

Where does the energy go during the interstellar NH₃ formation on water ice? A computational study

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Table S1. Computed reaction energies (ΔE_{rx}) and energy barriers (ΔE^\ddagger) for the sequential H-addition and H-abstraction reactions in the gas phase using different quantum chemical methods (PBE-D3(BJ), ω B97x-D3(BJ) and single points at CCSD(T)-F12) and different codes (CP2K and Orca). All the H-addition reactions have been found to be barrierless, namely, the products are spontaneously formed during the optimization process. Units are in kJ mol^{-1} .

	PBE-D3(BJ) CP2K	PBE-D3(BJ) Orca	CCSD(T)-F12//PBE-D3(BJ)m Orca	ω B97x-D3(BJ)m Orca	CCSD(T)-F12// ω B97x-D3(BJ)m Orca	
ΔE_{rx}	H-additions					
	N + H \rightarrow NH	-359.3	-367.2	-330.8	-351.5	-331.2
	NH + H \rightarrow NH ₂	-406.5	-415.4	-399.7	-411.5	-399.9
	NH ₂ + H \rightarrow NH ₃	-463.6	-472.3	-466.2	-473.4	-466.0
	H-abstractions					
NH + H \rightarrow N(⁴ S) + H ₂	-81.5	-70.9	-99.4	-98.2	-99.2	
NH + H \rightarrow N(² D) + H ₂	211.7	209.7	156.4	169.8	156.8	
NH ₂ + H \rightarrow NH(³ Σ^-) + H ₂	-34.3	-22.8	-29.9	-38.3	-30.3	
NH ₂ + H \rightarrow NH(¹ Δ) + H ₂	207.3	203.3	151.0	163.9	150.5	
ΔE^\ddagger	H-additions					
	Barrierless					
	H-abstractions					
	NH + H \rightarrow N(⁴ S) + H ₂	Barrierless	Barrierless	-	11.5	10.2
NH ₂ + H \rightarrow NH(³ Σ^-) + H ₂	1.1	2.9	28.9	26.4	29.6	

