USING MACHINE LEARNING TO MEET THE NEED FOR PRESSURE-BROADENING DATA IN EXOPLANETARY ATMOSPHERIC STUDIES

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The rapid growth of exoplanetary science has highlighted the need for large volumes of spectroscopic data. Simulations have demonstrated that dealing correctly with line broadening is crucial for understanding exoplanetary atmospheres[1]. The wide variety of atmospheres observed indicate that a wide variety of both active molecules and collision partners must be modelled. This work aims to fill this need. The HITRAN database[2] provides pressure-broadening parameters for all of its molecules. By comparison, the ExoMol database[3] currently only contains a very rudimentary treatment of line broadening[4], which urgently needs improving. The database contains many exotic species important on exoplanets, not covered by HITRAN. The molecules of interest form under unusual conditions and are difficult to study empirically. Pressure broadening is also computationally demanding for ab initio methods, where there are frequently no potential-energy surfaces available. Our solution is to use machine learning to provide *rotationally-dependent* estimates of line broadening parameters. This study collects HITRAN's line broadening data and trials various machine learning tools to extrapolate pressure-broadening parameters to new species; developing a method of automatic, large-scale production of missing data. To get an idea of the validity of our generated line broadening parameters, we compare them to rough semi-classical estimates containing no rotational dependence, that are easily computable for exotic molecular pairs. Our new calculated results will be used to update the ExoMol pressure-broadening diet[4] and populate the database.

[1] J.J. Fortney, T.D. Robinson, S. Domagal-Goldman et al., arXiv:1905.07064, (2019)

[2] I.E. Gordon, L.S. Rothman, R.J. Hargreaves, R. Hashemi et al., *J. Quant. Spectrosc. Radiat. Transf.*, **277**, 107949, (2022)

[3] J. Tennyson, Sergei N. Yurchenko, Ahmed F. Al-Refaie et al., *J. Quant. Spectrosc. Radiat. Transf.*, **255**, 107228, (2020)

[4] E.J. Barton, C. Hill, M. Czurylo et al., *J. Quant. Spectrosc. Radiat. Transf.*, **203**, Pages 490-495, (2017)