IDENTIFYING UNKNOWN MOLECULES WITH PROBABILISTIC DEEP LEARNING AND ROTATIONAL SPECTROSCOPY

KELVIN LEE, *Radio and Geoastronomy Division, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, USA*; MICHAEL C McCARTHY, *Atomic and Molecular Physics, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, USA*.

A major bottleneck in the analysis of broadband chirped-pulse microwave spectra is the identification of unknown molecules. Often, a set of molecular frequencies are fit to an effective Hamiltonian, whereby a set of spectroscopic parameters are used to infer the molecular carrier. These constants are reproduced with electronic structure calculations through a trial and error process, accompanied by chemical intuition involving the precursors used, and the reaction conditions (e.g. electrical discharges). As the size of the molecules increase, the combinatorics of many hundreds to thousands of possible isomers becomes an intractable problem for chemical intuition alone.

Since spectroscopic parameters are only weakly informative, we turn to statistical inference to complement conventional spectroscopic analysis. In this talk, I will discuss a new framework for identifying unknown molecules by performing inference on spectroscopic parameters with probabilistic deep learning. Using a series of decoder architectures, we are able to infer the approximate molecular composition/formula and what functional groups are present using only the rotational constants and derived quantities κ (the asymmetry parameter) and Δ (the inertial defect), and approximate magnitudes and projections of the dipole moments.