

Supplementary file for “AI-3000K Infrared Line List for Hot CO2”

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Notes for AI-3000K (05/2022 version) line list calculation and additional statistics.

Compared to preliminary 2021 versions, this latest 2022.May list has following updates or differences :

1. The intensity calculation now has built-in *P/R* consistency, no more need for Cs-sym intensity calc (and match) on 626 and 636. All 4 isotopologues have more self-consistent intensities computed.
2. Because the experiment validation and list comparisons are up to 3000K, and our analysis indicates the 4000K convergence probably requires more robust PES/DMS at higher energies (i.e., >40,000 cm⁻¹):
 - A. In the first step of individual isotopologue line list calculations (writing out base list), for every 0.01 cm⁻¹ interval, we adopted 99.99% for 296K and 1000K, 99.95% for 2000K, and 99.9% for 3000K and 4000K. In the 2nd step (generate lists for iso-mix) line list size reduction for every 0.01 cm⁻¹ interval, we adopted the same thresholds: 99.99% for 296K and 1000K, 99.95% for 2000K, and 99.9% for 3000K and 4000K.
Note that for 626, we run 0-36,000 cm⁻¹ and 0-40,000 cm⁻¹ intensity tests together, the S_{min} threshold selected for each 0.01 cm⁻¹ interval ensures the sum of intensity is converged for both ranges. In most (but not all) cases, S_{min}(40K) < = S_{min}(36K).
 - B. In the iso-mixing step, we still use 99% for the intensity_{sum} threshold at 4000K, but raise the 2000K threshold from 99.9% to 99.95%, and raise the 3000K threshold from 99% to 99.9%. As a result, the data size of the 2022.5 final list is effectively doubled. Now the 2000 .tgz files occupy ~400GB.
3. More conservative cutoffs were applied during the stage of identifying fake intensity, finding related upper levels, and rejecting all other transitions associated with those levels. Very small intensity reductions can be found near 20,000 cm⁻¹ at 3000K. No other differences were found at lower temperature or lower wavenumber range. Numerically equivalent (but not identical) to the 2021 list, especially below 10,000 cm⁻¹.

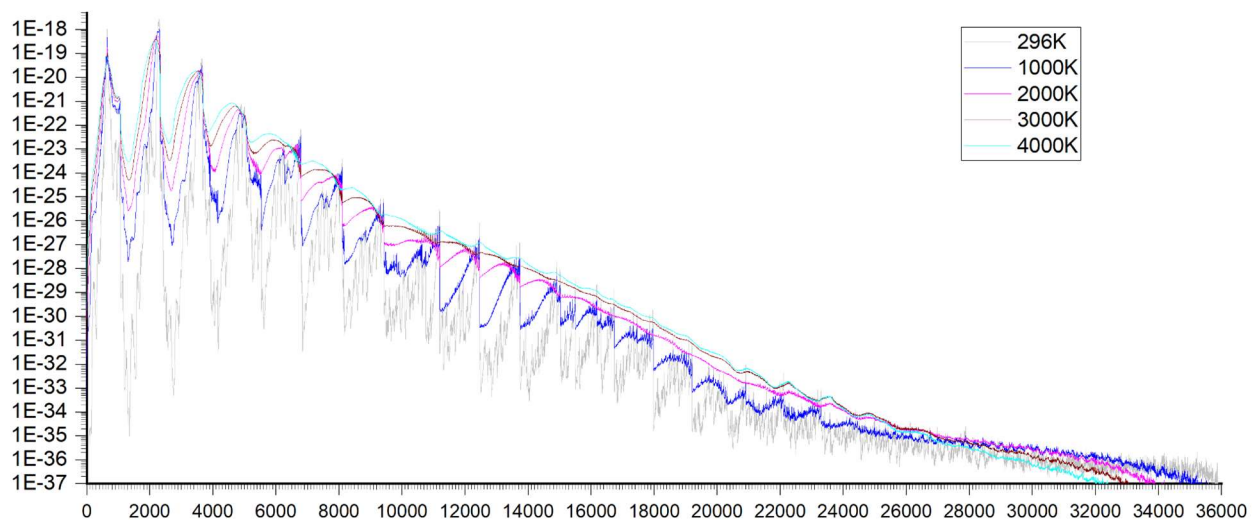
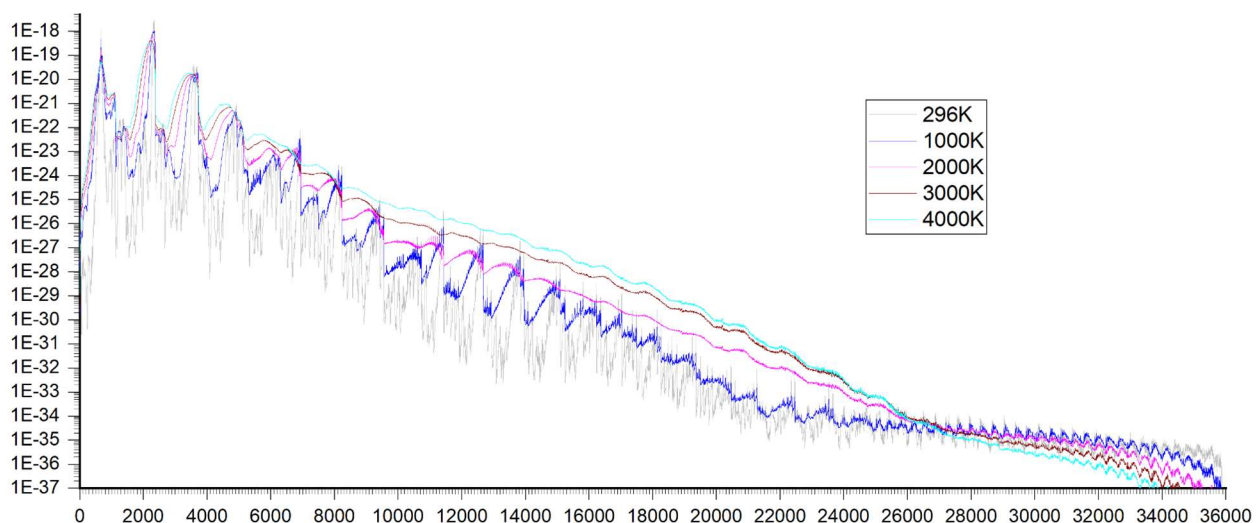
Statistics and Notes:

