

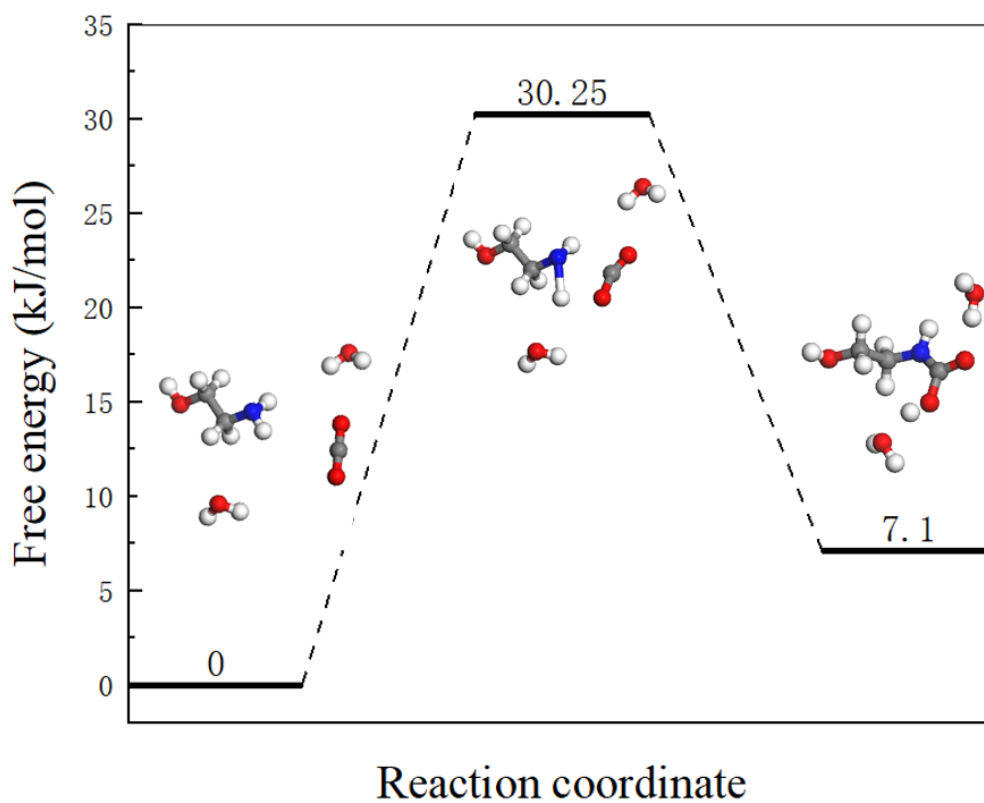


Figure S1. Energy barrier diagram for the first reaction step of MEA with the water-assisted Model. (Carbon, oxygen, hydrogen, and nitrogen atoms are represented by gray, red, white, and blue colors, respectively.)

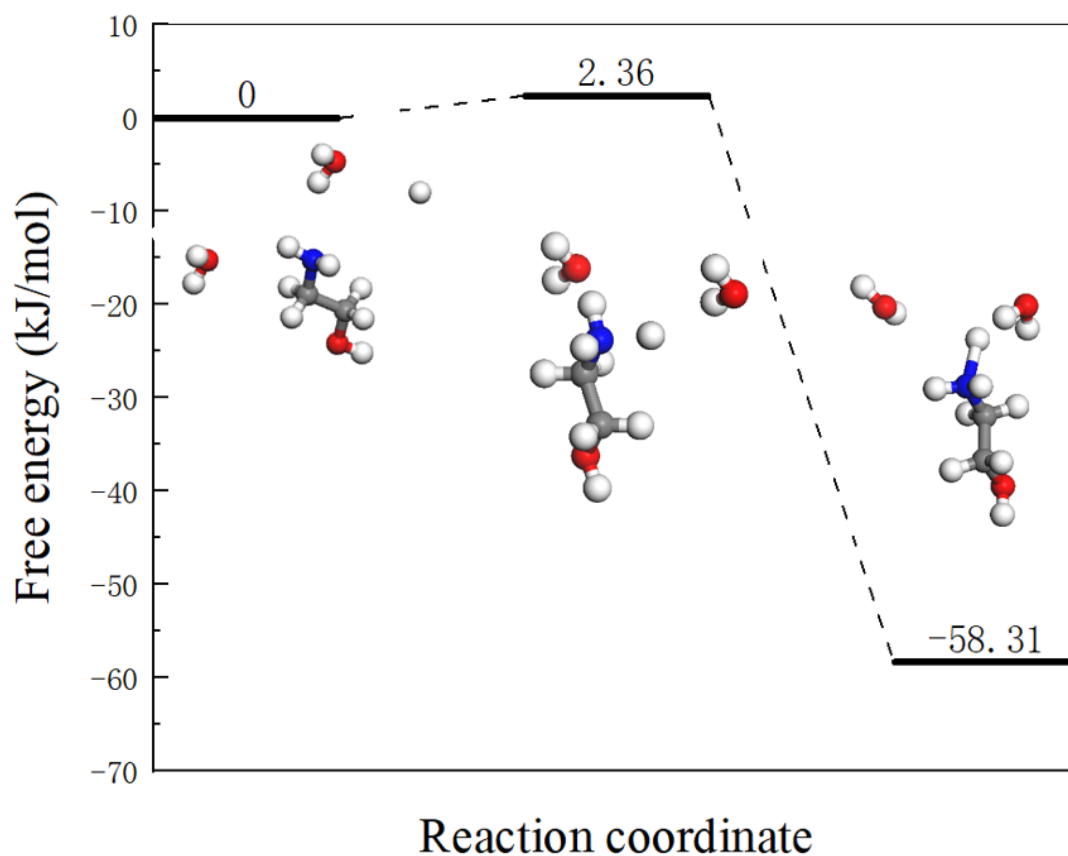


Figure S2. Energy barrier diagram for the second reaction step of MEA with the water-assisted model.(Carbon, oxygen, hydrogen, and nitrogen atoms are represented by gray, red, white, and blue colors, respectively.)

Table S1. Comparison of reaction free energy changes under different simulation models

Case	Simulation model	Reaction step	Free energy of intermediates (kJ/mol)	Free energy of final state (kJ/mol)
1	water-assisted model	1	30.25	7.1
2	implicit solvation model	1	32.02	7.4
3	water-assisted model	2	2.36	-58.31
4	implicit solvation model	2	1.41	-61.5