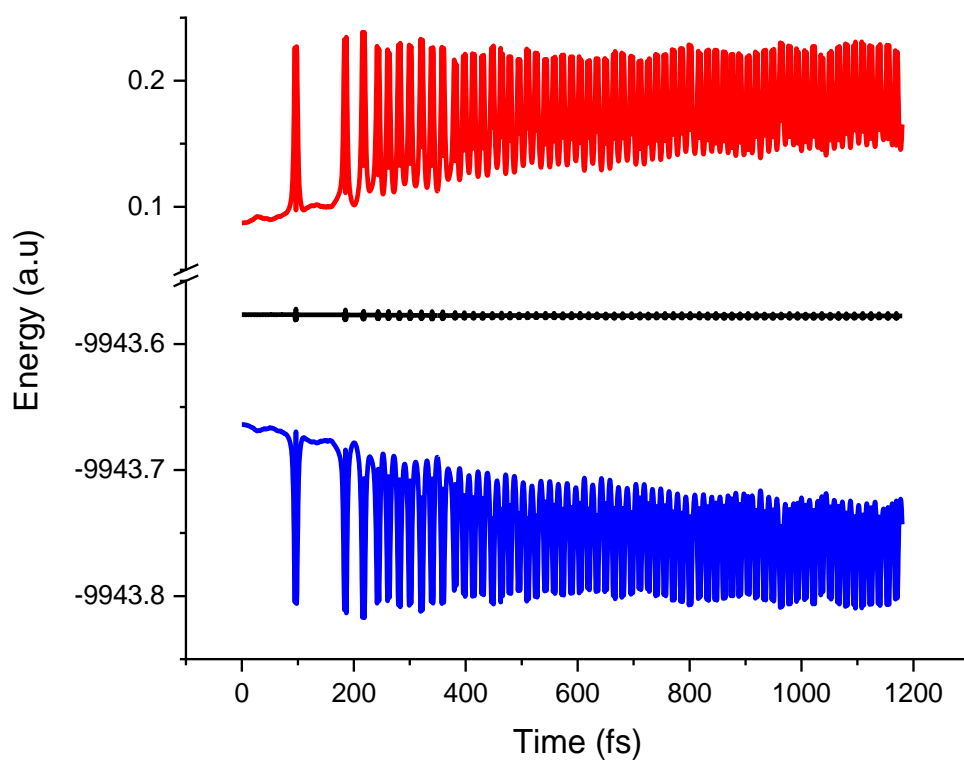


Figure S1. Evolution over time (in fs) of the potential energy (blue line), kinetic energy (red line) and total energy (black line) for the $\text{N} + \text{H} \rightarrow \text{NH}$ reaction on the amorphous water ice surface model. Note that the total energy is conserved due to the NVE microcanonical conditions. Energy units are in Hartrees (a.u.).

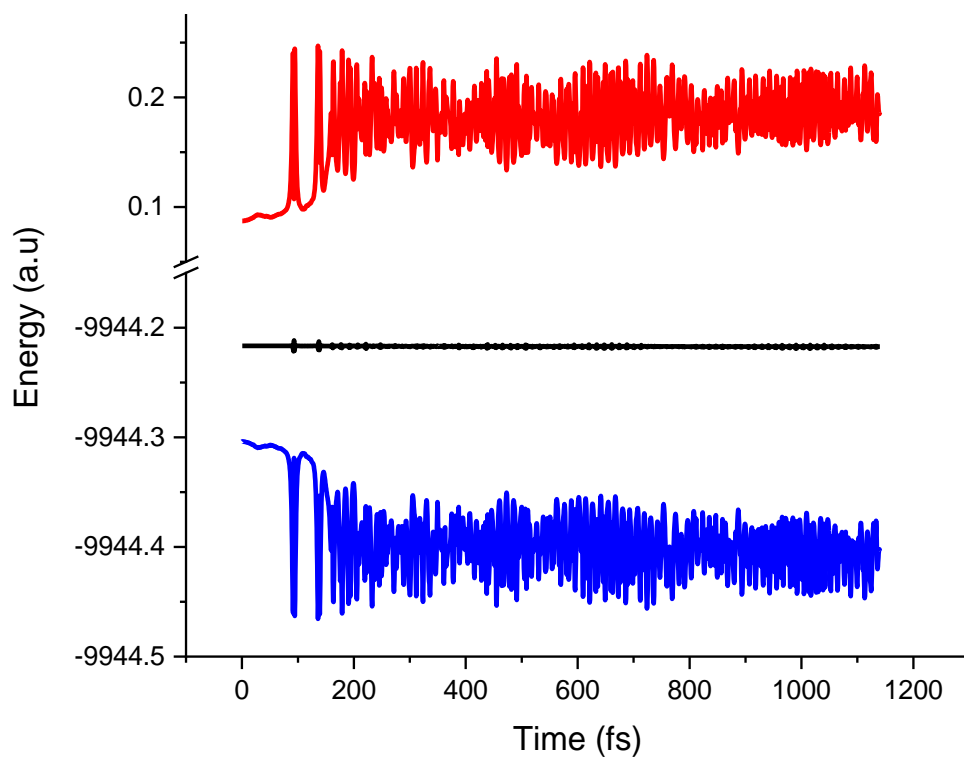


Figure S2. Evolution over time (in fs) of the potential energy (blue line), kinetic energy (red line) and total energy (black line) for the $\text{NH} + \text{H} \rightarrow \text{NH}_2$ reaction on the amorphous water ice surface model. Note that the total energy is conserved due to the NVE microcanonical conditions. Energy units are in Hartrees (a.u.).

