Enhanced Spectroscopic Detection of Molecules Combining IR Spectroscopy with Signal Processing

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Detection of molecules using various vibrational spectroscopies (IR or Raman) is important for many applications. Specifically, detection of dangerous substances needs to be successful at very low concentrations where the spectrum of the molecule of interest is masked by noise or other signals. In this application, a high quality experimental reference spectrum also may not be available.

We show by computational modeling that it must be possible to improve spectroscopic detection by combining vibrational spectroscopy with signal processing, specifically, with optimal filtration. We consider the vibrational spectrum as a signal on the energy axis and apply matched filtering on that axis. The matched filter is programmed using a computed spectrum. On the example of a nerve agent molecule, we show that this allows detecting a molecule by its vibrational spectrum even when the recorded spectrum is completely buried in noise, when conventional spectroscopic detection would fail (Fig. 1). Detection is predicted to be possible with signal-to-noise ratios in recorded spectra as low as 0.1. We study the importance of spectral range used for detection as well as of the quality of the computed spectrum used to program the filter, specifically, the role of anharmonicity and of parameters of the ab initio calculation used to model the spectrum. The use of the full spectral range rather than of a narrow spectral window with key vibrations is shown to be advantageous, as well as accounting for anharmonicity.

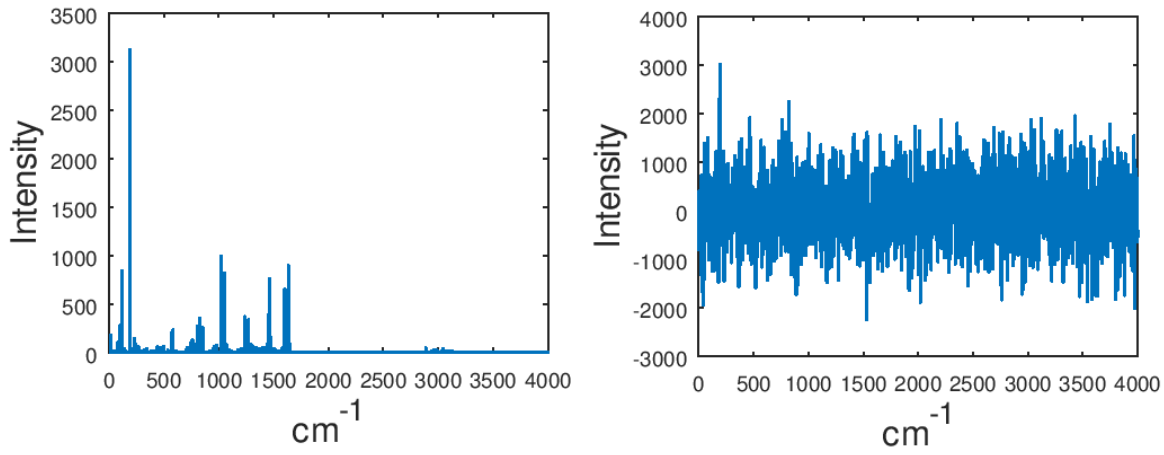

Fig. 1. Example of a molecular spectrum (left) and the same spectrum mixed with noise (right) where the detection is still possible with the proposed technique.