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Calculation of Proton Transfer Rates in Liquids Using Molecular Dynamics Simulations YIN GUO, Department of Physics, Oklahoma State University — We have been investigating a computational method that incorporates WKB tunneling calculations within the framework of classical molecular dynamics (MD) simulations. The computational cost is at the same level as the usual MD simulation, thus providing a practical and efficient dynamical approach for treating quantum tunneling. Building upon the earlier gas-phase studies, we extend the method to condensed phase materials. As a test case, the method is applied to a model system that represents proton transfer AH–B$\leftrightarrow$A$^-$–H$^+$B in liquid methyl chloride, where AH–B is a linear complex with parameters chosen to model a typical phenol-amine complex. The calculated results are compared with those of earlier studies on the same system by Azzouz and Borgis and by Hammes-Schiffer and Tully using different methods.

Yin Guo
Oklahoma State University

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