DETECTION OF TWO HIGHLY-STABLE SILICON NITRIDES BY CHIRPED-PULSE ROTATIONAL SPECTROSCOPY: HSiNSi and SiH_3NSi

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By means of chirped-pulse and cavity Fourier transform microwave spectroscopy of a supersonic molecular beam, the rotational spectra of two new silicon nitrides, HSiNSi and SiH_3NSi, have been detected in a discharge through dilute gas mixtures of either molecular nitrogen or ammonia and silane. Both molecules appear to be highly stable: they are by far the most readily observed silicon-nitrogen containing molecules in the 6-20 GHz frequency range, even though neither has apparently been the subject of prior experimental or theoretical studies. Density-functional calculations performed here confirm that both structures are deep minima on their respective potential energy surfaces, and each possesses a sizable dipole moment. Owing to their high abundance, in excess of 10^{12} molecules/gas pulse, extensive isotopic spectroscopy has been undertaken for both. Detection of other silicon-nitride clusters in the transition region from atomic constituents to Si_3N_4 by similar means may be promising.