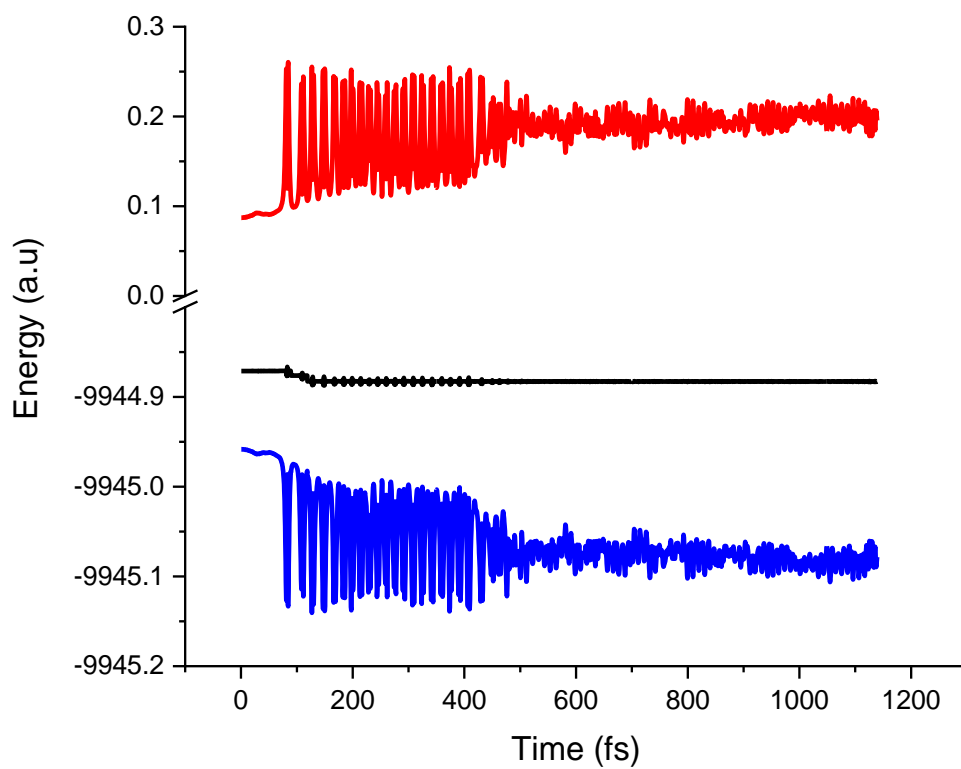


Figure S3. Evolution over time (in fs) of the potential energy (blue line), kinetic energy (red line) and total energy (black line) for the $\text{NH}_2 + \text{H} \rightarrow \text{NH}_3$ reaction from position Pos1 on the amorphous water ice surface model. Note that the total energy is conserved due to the NVE microcanonical conditions. Energy units are in Hartrees (a.u.).

