RESEARCH NEWS

Frequency Combs Tackle Large, Complex Molecules

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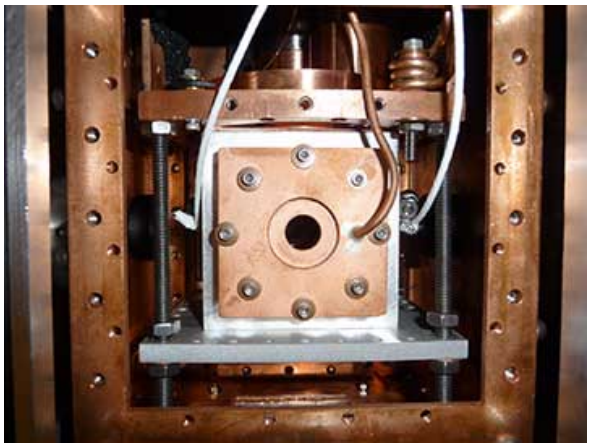

The JILA apparatus couples a mid-infrared frequency comb to an optical cavity containing a buffer gas chamber, in which samples are cooled to near absolute zero. “Calming down” the sample molecules by molecular cooling results in a cleaner, more rapidly interpreted “molecular fingerprint” in the frequency-comb spectra. [Image: Spaun/JILA]

Frequency-comb spectroscopy, recognized with a Nobel Prize in 2005, has brought unprecedented specificity and resolution to studies of molecular structure and dynamics. But it’s been difficult to apply to molecules consisting of more than 10 atoms or so. Physicists at the U.S. National Institute of Standards and Technology’s JILA unit in Boulder, Colo., and Harvard University, Cambridge, Mass., have now hit upon a method to bring the power of frequency combs to bear on much larger, more complex molecules (Nature, doi: 10.1038/nature17440 (http://dx.doi.org/10.1038/nature17440)). The secret: cool things down a bit.

Spectral congestion

In ordinary cavity-enhanced direct frequency-comb spectroscopy (CE-DFCS), a frequency comb—an “optical ruler” consisting of hundreds of thousands of equally-spaced spectral lines, usually created with a mode-locked laser—is coupled to a high-finesse optical cavity containing samples of the molecule of interest. Absorption of a fraction of the comb energy at the resonant frequencies of molecular-bond vibrations creates a “molecular fingerprint” that can be used to identify chemical species.

The setup offers a great mix of resolution (through the finely spaced lines of the comb) and sensitivity (through the cavity enhancement, which allows the comb light to make thousands of round trips within the cavity). The problem is that molecules larger than a few atoms have so many potential rotational and vibrational states (on the order of millions) that they can muddy up the exquisitely refined comb signal and make identifying the molecule a substantially dicier proposition—a complication with the very apt name of “spectral congestion.”

Cooling yields a “drastically simplified” view

To clean up the signal from large molecules, the JILA-Harvard team, led by OSA Fellow Jun Le, made a simple but powerful modification to the basic CE-DFCS approach. In the team's setup, the output from a mid-infrared frequency comb, spanning wavelengths from 2.8 to 4.8 μm, is coupled to a high-finesse optical cavity consisting of twin high-reflectivity mirrors surrounding a buffer gas cell containing the sample. The cell has two inlet ports—one port for piping in the large molecules to be identified, and the other for pumping in a supply of super-cold (5 to 10 K) helium buffer gas.

Multiple collisions between the warm sample molecules and the cold helium lowers the temperature of the sample molecules to the area of 10 K. The cooling dramatically reduces the rotational and translational degrees of freedom, resulting in a “drastically simplified” absorption spectrum that’s easier and much faster to interpret than a room-temperature signal. “Instead of just a glob of mountains in the signal,” Ye noted in a press release, “you can start to see the individual trees.”

Sensing, manufacturing and research applications

The team tested the system against a set of organic molecules, ranging in size from seven to 26 atoms, that feature a large suite of potential vibrational complexities, and that also are potentially important in applications like sensing explosives, producing pharmaceutical and plastics, and other areas. The researchers found that they could extract usable spectra at a rapid rate of 30 to 90 minutes per molecular species. And the signals for these complex molecules lined up extremely well with simulated spectra for each species.

The JILA scientists are now working to broaden the range of applications for the instrument—for example, through modifications to the buffer gas cell that will allow interrogation of more reactive molecular free-radical species, and over longer timeframes. Such modifications, they believe, could open up possibilities for using time-resolved frequency-comb spectroscopy to study chemical reactions in real time.

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