A SIMPLE FACTORIZATION SCHEME TO PREDICT IVR RATES IN MEDIUM-SIZED ORGANIC MOLECULES

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Other factors being equal, it has long been assumed that the IVR rate will decrease as the symmetry of the molecule increases. Recently, Callegari, et al. observed no trend: increasing rates of IVR in a progression from s-triazine to pyrrole to benzene in the first CH stretching overtone bands. The simple factorization method previously developed[a] has been applied to these systems. Using an anharmonic normal mode basis set for off-diagonal matrix element calculations and the MFD method[b], good agreement for the linewidths of pyrrole and s-triazine are obtained with only one adjustable parameter.

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[a] D. Madsen, R. Pearman, M. Gruebele, J. Chem. Phys, 106(14), 5874, (1997).

[b] M. Gruebele, J. Phys. Chem, 100, 12183, (1996).