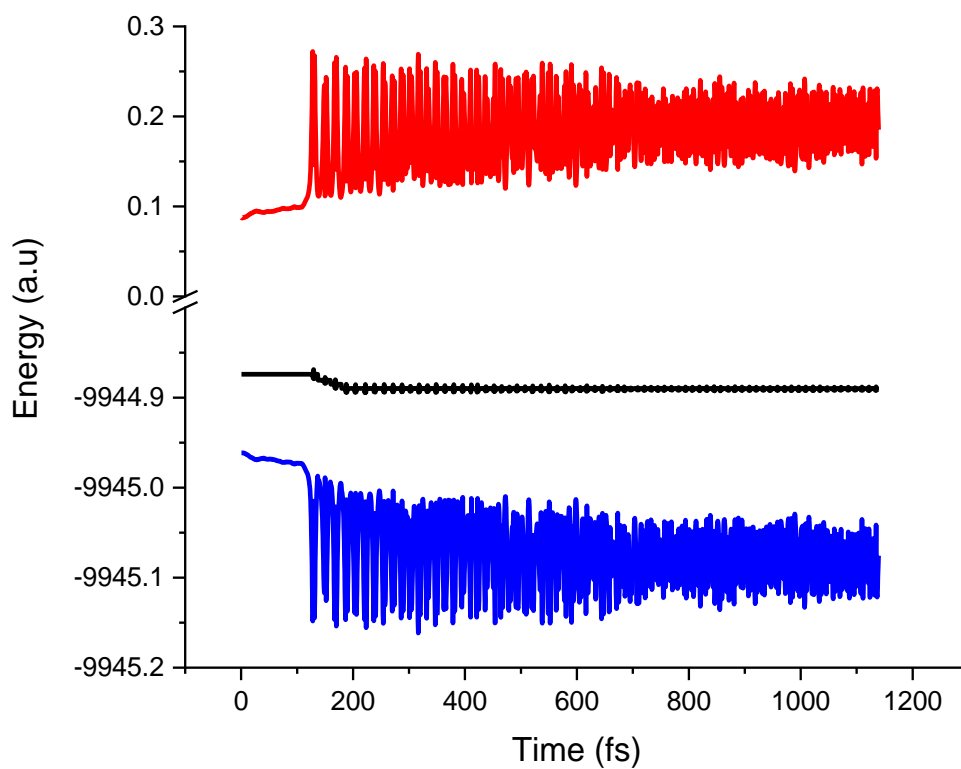


Figure S4. Evolution over time (in fs) of the potential energy (blue line), kinetic energy (red line) and total energy (black line) for the $\text{NH}_2 + \text{H} \rightarrow \text{NH}_3$ reaction from position Pos2 on the amorphous water ice surface model. Note that the total energy is conserved due to the NVE microcanonical conditions. Energy units are in Hartrees (a.u.).

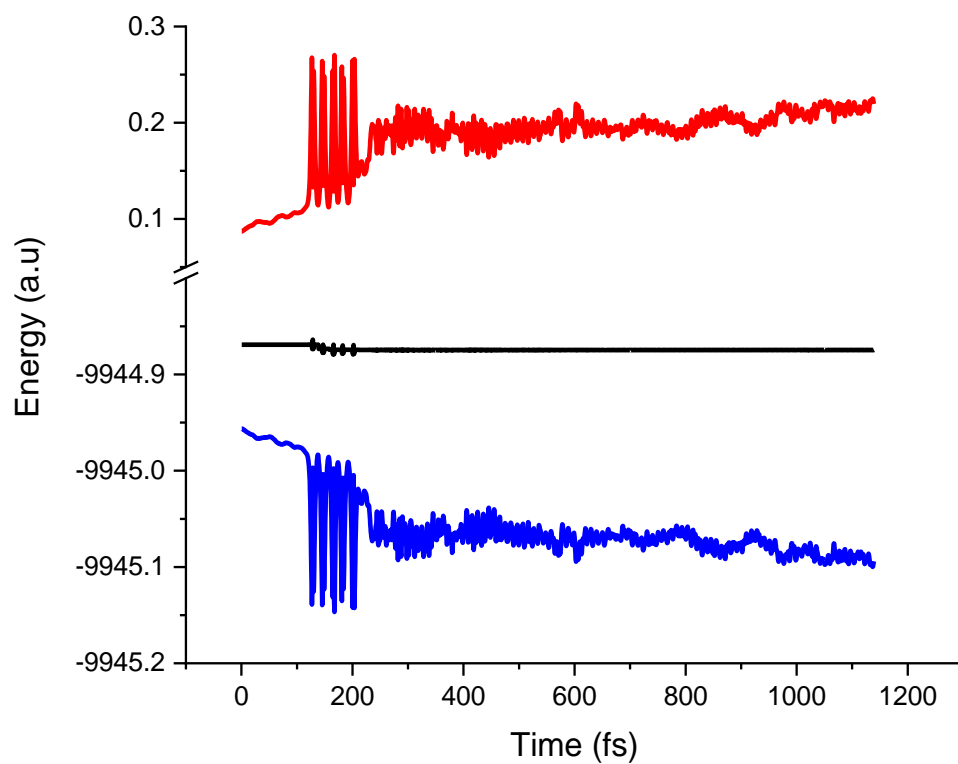


Figure S5. Evolution over time (in fs) of the potential energy (blue line), kinetic energy (red line) and total energy (black line) for the $\text{NH}_2 + \text{H} \rightarrow \text{NH}_3$ reaction from position Pos3 on the amorphous water ice surface model. Note that the total energy is conserved due to the NVE microcanonical conditions. Energy units are in Hartrees (a.u.).

