

PREDICTING THE ROTATIONAL DEPENDENCE OF LINE BROADENING USING MACHINE LEARNING

ELIZABETH R. GUEST, JONATHAN TENNYSON, SERGEI N. YURCHENKO, Department of Physics and Astronomy, University College London, London, United Kingdom.

Correct pressure broadening is essential for modelling radiative transfer in atmospheres, however data are lacking for the many exotic molecules expected in exoplanetary atmospheres. Here we explore modern machine learning methods to mass produce pressure broadening parameters for the molecules in the ExoMol database. To this end, state-of-the-art machine learning models have been used to fit to existing, empirical air-broadening data from the HITRAN database. A computationally cheap method for large-scale production of pressure broadening parameters is developed, which is shown to be reasonably (69%) accurate for unseen active molecules. This method has been used to augment the previously insufficient ExoMol line broadening data, providing air-broadening data for all ExoMol molecules, so that the ExoMol database has a full and more accurate treatment of line broadening. Suggestions are made for improved air broadening parameters for species present in atmospheric databases. Further work is in progress to incorporate data for line broadening by other perturbative species. This should lead to a final pipeline which can provide reasonable estimates of pressure broadening for any active-perturbing molecule pair.