How to Characterise Uncertainties in Molecular Opacities: An ExoMol Study

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Accurate molecular opacities are paramount for reliable exoplanet atmospheric characterisation and the interpretation of observed spectra. The ExoMol opacities (ExoMolOP) are based on line lists for over 100 molecules and 300 isotopologues, amounting to nearly a trillion individual transitions. The quality of the lines provided can vary significantly, ranging from high spectroscopic resolution to being only applicable for low-resolution applications. This information is recorded in individual line uncertainties, provided alongside the description of molecular or atomic states. However, this information is not propagated to the opacity tables. As a result, high-quality spectroscopic regions can be mixed with low-quality data. In this talk, I will discuss ideas on how uncertainties of the molecular opacities can be defined and present our methodology for a robust propagation of the line uncertainties to the molecular cross sections. The associated data format for storing this information in the database, as well as prospects for integrating these uncertainties into atmospheric retrievals, will also be discussed.