

Spectral Signatures of Hydrogen Thioperoxide (HOSH) and Hydrogen Persulfide (HSSH): Possible Molecular Sulfur Sinks in the Dense ISM

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Abstract

Molecular sulfur in the dense interstellar medium (ISM) has eluded astronomical observation for nearly 50 years; but, somewhere there exists a molecular sulfur sink in the dense ISM where it may be hiding. Recent discovery of hydrogen peroxide (HOOH), and its suggested formation pathway, may provide a natural starting point for this investigation in the form of two sulfur-bearing analogs of HOOH: hydrogen thioperoxide (HOSH) and hydrogen persulfide (HSSH). The present theoretical study couples the accuracy in the anharmonic fundamental vibrational frequencies from explicitly correlated coupled cluster theory with the accurate rotational constants generated by canonical high-level coupled cluster theory to produce rovibrational spectra for use in the potential astronomical observation of HOSH and HSSH. The ν_6 mode for HSSH at 886.1 cm^{-1} is within 0.2 cm^{-1} of gas phase experiment, and the B_0 rotational constant for HSSH of 6979.5 MHz is within 9.0 MHz of the experimental benchmarks implying that the current methodology is accurate and reliable. The most intense vibrational transition for each molecule are the torsions, with HOSH having the more intense transition of 117 km/mol compared to HSSH's intensity of 23 km/mol . Further more HOSH has a larger net dipole moment of 1.60 D compared to HSSH's 1.15 D . While HOSH may be the more likely candidate of the two for possible astronomical observation *via* vibrational spectroscopy due to the notable difference in their intensities, both HSSH and HOSH have large enough net dipole moments to be detectable by rotational spectroscopy to discover a possible molecular sulfur sink in the dense ISM.