MATRIX ISOLATION VS. QUANTUM CHEMISTRY FOR PREDICTING VIBRATIONAL FUNDAMENTALS OF SMALL FREE RADICALS

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The average deviations from the gas-phase band centers of vibrational fundamental frequencies of 33 small molecular free radicals, recently calculated by Byrd, Sherrill, and Head-Gordon [a] using several commonly employed computational levels and basis sets, will be compared with the corresponding values characteristic of measurements in argon and neon matrices. Strategies will be suggested for estimating values for the ground-state vibrational fundamentals of small free radicals when detailed gas-phase data are not available.

[a] E. F. C. Byrd, C. D. Sherrill, and M. Head-Gordon, J. Phys. Chem. A 105, 9736 (2001).