SPECTROSCOPY OF OCS IN PURE AND HYDROGEN-DOPED HELIUM CLUSTERS: MICROSCOPIC QUANTUM THEORETICAL TREATMENT

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We present a comprehensive theoretical analysis of the spectroscopy of the OCS molecule in low temperature quantum fluid clusters, employing path integral, spectral evolution, and hydrodynamic calculations. Calculations of the rotational energy level structure of OCS in superfluid clusters of ^{4}He, and the modifications of this that are induced by complexing with hydrogen molecules are presented from several complementary quantum methodologies. We summarize the insights gained into the extent of rigidity of the complexes of OCS with He and with H_2, the effect of molecular rotation on quantum calculations of the solvating helium density, and implications for microscopic analysis of spectroscopically measured rotational constants for OCS and its complexes in helium clusters.