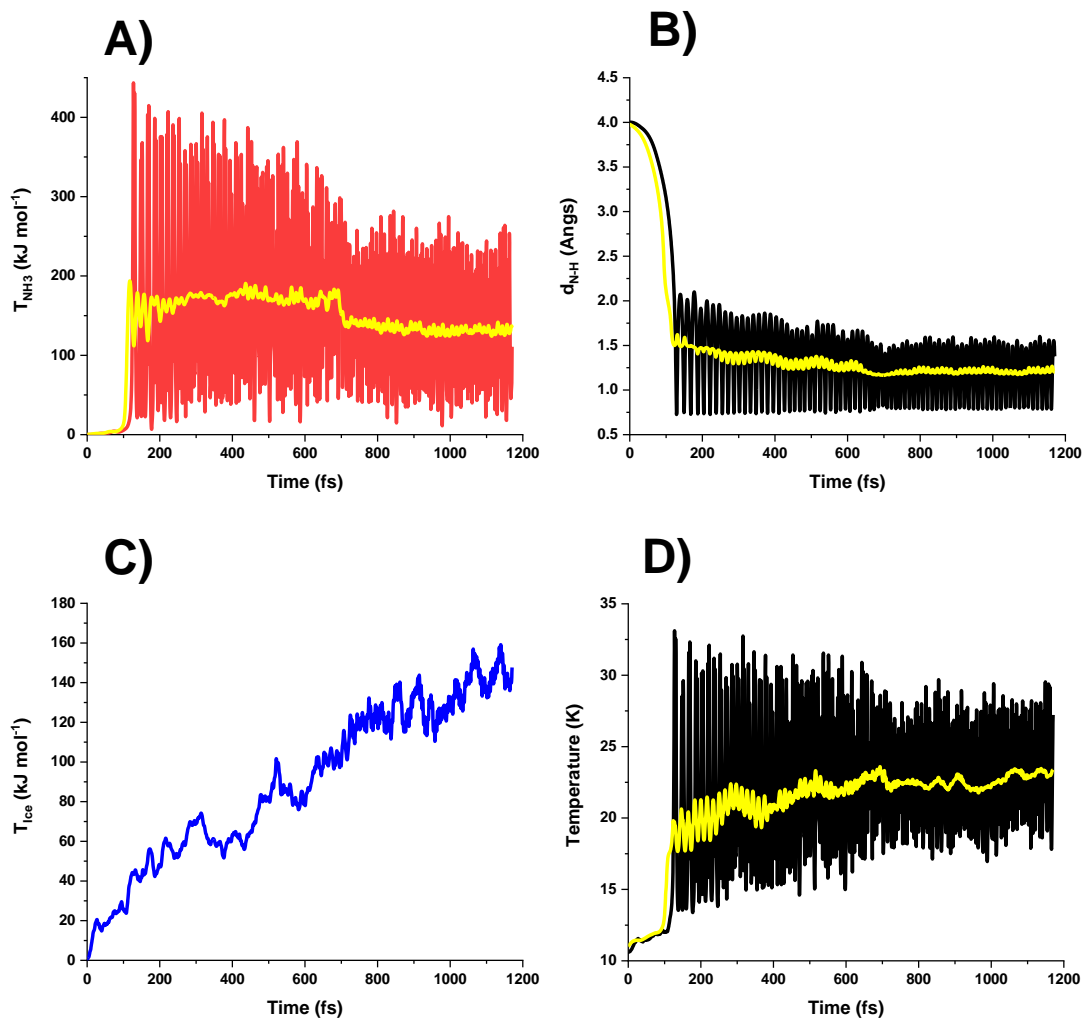


Figure S6. Results of the NVE AIMD simulations for the third H-addition $\text{NH}_2 + \text{H} \rightarrow \text{NH}_3$ from position Pos2: A) initial structure of the simulation; B) evolution of the kinetic energy of NH; C): evolution of the N-H distance; D) evolution of the kinetic energy of the ice; and E) evolution of the temperature of the ice. Instantaneous and averaged values (in yellow) are reported.