COMPUTATIONAL INFRARED SPECTROSCOPY OF PHOSPHORUS-CONTAINING POTENTIAL BIOSIGNATURES

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Phosphine is now well established as a biosignature, which has risen to prominence with its recent tentative detection on Venus. To follow up this discovery and related future exoplanet biosignature detections, it is important to spectroscopically detect the presence of phosphorus-containing (P-molecules) atmospheric molecules that could be involved in the chemical networks producing, destroying or reacting with phosphine. Here, we present a high-throughput approach utilising established computational quantum chemistry methods (CQC) to produce a database of approximate infrared spectra for 958 P-molecules that could be spectroscopically detected in planetary atmospheres. We performed the calculations with the strongly performing harmonic ωB97X-D/def2-SVPD model chemistry for all molecules and tested the more sophisticated and time-consuming GVPT2 anharmonic model for 250 smaller molecules. Limitations to our automated approach, particularly for the GVPT2 method, are considered along with pathways to future improvements. Our CQC calculations significantly improve on existing spectroscopic data by providing quantitative intensities, new data in the fingerprint and higher frequency regions, and improved data for fundamental transitions based on the specific chemical environment.