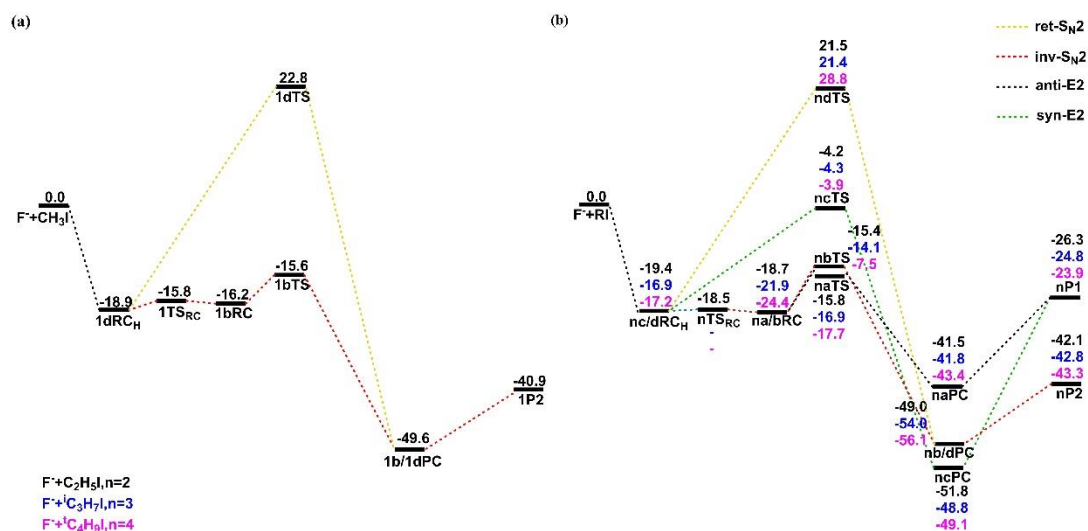


Effects of Methyl Substitution and Leaving Group on E2/S_N2 Competition for Reactions of F⁻ with RY (R = CH₃, C₂H₅, ⁱC₃H₇, ^tC₄H₉; Y = Cl, I)

Wenqing Zhen, Siwei Zhao, Gang Fu, Hongyi Wang, Jianmin Sun, Li Yang *
and Jiaxu Zhang *

State Key Laboratory of Urban Water Resource and Environment, School of Chemistry and Chemical Engineering, Harbin Institute of Technology, Harbin 150001, China; 20b925102@stu.hit.edu.cn (W.Z.); 18b925114@stu.hit.edu.cn (S.Z.); 20b925088@stu.hit.edu.cn (G.F.); wanghongyi999123@163.com (H.W.); sunjm@hit.edu.cn (J.S.)
* Correspondence: yangli2014@hit.edu.cn (L.Y.), zhjx@hit.edu.cn (J.Z.)



