## Molecular Simulations for the Spectroscopic Detection of Atmospheric Volatiles

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Unambiguously identifying molecules in spectra is of fundamental importance for a variety of scientific and industrial uses; a compelling modern focus is the spectroscopic detection of volatiles in exoplanet atmospheres. Analyses of observational spectra require information about the spectrum of each of its putative components. However, spectral data currently only exist for a few hundred molecules and only of fraction of those have complete spectra (e.g. $H_2O$, $NH_3$). Consequently, remote detections of molecules are vulnerable to false positives, false negatives and miss-assignments. There is a key need for spectral data for a broad range of molecules.

Using a combination of experimental measurements, organic chemistry, and quantum mechanics, ATMOS (Approximate Theoretical MOlecular Spectra) is a programme that:
a) Provides approximate spectral data (band centres and relative intensities) for thousands of molecules in seconds.
b) Assesses hundreds of molecules simultaneously, highlighting patterns and any distinguishing features. Traditional methods for obtaining spectra are extremely costly and time-consuming (i.e. months/years per molecule); ATMOS will inform prioritisation protocols for future high accuracy studies.
c) Demonstrates that, at low resolution, individual spectral features could belong to a large number of molecules. Molecular detections in spectra are often made by assigning one, or a few, spectral features to a given molecule. ATMOS can highlight ambiguities in such molecular detections and also direct observations towards spectral regions that reduce the degeneracy in molecular identification.

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