# Extrapolating and Interpolating Hydrocarbon Cross Sections

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## Hydrocarbons Line Lists

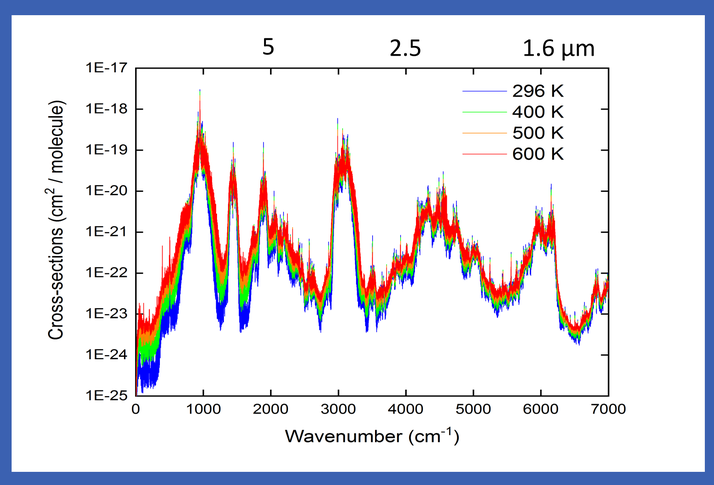
**Hydrocarbons are an important class of molecules for exoplanetary atmospheres.**

**We have computed hot line lists for $CH_4$, $C_2H_2$ and $C_2H_4$ so far.**

**This is expensive however requiring Tbs of data and 100s of hours of CPU time!**

**Ethylene has relatively little temperature variation[1]:**

**Can we approximate temperature dependence in a quicker and cheaper way?**




## Fitting Model

**For each measurement interval we fit the temperature dependence of the cross section to a cubic polynomial:**

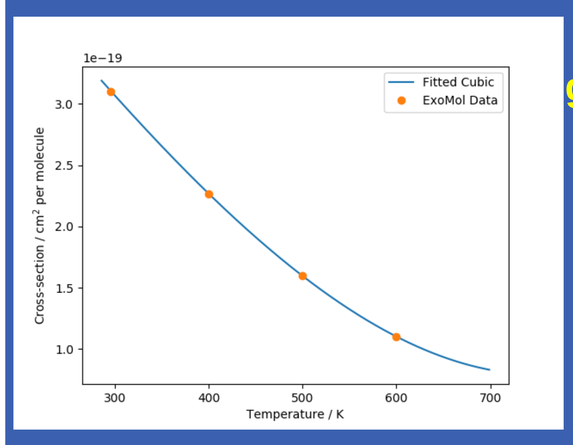
$$\sigma\ (T)_v = a + b*T + c*T^2 + d*T^3$$

**Cross sections taken from experimental data or calculated line lists as a model.**

**Check accuracy of interpolation and extrapolation using Integrated cross section:**

$$\int \sigma(T)_v = \text{constant}$$

## Ethene

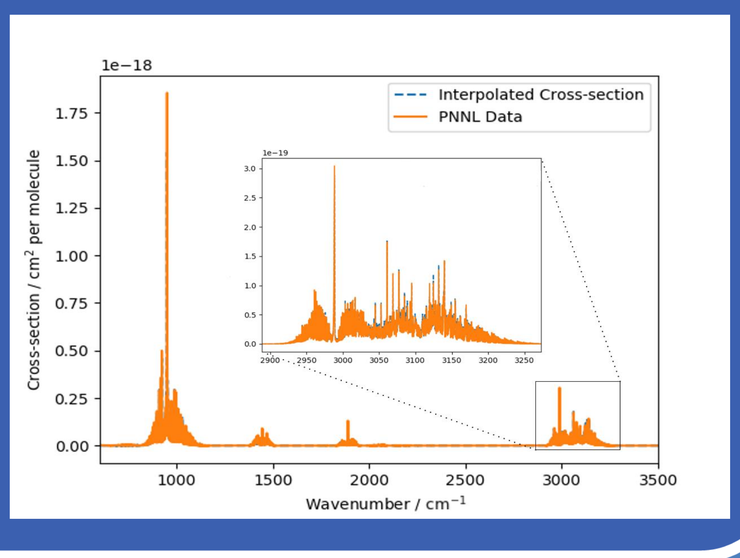



**Data taken from $C_2H_4$ line list[1] generated at 0.1 $cm^{-1}$ resolution.**

**Fit for Q-branch at 2945 $cm^{-1}$.**

**Comparison of fit to PNNL data at 323 K.**

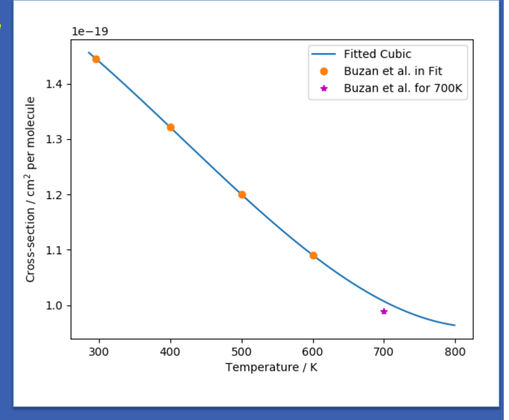
**Interpolation is very good and integrated opacity < 1.6% different.**

