Department of Physics
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Application of Complete Experimental Catalogs to Astrophysical Problems

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Abstract: There is a broad consensus that many, if not most, of the unidentified spectral lines in astrophysical spectra are due to transitions in highly perturbed excited vibrational states of a relatively small number of molecules, the astrophysical weeds. We have previously discussed a new experimental approach to address this problem. This approach does not require the time prohibitive assignment and quantum mechanical analysis of the traditional catalog method. However, the spectroscopic completeness of this approach results in a much larger database. These data can be transfer to the astrophysical community in a variety of ways, but because an order of magnitude larger number of lines is included, consideration must be given to implementation strategies. Strawman tools and evaluations of these tools will be presented. Feedback from the astrophysical community will be solicited.

Number of lines/GHz within 0.5% of strongest line as a function of molecules and source temperature

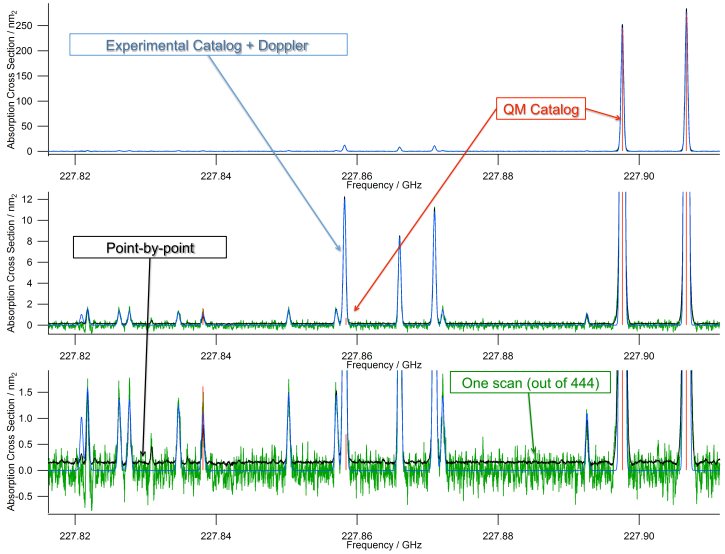
Molecule	150 K		300 K		500 K	
	Experiment	Catalog	Experiment	Catalog	Experiment	Catalog
Ethyl Cyanide	30	7.7	74	9	113	10
Vinyl Cyanide	11	8.7	38	11	58	14
Methyl Cyanide	1.8	2.3	4.2	1.9	9	1.8
Dimethyl Ether	26	14	40	9.9	75	8.4

Dissemination

1. All ~400 spectral scan (per molecule) available in archival literature (~10^6 points by one column by ~400 spectra)
2. Standard astrophysical data format (S_{ij} and E_l) available in archival literature and available to catalogs (~10^3 by two columns)
3. Point-by-point constants (S_{ij} and E_{ij}) available in archival literature and available to catalogs (10^6 points by two columns)

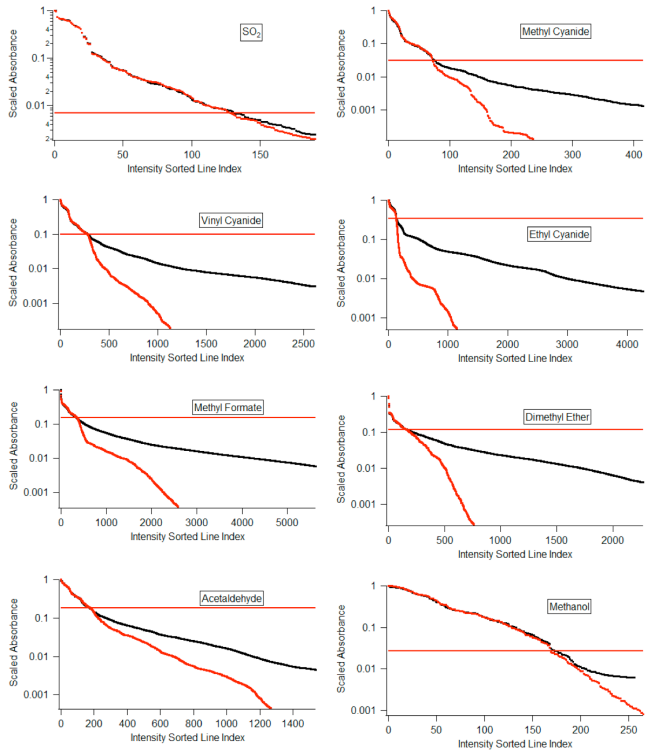
Astrophysical Simulation Strategies

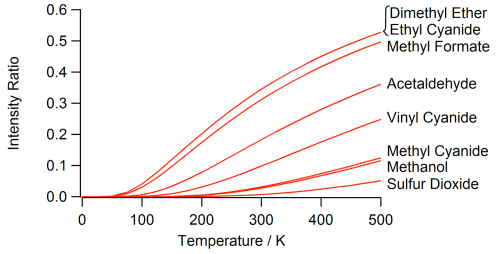
1. Simulation from experimental catalog
   - -Same as current QM catalog procedure – just more lines (2895 vs 618)
   - -Isotopic and vibrational temperature adjustments via non-perturbed ground state analyses
2. Simulation from frequency point-by-point catalog
   - -Same numerics, but 2.4 million points
   - -Must convolve astrophysical lineshape with laboratory Doppler width
   - -Another order of magnitude more lines (~30 000)



The portion of the vinyl cyanide spectrum between 227.82 and 27.92 GHz at 300K. The green trace is a single scan at 300 K, the blue scan is a simulation based on *all* of the 2895 catalog lines, and the black trace a simulation based on the point-by-point analysis of the 444 temperature scans. The red stick spectra represent the lines that are included in the QM catalogs. Except for the highest magnifications, differences are only observable with respect to the QM catalog.

Catalog and experimental spectral density as a function of intensity
Red line is vibrational Boltzmann factor for first omitted state





Ratio of Strongest Non-Catalog Line to Strongest Catalog Line as a Function of Temperature