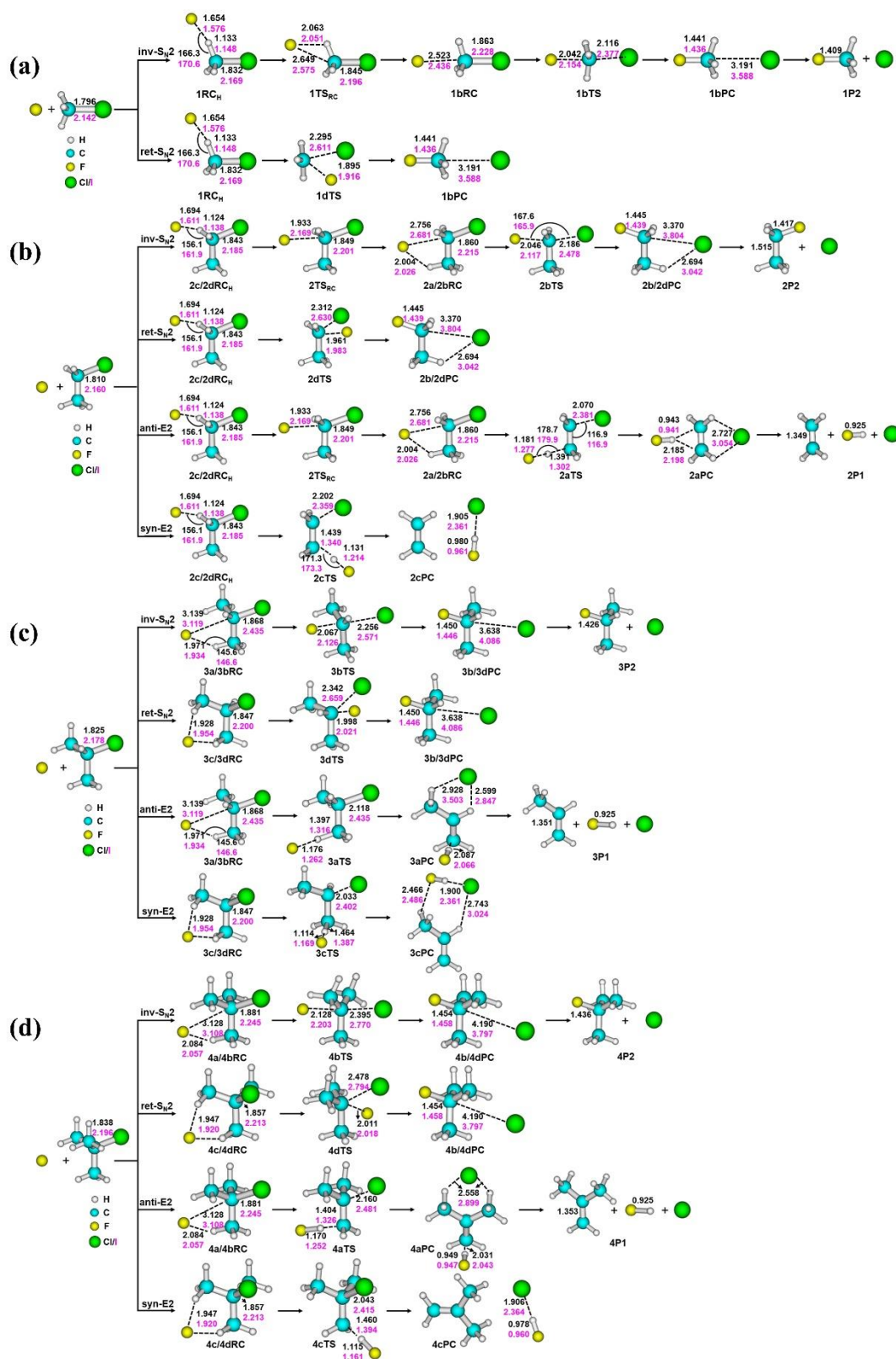


Figure S2. Stationary point structures of E2 and S_N2 pathways for (a) $F + CH_3Y$, (b) $F + C_2H_5Y$, (c) $F + {}^iC_3H_7Y$, (d) $F + {}^iC_4H_9Y$ (Y = Cl, I) reaction optimized at the MP2/aug-cc-pVDZ(ECP/d) theoretical level. Bond distances are in Å, and black/pink line represents Y = Cl / I.

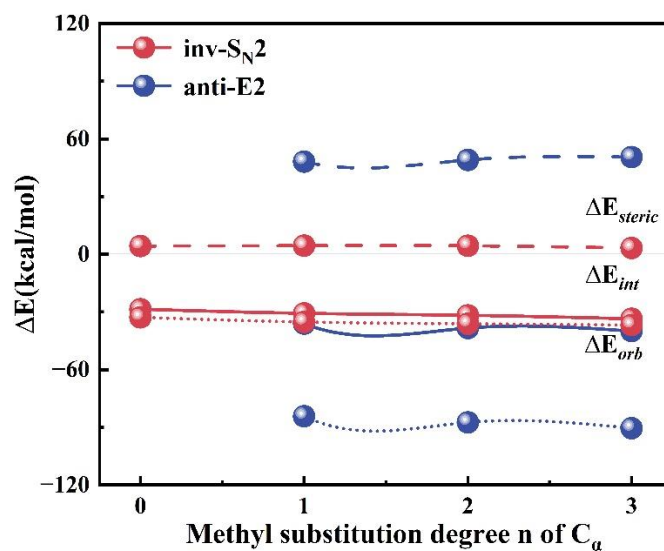


Figure S3. Interaction energy decomposition according to formula $\Delta E_{int} = (\Delta E_{els} + \Delta E_{xc} + \Delta E_{Pauli}) + \Delta E_{orb} = \Delta E_{steric} + \Delta E_{orb}$. ΔE_{els} is electrostatic interaction term, ΔE_{xc} is the change of exchange-correlation energy during complexation process, and ΔE_{Pauli} is the Pauli repulsion effect between electrons in occupied orbitals of the fragments and is invariably positive. They combine to form steric term ΔE_{steric} (Dashed line). ΔE_{orb} is orbital interaction term and represented by short dotted line. The full line represents ΔE_{int} .