

Table S3. The Gibbs free energy change of each reaction step of Path 1 for electrocatalytic NO₃RR to NH₃ by Co NPs.

Reaction step	ΔG	U_L
*	0	
* + NO ₃ ⁻ → *NO ₃ + e ⁻	-4.49	
*NO ₃ + H ⁺ + e ⁻ → *NO ₃ H	-2.55	
*NO ₃ H + H ⁺ + e ⁻ → *NO ₂ + H ₂ O	0.14	
*NO ₂ + H ⁺ + e ⁻ → *NO ₂ H	0.41	
*NO ₂ H + H ⁺ + e ⁻ → *NO + H ₂ O	-0.30	
*NO + H ⁺ + e ⁻ → *NOH	0.43	-0.43
*NOH + H ⁺ + e ⁻ → *N + H ₂ O	-1.00	
*N + H ⁺ + e ⁻ → *NH	-2.71	
*NH + H ⁺ + e ⁻ → *NH ₂	-0.17	
*NH ₂ + H ⁺ + e ⁻ → *NH ₃	-0.02	
*NH ₃ → * + NH ₃	0.26	