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Vibrational and Rotational Spectral Data for Possible Interstellar Detection of AlH_3OH_2, SiH_3OH, and SiH_3NH_2[1] ALEXANDRIA WATROUS, BRENT WESTBROOK, MEGAN DAVIS, RYAN FORTENBERRY, University of Mississippi — This is the first full set of vibrational and rotational spectral data needed to aid in the detection of AlH_3OH_2, SiH_3OH (silanol), and SiH_3NH_2 (silylamine) in astrophysical or simulated laboratory environments through the use of quantum chemical computations at the CCSD(T)-F12b level of theory employing quartic force fields for the three molecules of interest. Previous work has shown that SiH_3OH and SiH_3NH_2 contain some of the strongest bonds of the most abundant elements in space. AlH_3OH_2 also contains highly abundant atoms and represents an intermediate along the reaction pathway from H_2O and AlH_3 to AlH_2OH. All three of these molecules are also polar with AlH_3OH_2 having the largest dipole of 4.58 D and the other two having dipole moments in the 1.10–1.30 D range, large enough to allow for the detection of these molecules in space through rotational spectroscopy. The molecules also have substantial infrared intensities with many of the frequencies being over 90 km mol^{-1} and falling within the currently uncertain 12–17 μm region of observed infrared spectra.

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Alexandria Watrous
University of Mississippi

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