ADIABATIC DIFFUSION MONTE CARLO STUDIES FOR THE Ne_2SH/D ($^2\Sigma^+, v = 0$) VAN DER WAALS COMPLEXES

HEE-SEUNG LEE, JOHN M. HERBERT AND ANNE B. MCCOY, *Department of Chemistry, The Ohio State University, Columbus, OH 43210*.

Two adiabatic extensions to the diffusion Monte Carlo approach(ADMC) [a] are presented. In the first, an adiabatic form of the finite field method is developed for the systematic evaluation of expectation values. In addition, an adiabatic flexible node method for calculating excited state energy is described. The above methods are tested by applying to NeSH[b] and Ar_2HCl[c] complexes where comparisions to results of variational calculation can be made. Our results show that the agreement between ADMC and variational calculation is better than 1% relative error.

Application of ADMC to the structure and spectroscopy of Ne_2SH/D van der Waals complexes will also be discussed. The spectra of these systems have been recorded recently,[d] but not fully assigned. As such, this work will provide valuable insights into the interpretation of complicated spectra of these very floppy systems.

---

[a] H. -S. Lee, J. M. Herbert and A. B. McCoy, *J.Chem.Phys.* **110**, in press

[b] C. C. Carter, T. A. Miller, H. -S. Lee, A. B. McCoy and E. F. Hayes, *J.Chem.Phys.* **110**, 5065

[c] A. R. Cooper and J. M. Hutson, *J.Chem.Phys.* **98**,5337

[d] C. C. Carter and T. A. Miller (unpublished)