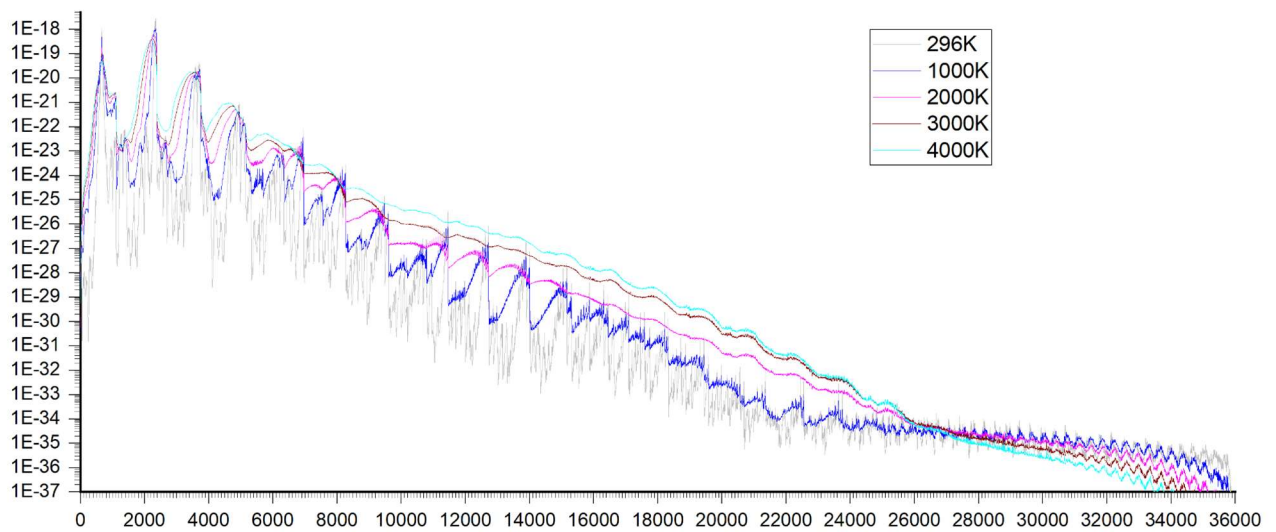
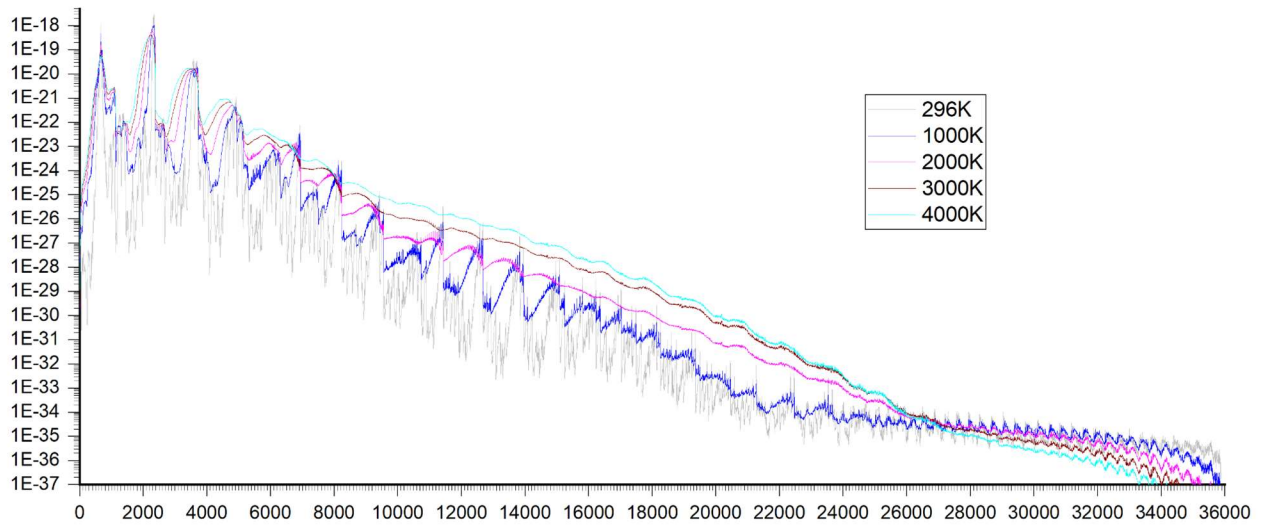
1. The 2021 version of convert.f90 works fine. The v5 version of energy level lists are almost numerically identical to the v4 version. Should not cause any discernible differences in simulation or analysis.
2. Number of transitions: (628 becomes more significant than 636 at higher temperature and higher wavenumber)

