ExoMol: Molecular line lists of Exoplanets and other atmospheres

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Spectral characterization of astrophysical objects cool enough to form molecules in their atmospheres (cool stars, extrosolar planets and planetary discs) requires considerable amounts of fundamental molecular data. The existing molecular line lists (with some exceptions) are generally not sufficiently accurate and complete. The ExoMol project is actively generating comprehensive line lists for *all* molecules likely to be observable in exoplanet atmospheres in the foreseeable future. This is a huge undertaking which will mean providing in excess of 10^{11} spectral lines for a large variety of molecular species, see Tennyson and Yurchenko (*Mon. Not. R. Astron. Soc.*, **425**, 21 (2012))

The physics of molecular absorptions is complex and varies between different classes of absorbers. The project is therefore divided into following topics (a) diatomic, (b) triatomics, (c) tetratomics, (d) methane and (e) larger molecules. Special techniques are being developed to treat each case. The majority of diatomic systems to be tackled are open shell species involving a transition metal atom; the opacity is provided by the transitions between the many low lying electronic states of the system. The calculation of rotation-vibration line lists for closed-shell triatomic systems is now relatively straightforward provided enough care is taken in deriving the potential energy and dipole surfaces. An H_2S line list is nearing completion and studies on C_3 have started. Accurate rotation-vibration line lists for hot tetratomic molecules such as ammonia (complete), phosphine (nearing completion), acetylene (initial study published), hydrogen peroxide (initial study complete), SO_3 (room temperature line list complete) and formaldehyde, test what is computationally possible at present. An initial line list for hot (1000 K) methane has been completed and is being improved. Work on systems larger than this is just commencing. Data from this project can be accessed at *www.exomol.com*.