INTERMOLECULAR POTENTIAL AND 4-DIMENSIONAL BOUND STATE CALCULATIONS OF H_2-OCS COMPLEXES

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The interaction between molecular hydrogen and carbonyl sulfide was studied through *ab initio* calculations and 4-D bound state calculations of $p$$H_2$-OCS, $o$$H_2$-OCS, $p$$D_2$-OCS, $o$$D_2$-OCS, and HD-OCS. The intermolecular potential surface (IPS) encompasses all four intermolecular degrees of freedom and was briefly presented previously.[a] The focus of this talk will be on bound state calculations performed on the IPS in order to understand the observed microwave spectra of the complexes. Although the spectra of complexes involving $j = 0$ hydrogen is well understood using a pseudo 2-D potential generated by averaging the 4-D potential over a spherical hydrogen distribution, the spectra of the complexes involving $j = 1$ hydrogen is much more complicated and requires 4-D bound state calculations on the full IPS. In addition to the specific examination of hydrogen-OCS complexes a more general exploration of the bound states of hydrogen-molecule complexes will be presented, in particular focusing on the transition from an isotropic to an anisotropic potential with respect to hydrogen rotation, and on the role geometry plays in the angular momenta of the bound states.

[a] Higgins, *et al.* 61th International Symposium on Molecular Spectroscopy (2006)