Computing molecular line lists for atmospheric applications: completeness versus accuracy

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The ExoMol team at UCL is the world leader in providing spectroscopic data for hot atmospheric applications. The ExoMol database hosts molecular line lists for about 90 molecules plus many isotopologues. The ExoMol data base (www.exomol.com) has become the go to place for data on hot molecules for studies of hot environments.

Production of ExoMol line lists is based on the application of rigorous quantum mechanical methods informed by laboratory experiments, rather than on direct measurements. The ExoMol philosophy has therefore been to make a rigorous quantum mechanical formulation of the spectroscopic problem for each molecule, to use the best practicable method for solving this problem, and to then use any available experimental data to improve our spectroscopic model. We describe this as "first principles theory informed by experiment". Methods of producing highly accurate molecular line list for modern high-resolution spectroscopic applications to meet the competing demands of completeness versus accuracy will be discussed.