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ExoMol: Large-scale production of line lists for molecules important for modelling of planetary atmospheres

S. N. Yurchenko and J. Tennyson
Department of Physics and Astronomy, University College London, London, WC1E 6BT, UK (s.yurchenko@ucl.ac.uk)

Abstract

The spectral characterization of astrophysical objects cool enough to form polyatomic molecules (the atmospheres of planets, brown dwarfs, planetary discs etc.) requires a huge amount of fundamental molecular data. With a few exceptions the existing molecular line lists are not sufficiently accurate and complete. The aim of ExoMol [1] is to generate comprehensive line lists for all molecules likely to be observable in exoplanet atmospheres in the foreseeable future (see *www.exomol.com* for more details).

We identified the following 40 species that are important sources of opacity in (exo)planets and brown dwarfs and where there is currently a lack of fundamental data on wavelength and temperature-dependent absorption:

- Diatomics: AlO, AlH, BeH, CaH, C_2, CrH, FeH, HF, HCl, KCl, MgH, MgO, NaH, NaCl, NiH, O_2, SiO, SiH, S_2, SH, TiH, TiO, VO, YO
- Triatomics: C_3, H_2S, SO_2
- Tetratomics: H_2CO, H_2CS, HCCH, HOOH, PH_3, SO_3
- Pentatomics: CH_4, HNO_3
- Larger molecules: C_2H_4, C_2H_6, C_3H_8, P_2H_2, P_2H_4

The production of comprehensive and very large rotation-vibration and rotation-vibration-electronic line lists requires a mixture of first principles quantum mechanical methods and empirical tuning based on laboratory spectroscopic data and makes extensive use of state-of-the-art computing. These and other aspects of molecular line lists, their production and astrophysical applications will be discussed. The contribution will make specific reference to molecules for which line lists have recently been completed or are nearing completion: phosphine, hydrogen sulphide, hydrogen peroxide, methane, formaldehyde, nitric acid as well as to a number of diatomic molecules of astrophysical importance, see Fig. 1.

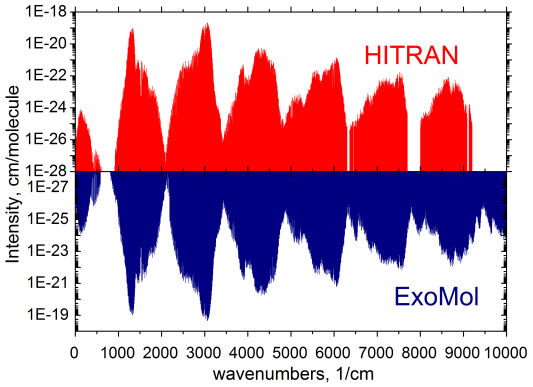

Figure 1: Absorption spectrum of CH_4 at $T = 300$ K (log-scale): Experiment (HITRAN) *vs.* Theory (ExoMol)

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Acknowledgements

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References

[1] J. Tennyson and S. N. Yurchenko. ExoMol: molecular line lists for exoplanet and other atmospheres. 425:21–33, 2012.