

# Rotationally Resolved Spectroscopy for Interstellar Chemistry and Precise Molecular Structure Determination

**Don McNaughton**

*School of Chemistry, Monash University, Clayton, Victoria, Australia 3800*

**E-mail: donald.mcnaughton@monash.edu**

## Abstract

Much of the direct knowledge of interstellar chemistry arises from the powerful combination of radio and mmwave telescopes, rotational resolved spectroscopy and computational and theoretical modelling. Precise molecular structures can also be calculated through the combination of rotational spectroscopy and computational chemistry. Over the last 50 years developments in each of these scientific disciplines has resulted in the identification of around 200 molecules in the interstellar medium or circumstellar shells, and a convergence in the values of the molecular structural parameters derived by experiment and theory. A number of example chemical systems from cm-wave, mm-wave and Far-IR spectroscopy will be explored to outline these developments and the current state of the art in the area.

Propadienone: Is the heavy atom chain bent or linear and why despite being the lowest in energy is it the only one of three  $C_3H_2O$  isomers not detected in the ISM?

Glycine has many conformers, none of which has yet been detected in the ISM despite a number of searches and a raft of computational studies.

Cyano-substituted molecules: The cyano group is ubiquitous in the molecules detected in the ISM primarily because it provides a large dipole moment leading to strong signals. The largest ISM molecules apart from  $C_{60}$  and  $C_{70}$  are the long chain cyanopolynes. Does it provide a way to detect aromatic systems in the ISM?

Sulfur containing species are rare. Which are the best candidates?

Precise molecular structures and the role of computational chemistry in determining them – semi-experimental structures. Eg. The ‘privileged’ drug precursor 8 hydroxyquinoline.

**Keywords:** Microwave spectroscopy, molecular structure, interstellar molecules