

Indirect dynamics in $S_N2@N$. Insight into the influence of central atom

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Table S1. Average fractions of $F^- + NH_2Cl \rightarrow NH_2F + Cl^-$ product energy partitioning^a

	f_{rot}'	f_{vib}'	f_{trans}'	f_{int}'
$E_{coll} = 300K (0.9 \text{ kcal/mol})$				
Direct rebound	0.07 ± 0.03	0.45 ± 0.10	0.48 ± 0.10	0.52 ± 0.10
Direct stripping	0.03 ± 0.01	0.28 ± 0.14	0.70 ± 0.13	0.30 ± 0.13
Indirect	0.22 ± 0.02	0.53 ± 0.02	0.26 ± 0.02	0.74 ± 0.02
Total	0.21 ± 0.02	0.51 ± 0.02	0.28 ± 0.02	0.72 ± 0.02
$E_{coll} = 40 \text{ kcal/mol}$				
Direct rebound	0.15 ± 0.08	0.28 ± 0.07	0.57 ± 0.09	0.43 ± 0.09
Direct stripping	0.17 ± 0.01	0.22 ± 0.04	0.61 ± 0.03	0.39 ± 0.03
Indirect	0.11 ± 0.02	0.56 ± 0.03	0.33 ± 0.03	0.67 ± 0.03
Total	0.13 ± 0.02	0.46 ± 0.04	0.42 ± 0.03	0.58 ± 0.03

^aThe f 's are fractions of energy partitioned to rotational, vibrational, relative translational, and internal (rotation + vibration) energy. Total is the combined partitioning for the individual mechanisms.

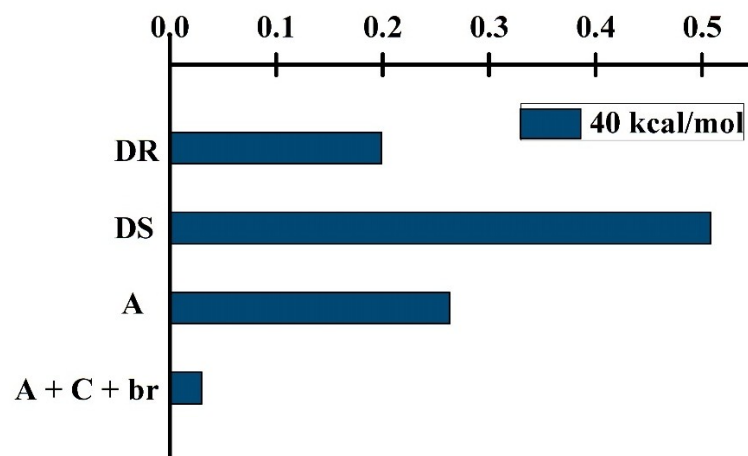


Figure S1. Fractions of the atomistic mechanisms for $\text{F}^- + \text{NH}_2\text{Cl} \rightarrow \text{HF} + \text{NHCl}^-$ proton transfer reaction at a collision energy of 40 kcal/mol. DR, direct rebound; DS, direct stripping; A, F^- - $\text{H}\text{N}\text{H}\text{Cl}$; C, NHCl^- - HF ; br, barrier recrossing. DR and DS are direct mechanisms, and others are indirect events.

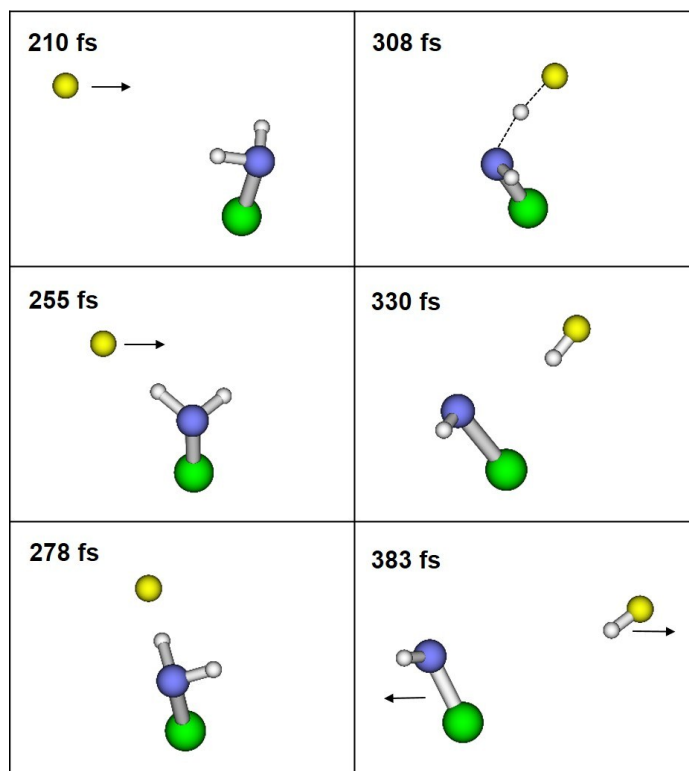


Figure S2. Atomistic dynamics of a typical trajectory for the direct stripping mechanism that dominates the $\text{F}^- + \text{NH}_2\text{Cl} \rightarrow \text{HF} + \text{NHCl}^-$ proton transfer reaction at a collision energy of 40 kcal/mol.

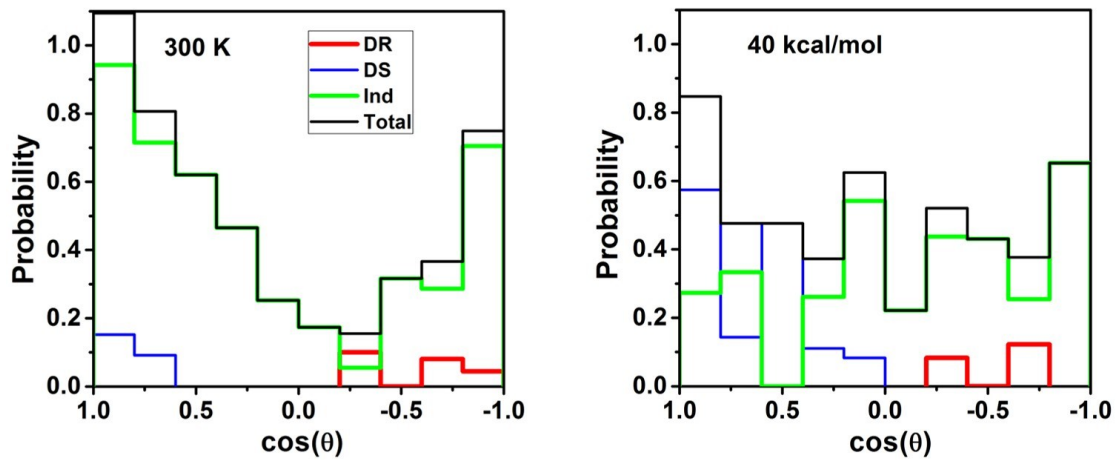


Figure S3. Velocity scattering angle distributions for the $F^- + NH_2Cl \rightarrow NH_2F + Cl^-$ S_N2 reaction at 300 K and 40 kcal/mol collision energies. The results are illustrated for the individual direct rebound (red), direct stripping (blue), and indirect (green) mechanisms and for the total scattering (black).