

Abstract Submitted  
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**Rotational Spectra of Methane in Helium-4** ROBERT ZILLICH, Kepler University, Linz, BIRGITTA WHALEY, University of California, Berkeley — We extend correlated basis function (CBF) theory, in combination with diffusion Monte Carlo simulations, to spherical top molecules solvated in superfluid  $^4\text{He}$  droplets. Similarly to our previous CBF work on linear molecules, the rotational excitations of a spherical top molecule are renormalized by a self energy which contains the  $^4\text{He}$  density modulation around the molecule as coupling. Due to the high symmetry of this density in the case of solvated spherical molecules the rotation- $^4\text{He}$  coupling turns out to be weak, and the corresponding reduction of the effective rotational constant is small. Furthermore, unlike for linear molecules, for spherical top molecules the symmetry of the gas phase rotational spectrum is not preserved. Instead, for excitations of total angular momentum  $J \geq 2$ , we find that the self energy induces a splitting of the rotational energies. We present results for the rotational spectrum of solvated  $\text{CH}_4$  and  $\text{CD}_4$  for several available He- $\text{CH}_4$  potential energy surfaces, and compare with experimental results measured recently. We propose to measure spectra of partially substituted methane (e.g.  $\text{CDH}_3$ ) to investigate the effect of symmetry breaking on the rotation- $^4\text{He}$  coupling strength.

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