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# Competitive dynamics of E2 and $S_N2$ reaction driven by leaving group and collision energy

Siwei Zhao, Gang Fu, Wenqing Zhen, Hongyi Wang, Meiling Liu, Li Yang,* and Jiaxu Zhang*

State Key Laboratory of Urban Water Resource and Environment

MIIT Key Laboratory of Critical Materials Technology for New Energy Conversion and Storage, School of Chemistry and Chemical Engineering,

Harbin Institute of Technology,

Harbin 150001, P. R. China

Author E-mail Address: yangli2014@hit.edu.cn and zhjx@hit.edu.cn

Table S1 Selected bond distances (Å), geometric looseness (%$L_{E2}$), and geometrical asymmetry (%$AS_{E2}$) of anti-E2-TS structures for $F^-$ + $CH_3CH_2Y$ (Y = Cl, Br[22], I[34]) reactions as optimized by M06/aug-cc-pVDZ and M06/ECP/d methods.

| Substitution | $r^{TS}(F–H_\beta)$ | $r^{TS}(C_\alpha–Y)$ | $r^{Product}(F–H_\beta)$ | $r^{Reactant}(C_\alpha–Y)$ | %$(F–H_\beta)$ | %$(C_\alpha–Y)$ | %*L* | %*AS* |
|---|---|---|---|---|---|---|---|---|
| $CH_3CH_2Cl$ | 1.231 | 2.042 | 0.918 | 1.813 | 34.0 | 12.6 | 46.7 | 21.4 |
| $CH_3CH_2Br$ | 1.271 | 2.225 | 0.918 | 1.969 | 38.4 | 13.0 | 51.4 | 35.4 |
| $CH_3CH_2I$ | 1.311 | 2.424 | 0.918 | 2.161 | 42.8 | 12.2 | 55.0 | 30.6 |