Effect of microsolvation on a $S_{\rm N}2$ reaction. Indirect atomistic dynamics and

weakened suppression of reactivity

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	DR	DS	Ind	Total	Expt.
			$E_{coll} = 0.32 \text{ eV}$		
$F(H_2O)$	0.62±0.02	0.46±0.04	0.75±0.01	0.69±0.01	
F-	0.54±0.03	0.55±0.04	0.79±0.02	0.69±0.02	0.70±0.10
			$E_{coll} = 1.53 \text{ eV}$		
$F^{-}(H_2O)$	0.64±0.03	0.56±0.06	0.82±0.02	0.73±0.02	
F-	0.63±0.02	0.66±0.02	0.85±0.07	0.66±0.01	0.59±0.08

Table S1. Average fractions of product energy partitioned to internal excitation for F⁻ (H₂O) + CH₃I \rightarrow CH₃F + I⁻ + H₂O scattering^a and comparison with unsolvated reaction^b.

^aResults are reported for the individual direct rebound (DR), direct stripping (DS), indirect (Ind) mechanisms, and for the total reaction.

^brefs 23 and 24.



Figure S1. H_2O -leaving time as a function of displacement occurrence time for the F-(H_2O) + $CH_3I \rightarrow CH_3F + I^- + H_2O$ reaction at 0.32 eV collision energy, in comparison to 300 K data. Trajectories at these two energies show similar features for this information (see text). The results are illustrated for direct rebound (DR), direct stripping (DS), and indirect (Ind) scatterings.

 $F(H_2O)$



Figure S2. Velocity scattering angle distributions at different collision energies for the F- $(H_2O)_n + CH_3I \rightarrow CH_3F + I^- + nH_2O$ (n = 0 and 1) reactions. The data for direct rebound (red), direct stripping (pink), and indirect (green) mechanisms and for the total scattering (blue) of solvated system are presented in left pannels. Each individual distribution is proportional to its contribution to the atomistic dynamics whose sum is normalized to unity. Right pannels denote the total distributions of unsolvated scattering from the silumlation (blue) and experiment (black).^{23,24}