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Characterizing Exoplanet Atmospheres : A Complete Line List for Phosphine

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Abstract

The ability to characterise the atmospheres of cool stars, brown dwarfs and exoplanets requires fundamental data for all species contributing significantly to their opacity. However, with notable exceptions such as water and ammonia, existing molecular line lists are not sufficiently accurate or complete to allow for a full spectroscopic analysis of these bodies.

ExoMol (www.exomol.com [1]) is a project that aims to rectify this by generating comprehensive line lists for all molecules likely to be detected in the atmospheres of cool astrophysical objects in the foreseeable future. The spectral data is generated by employing ab initio quantum mechanical methods, performing empirical refinement based on experimental spectroscopic data and harnessing high performance computing.

Here we present our work on phosphine, (PH_3), an equilateral pyramidal molecule (the phosphorus analogue to ammonia). Phosphine is known to be important for the atmospheres of giant-planets, cool stars and many other astronomical bodies. Rotational transition features of phosphine have been found in the far-infrared spectra of Saturn and Jupiter [2, 3], where it is a marker for vertical convection zones. A computed room temperature line list of phosphine is presented here [4], illustrated in the accompanying figure 1. This line list is a precursor to a high temperature equivalent to be produced in the near future, necessary for the analysis of cool stars and brown dwarfs. All the transitions' energy levels and Einstein A-coefficients were computed using the program TROVE [5].

Acknowledgements

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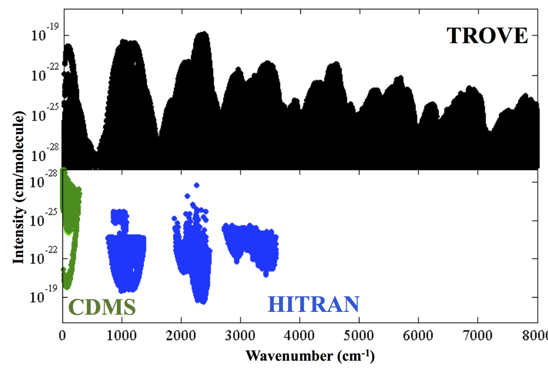

Figure 1: Comparison of the intensities (cm/molecule, log scale) and wavenumber (cm^{-1}) of transitions between TROVE and experimental data (HITRAN and CDMS). The full range of calculations contained 137 million lines versus the 20,000 experimental lines.

References

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