A NEW PERSPECTIVE ON ISOMERIZATION DYNAMICS ILLUSTRATED BY HCN $\rightarrow$ HNC

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We present a number of delocalized, "isomerization", wavefunctions for HCN/HNC based on exact three degree of freedom calculations using a high quality global ab initio potential energy surface [Bowman, J. M.; Gazdy, B.; Bentley, J. A.; Lee, T. J.; Dateo, C. E. J. Chem. Phys. 1993, 99 , 308.]. We suggest new notation for "assigning" these states. We will also discuss the role of delocalized states in isomerization dynamics, and illustrate the ideas by considering isomerization in HCN. We analyze results from an earlier study, where HCN was treated as a semi-rigid bender, and isomerization was induced by collision with an Ar atom, and suggest a new theory to obtain the cumulatiave isomerization reaction probability.