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Toward the Infrared Spectroscopic Observation of SiH^+_5: The Silanium Ion

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Abstract

Ab initio quantum mechanical methods, including the self-consistent field, single and double excitation configuration interaction, and single and double excitation coupled cluster, have been applied to six stationary points on the SiH^+_5 potential energy hypersurface. Equilibrium geometries were determined using analytic energy first derivative techniques. Relative energies of stationary points have been obtained. Harmonic vibrational frequencies of the global minimum were obtained at all levels of theory. Basis sets used include double-zeta plus polarization and triple-zeta plus double polarization. SiH^+_5 should be regarded as involving weakly bound H_2 and SiH^+_3 subunits, with a dissociation energy of only about 10 kcal/mol. Pseudorotation was found to be unfavorable in the SiH^+_5 ion.