

Can We Find Interstellar Nitrogen Hiding in Exotic Molecules?

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Abstract: The nitrogen molecule is one of the most strongly bound systems known. It also makes up a vast majority of the Earth's atmosphere. However, the origin of this molecule in the atmosphere is still largely unknown. Is the nitrogen primordial to the Earth or was it formed through biological or geological processes? One way to find out is through observation of stellar systems similar to the early solar system. The chief issue is that N_2 is not observable through vibrational or rotational means due to a lack of a permanent or induced dipole moment, and electronic observation is difficult to quantify. As a result, molecular tracers must be observed, instead. Dinitrogen bonds are notoriously unstable making laboratory synthesis and observation is difficult for such species. However, quantum chemical techniques are not hampered in such ways making them ideal for spectral prediction and structural analysis. This work will discuss the structure, binding, and relative energetics of the $NNHNN^+$, $NN-HCO^+$, and $CO-HNN^+$ proton-bound complexes where the proton-shuttle motion is exceptionally bright. Additionally, the rovibrational spectra and relative energies of $HNNS$ radicals will be described where previous work has predicted these species to be intermediates in the formation of N_2 and the recently observed SH radical.