ROTATIONAL SPECTROSCOPY OF SILICON-NITROGEN MOLECULES: SiH_3NC AND NH_2Si

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Silicon-nitrogen compounds are an important class of molecules, with implications in fields ranging from molecular astrophysics as refractory species in evolved stars, and in terrestrial applications such as chemical vapor deposition. In this talk, we present the gas-phase detection and microwave rotational spectroscopy of two new silicon-nitrogen molecules: silyl isocyanide (SiH_3NC, $\tilde{X}\ ^1A_1$) and aminosilane (H_2NSi, $\tilde{X}\ ^2B_2$). Both species are readily produced in an electrical discharge, combining silane (SiH_4) with either methyl cyanide (CH_3CN) or ammonia (NH_3) to produce the species of interest. Using Fourier-transform and double resonance microwave spectroscopy, we were able to measure the three lowest rotational transitions (at 10, 20, 30 GHz) for SiH_3NC, and for H_2NSi, the two lowest transitions at 30 and 60 GHz. By substituting the precursors for rare-isotope enriched ones (e.g. $^{15}NH_3$), we were able to extend the measurements to several isotopologues: $SiH_3^{15}NC$ and $SiH_3N^{13}C$ for silyl isocyanide, and $H_2\ ^{15}NSi$, D_2NSi for aminosilane. The experiments are supplemented by high level quantum chemical calculations, which provided predictions of rotational constants, multipole moments, and in the case of aminosilane, the spin-rotation interaction tensor elements.