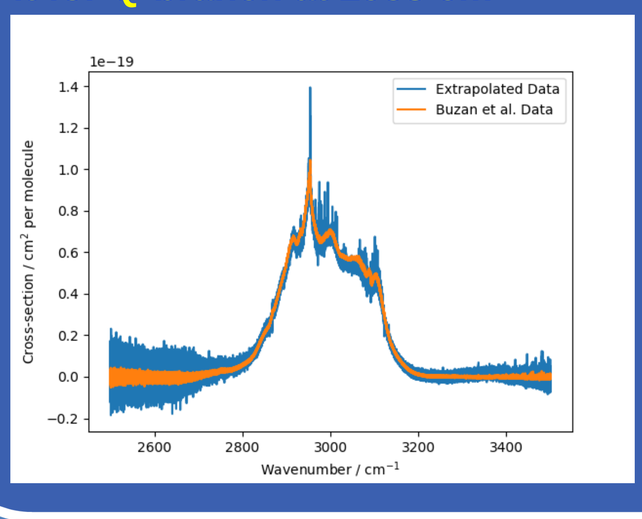



## Propene

**Experimental data from Buzan *et al.* at 0.05 $cm^{-1}$ resolution in 3 μm range for 296, 400, 500, 600 and 700 K.[3]**

**Fit for Q-branch at 2953 $cm^{-1}$.**



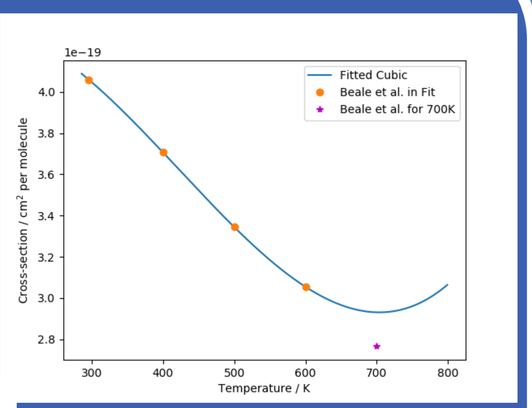



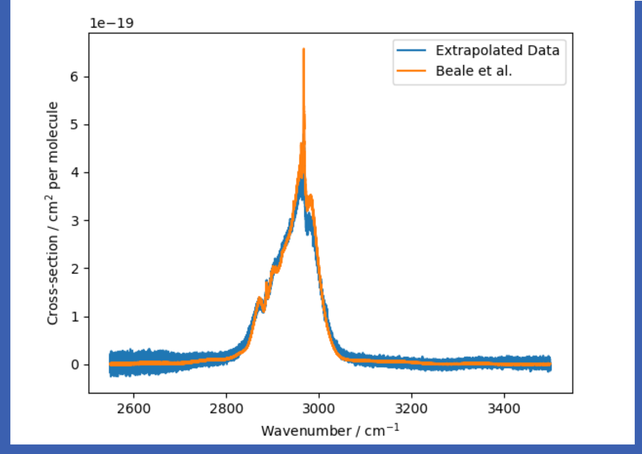

**700 K experiment and extrapolated fit. The integrated cross section differs by < 1%.**

## Propane

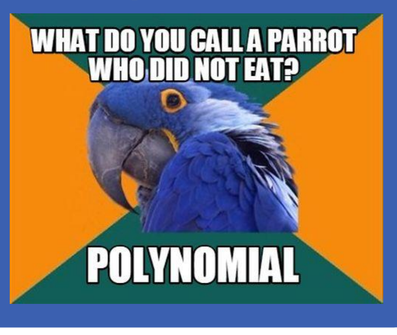
**Experimental data from Beale *et al.* at 0.05 $cm^{-1}$ resolution at 296, 400, 500, 600 and 700 K.[4]**

**Fit for R-branch at 2982 $cm^{-1}$.**




**700 K experiment and extrapolated. The integrated cross section differs by < 1%.**




## Discussion

- **Appears that many hydrocarbons have absorption cross sections which have simple temperature dependence.[2]**
- **Polynomial function fit to experimental data can reliably interpolate and extrapolate band shape while retaining integrated cross section.**
- **May be possible to use lower temperature measurements to extrapolate to higher data using e.g. linear or exponentials functions.**

**References: 1. Mant *et al.*, MNRAS, 478 (2018) 2. Klingbeil *et al.*, JQSRT, 107 (2007) 3. Buzan *et al.*, Mol. Astro. Phys. 3-4 (2016), 4. Beale *et al.*, JQSRT, 182 (2016).**