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***Ab Initio* Molecular Metadynamics Study of the Base-Catalyzed Hydrolysis of N-Methylacetamide**[1] SUFIAN ALNEMRAT, IGOR VASILIEV, HAOBIN WANG — We apply the first principles metadynamics simulation technique implemented in the Car-Parrinello molecular dynamics package to study the base-catalyzed hydrolysis of N-methylacetamide in aqueous solution. Our calculations are carried out in the framework of density functional theory combined with the hybrid BLYP exchange-correlation functional The free energy surfaces and hydrolysis reaction pathways for N-methylacetamide are examined in the presence of a hydroxide ion, and 4, 16, 32, and 64 water molecules. We find that at least 32 water molecules must be explicitly included in metadynamics simulations to accurately describe the mechanism of the hydrolysis reaction of N-Methylacetamide Our theoretical estimate for the dissociation energy of N-Methylacetamide is in good agreement with the results of previous experimental and theoretical studies.

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