Extrapolating and Interpolating Hydrocarbon Cross Sections

Brendan Devlin-Hill, Barry Mant,[1] *and Sergey Yurchenko, UCL*

The calculation of line lists for large molecules is very intensive in terms of CPU time and memory. Our recent ethylene line[2] list required 100s of hours of CPU time and terabytes of data. However, for many larger hydrocarbons it appears infrared absorption cross sections show simple temperature dependence.[3] We present work on modeling the temperature dependence of ethylene, propene and propane absorption cross sections using model Exomol line list[2] and experimental data.[4,5] A simple polynomial fit to infrared cross sections is shown to give reliable interpolation between measured temperatures and modest extrapolation to higher temperatures. This simple model can reproduce band shapes relatively well as well as retain integrated absorption cross sections. This method, as well as more sophisticated models,[6] should allow the temperature dependence of many hydrocarbons to be accounted for in a cheap and simple manner.

[1]b.mant@ucl.ac.uk

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