Efficient compression of molecular line lists: application of 'super-energies' to the ExoMol database
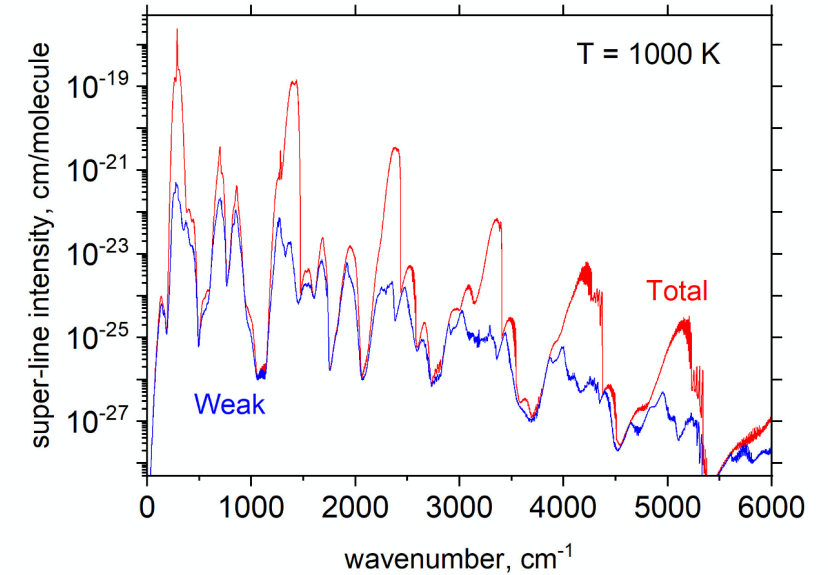
- Aim: compress the temperature dependent weak lines of the spectrum

- Method: for each line, find the lower state energy $\widetilde{E}_i$ and the Einstein-A coefficient A_{fi}

$$I(T) = \frac{A_{fi}}{8\pi\widetilde{\nu}_{fi}^2} \frac{g_f^{tot}}{Q(T)} \exp\left(-\frac{c_2\widetilde{E}_i}{T}\right)\left[1 - \exp\left(-\frac{c_2\widetilde{\nu}_{fi}}{T}\right)\right]$$
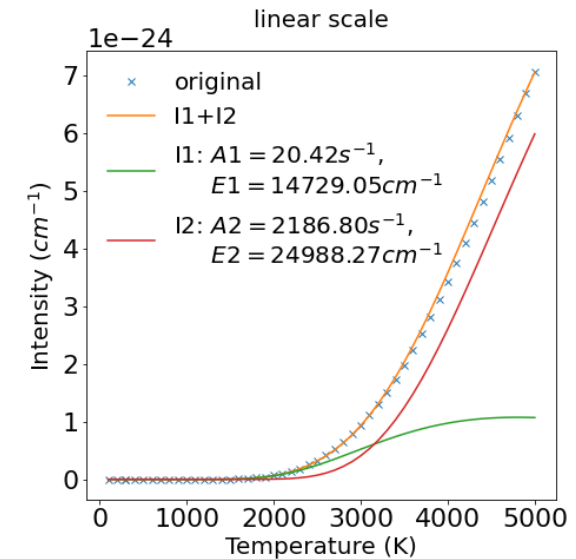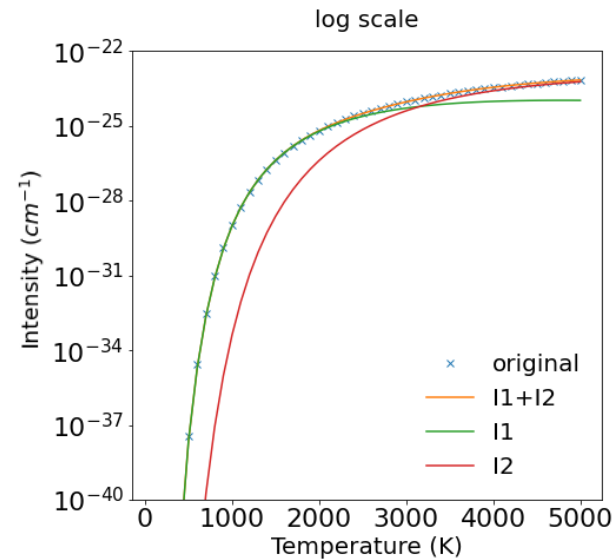
$$I(T) = I_1(T) + I_2(T)$$

4 parameters in total: 2 energies and 2 Einstein coefficients

- Result: compressed H_2O, SiO_2 and KOH

Line list example

H_2O super-lines using the super-energy method for $\widetilde{\nu}_k = 1048.97184$ cm^{-1}