POPULATING THE EXOMOL DATABASE WITH LINESHAPE PARAMETERS: COLLISIONAL BROADENING AND SHIFTING OF ACETYLENE

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Collisional lineshape parameters are one of the indispensable data inputs necessary to produce absorption/emission cross-sections which are required in radiative transfer calculations and spectral retrievals. To be exhaustive, these parameters need to be calculated for a number of "radiating molecule – collisional perturber" pairs and at different temperatures. Of particular interest to a burgeoning field of exoplanetary science are the parameters at temperatures higher than those usually required for terrestrial studies, typically around 500–3000 K.

We discuss our recent progress in using a semiclassical method called Modified Complex Robert-Bonamy (MCRB) approach in calculating broadening and shifting coefficients of acetylene (C_2H_2) for several perturbers (H_2, He, N_2 and C_2H_2) for a large range of temperatures. This report is a part of the ongoing work to populate the ExoMol database with lineshape parameters, including the line list for acetylene aCeTy containing over 3 billion transitions, with little or no line broadening information. Comparisons with a large pool of existing theoretical and experimental acetylene data are shown. In addition, discussed are the difficulties arising when modelling vibrational dependence of lineshape parameters.

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