

Table S4. The Gibbs free energy change of each reaction step of Path 4 for electrocatalytic NO₃RR to NH₃ by Co SACs.

Reaction step	ΔG	U_L
*	0	
* + NO ₃ ⁻ → *NO ₃ + e ⁻	-2.26	
*NO ₃ + H ⁺ + e ⁻ → *NO ₃ H	0.12	
*HNO ₃ + H ⁺ + e ⁻ → *NO ₂ + H ₂ O	-1.85	
*NO ₂ + H ⁺ + e ⁻ → *NO ₂ H	0.72	-0.72
*NO ₂ H + H ⁺ + e ⁻ → *ON + H ₂ O	-0.66	
*ON + H ⁺ + e ⁻ → *ONH	0.27	
*ONH + H ⁺ + e ⁻ → *ONH ₂	-0.96	
*ONH ₂ + H ⁺ + e ⁻ → *O + NH ₃	0.10	
*O + H ⁺ + e ⁻ → *OH	-1.02	
*OH + H ⁺ + e ⁻ → *H ₂ O	-0.04	
*H ₂ O → * + H ₂ O	0.34	