

Abstract Submitted
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High Magnetic Field calculations of Molecular Hydrogen Dissociation¹ JONATHAN JERKE, Texas Southern Univ, SAMINA MASOOD, University of Houston Clear Lake, CHRIS TYMCZAK, Texas Southern Univ — The dissociation curves of molecular Hydrogen in a 1 and 10 milli au magnetic field are calculated in a Generalized Hartree Fock theory, GHF. In GHF, the electrons are allowed to spin in any direction at each point in space, i.e. torsional spin waves. Torsional spin wave magnitude on the atomic cores, as well as the transition from a covalent bond to two doublets, is observed. The vibrational spectra of the ground state is also reported. By comparison, based on absolute accuracy of matrix elements and zero field calculations, these calculations of electronic structure achieve 3-4 significant digits on absolute energy in a generalized Hartree Fock calculation.

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