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The role of vibrations in the kinetics of conformational isomerization of biomolecules and clusters DAVID LEITNER, JOHNSON AGBO, University of Nevada, Reno, DAVID EVANS, DAVID WALES, Cambridge University — The kinetics of conformational isomerization of sizable molecules and clusters depends both on the topography of the potential energy surface (PES), in particular barriers that separate minima corresponding to specific conformers, and the vibrational dynamics of each conformer. Incorporation of the vibrational contribution can be finessed by assuming rapid vibrational energy flow within a basin of the PES and adopting Rice-Ramsperger-Kassel-Marcus (RRKM) theory to calculate isomerization rates between pairs of conformers. However, RRKM theory often overestimates rates of conformational change due to insufficiently rapid vibrational energy flow. In this case, isomerization rates can be computed by applying a theory for quantum energy flow in many-oscillator systems to calculate corrections to RRKM theory. As an example we discuss the influence of vibrational energy flow on the kinetics of conformational isomerization of the dipeptide NATMA.

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