ExoMol: molecular line lists for exoplanet and other hot atmospheres

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The ExoMol database (www.exomol.com) provides comprehensive line lists of molecular transitions (line lists) which are valid over extended temperatures ranges [1]. The database currently contains line lists for 90 molecules (250 isotopologues) and a total of about 10^{12} transitions [2]. The database stores energy levels (and hence transition frequencies) and Einstein *A* coefficients with other key properties, including lifetimes of individual states, temperature-dependent cooling functions, Landé *g*-factors, partition func- tions, cross sections, and transition dipoles with phase relations. Recently we have started including temperature-dependent photodissociation cross sections [3].

The basic methodology we use starts with detailed electronic structure calculations of potential energy and dipole moment surfaces, plus spin-orbit and other couplings where required. Variational methods are used to treat the nuclear motion and potentials are generally tuned to reproduced observed data. Conversely transition intensities can often be predicted using *ab initio* dipole moments to accuracies competitive with the best experiments [4]. While for many closed shell molecules using tuned potentials and *ab initio* dipoles gives excellent results, this is not true in all cases. Particularly challenging are diatomic molecules containing a transition metal. Many of these molecules have low-lying electronic states which are known to absorb strongly in the atmospheres of cool stars and brown dwarfs, and are thought to be important in exoplanetary atmospheres. Current electronic structure programs struggle to give accurate results for these species and experimental data is usually at best partial.

The recent development of cross correlation spectroscopy to identify molecules in the atmospheres of exoplanets has emphasized the need for highly accurate transition frequencies. In general these can only be achieved using experimental data for which we use the MARVEL (measured active vibration rotation energy levels) procedure [5]. For some molecules, VO for example, it is necessary to explicitly include hyperfine effects in the spectroscopic model. We have therefore extended our diatomic nuclear motion program Duo to include a full treatment of hyperfine interactions [6] but have found the treatment of these effects in electronic structure codes to be very patchy [7].

References

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