Cold molecules are a new frontier for quantum physics and chemistry. In the microwave regime, we observe discrete spectra of the molecules’ rotational transitions, with 100 to 5,000 distinguishable lines in a typical spectrum. The assigned microwave spectrum provides an accurate measurement of the rotational constants $A$, $B$, and $C$ of a molecule; these constants are related to the principal moments of inertia $I_x$, $I_y$, and $I_z$ via:

$$A = \frac{\hbar}{8\pi I_x}, \quad B = \frac{\hbar}{8\pi I_y}, \quad C = \frac{\hbar}{8\pi I_z}$$

If we know a molecule’s rotational constants, generating the molecule’s theoretical spectra is a simple matter of running decades-old software.

The challenge is, if we have a spectra of an unknown mixture, how do we figure out which rotational constants belong to the molecules in the mixture? As rotational constants uniquely identify a molecule, this is the same as asking what molecules are in the mixture. This problem, called the assignment problem, has for decades eluded all but a few human experts.

The heart of the assignment problem is to correctly “guess” a set of line assignments. An assignment is a pairing between a frequency and the quantum numbers $J$, $K_a$, and $K_c$ of its two states. To find the three rotational constants, we must guess at least three lines to provide a solvable system.

We vastly reduce the number of guesses required through pattern finding. As an example, consider the 14858.2 MHz line of $\beta$-pinene above. Note that 14858.2 + 17205.3 – 16405.7 – 15657.8 = 0. By only considering four lines that add up to approximately zero, we have significantly narrowed our search space. These four lines are actually part of a larger structure, which we’ve termed a scaffold:

$$A = 14858.2, \quad B = 17205.3, \quad C = 16405.7, \quad D = 15657.8$$

We are working towards the ability to calculate the $x$, $y$, and $z$ positions of atoms in the molecular backbone. This would have far-reaching ramifications for atomic, molecular and optical physics; astrochemistry; molecular biology; pharmaceuticals; forensics; and many more scientific fields.

**ACKNOWLEDGMENTS**

Dave Patterson        Sathya Guruswamy        Samantha Davis        Jin Kim