HOW DIFFERENT ARE *ORTHO* AND *PARA* HYDROGEN? A COMPUTATIONAL EXAMINATION OF POTENTIALS, BOUND STATES, AND SCATTERING OF HYDROGEN COMPLEXES

KELLY J. HIGGINS, *Spectral Sciences, Inc., Burlington, MA 01803*; WILLIAM KLEMPERER, *Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA 02138*.

The interaction between molecular hydrogen and other molecules is studied through *ab initio* calculations with a focus on differences in behavior between *ortho* and *para* hydrogen. These differences manifest themselves in various ways, including in the rotational spectra of complexes[a,b] and in pressure broadening cross sections.[c] Two specific systems, H_2-HCN and H_2-OCS, will be examined. For H_2-HCN, a new 4-D potential surface will be presented along with bound state and scattering calculations, while for H_2-OCS new calculations utilizing a previously presented potential[d] will be discussed. These two systems display markedly different ground state geometries that lead to different behavior of the *ortho* and *para* hydrogen complexes. In addition to the specific systems a more general discussion will examine the effect of potential anisotropy and ground state geometry on the properties of hydrogen complexes and how the differences between *ortho* and *para* interactions can be used.

[a] Z. Yu, *et al.*, J. Chem. Phys. **127**, 054305 (2007).
[b] M. Ishiguro, *et al.*, J. Chem. Phys. **115**, 5155 (2001).
[c] M. Mengel, D.C. Flatin, and F. C. De Lucia, J. Chem. Phys. **112**, 4069 (2000).
[d] K.J. Higgins, Z. Yu, and W. Klemperer, 62nd International Symposium on Molecular Spectroscopy (2007).