The ExoMol project: molecular line lists for the opacity of exoplanets and other hot atmospheres

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The ExoMol project aims to provide comprehensive line lists for models of hot astronomical bodies which contain molecules [1]. These line lists can be huge: in excess of 10 billion lines for molecules such as methane or CH_3Cl. Studies show that as the temperature increases treating the very large number of weak lines is essential to model opacities correctly [2].

Line lists are computed using variational nuclear motion programs starting from *ab initio* potential energy and dipole moment surfaces. *Ab initio* dipoles can be computed with an accuracy than means the uncertainty in the resulting intensities is competitive with the best experiment [3]. However, even the best *ab initio* potentials give transition frequencies which are far from true spectroscopic accuracy. This particularly true for species containing transition metal atoms [4], some of whom, such as TiO, are known to be important in stellar atmospheres and are thought to control thermal inversion in some classes of exoplanets. As a result extensive use is made of experimental data to improve potential energy surfaces and other aspects of the calculation.

The calculated line lists for over 50 molecules are available as part of the ExoMol database (www.exomol.com) [5]. For each molecule/isotopologue of interest the database provides energy levels (and hence transition frequencies) and Einstein A coefficients, along with other key properties including lifetimes of individual states, temperature-dependent cooling functions, Landé g-factors, partition functions, cross sections, k-coefficients and transition dipoles with phase relations. These data are widely used not only for astrophysics but also terrestrial applications ranging from combustion modelling to molecular steering.

References

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