

## Machine Learning for Isotopologue Extraction

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Accurate isotopologue line lists are essential for modelling and interpreting high-resolution astronomical spectra, particularly for molecules like carbon monoxide (CO) that play a key role in the atmospheres of exoplanets, brown dwarfs, and cool stars. Existing approaches to isotopologue extrapolation used by ExoMol typically apply corrections based on variational calculations for the main isotopologue, assuming mass-dependent shifts and shared residuals across isotopologues.[1] While this method is effective and has proved useful,[2] it can struggle with higher accuracy requirements at elevated vibrational or rotational states, and/or for minor isotopologues.

In this work-in-progress, the application of machine learning (ML) techniques is explored to improve isotopologue extrapolation for CO. Predicting isotopologue rovibrational energy levels and transition frequencies using ML on a combination of variational calculations, hybrid line list data, and available experimental results. By learning patterns in the residuals between computed and corrected energy levels, these models are expected to generalize to isotopologues with sparse experimental data, such as  $^{12}\text{C}^{17}\text{O}$ ,  $^{13}\text{C}^{17}\text{O}$  or  $^{13}\text{C}^{18}\text{O}$ . Several machine learning architectures are currently being evaluated including kernel-based methods and neural networks, with plans to benchmark against traditional extrapolation techniques in terms of accuracy and robustness across a range of energy levels.

[1] O.L. Polyansky, A.A. Kyuberis, L. Lodi, J. Tennyson, R.I. Ovsyannikov and N.F. Zobov, *Mon. Not. R. astr. Soc.*, 466, 1363-1371.(2017).

[2] Ya.V. Pavlenko, S.N. Yurchenko, L.K. McKemmish and J. Tennyson, *Astron. Astrophys.*, 42, A77 (2020).