	626	636	628	627	Sum
296K	8679292	4102781	9187117	5896321	
1000K	574267343	129459222	208009376	94383807	
2000K	11581289410	1259622929	2252742848	717929106	
3000K	27397362378	2691372006	4578190786	1294391142	
4000K	16955873906	815640117	1041707073	203707345	

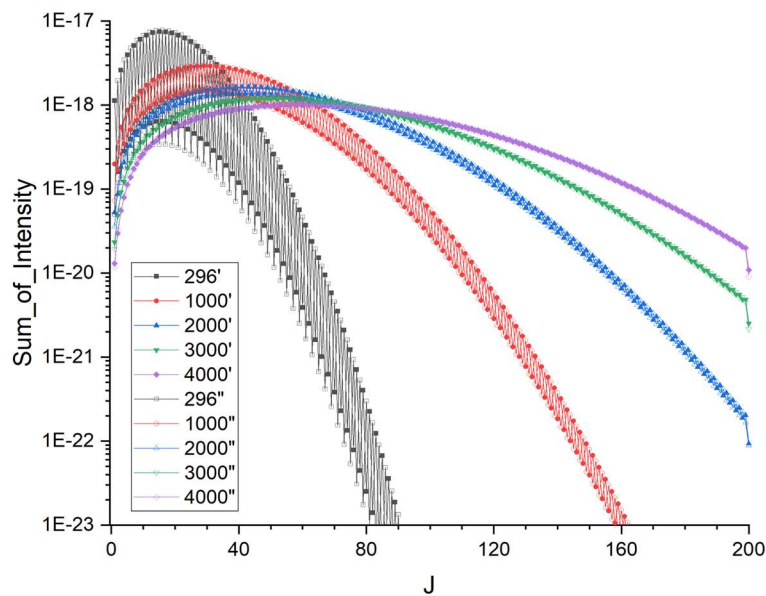
Total 27548493437 +2780854018 +4801316888 +1418062103 = 36,548,726,446 lines

3. Overview of the Al-3000K line lists for the 4 isotopologues, in the order of 626, 636, 628, and 627

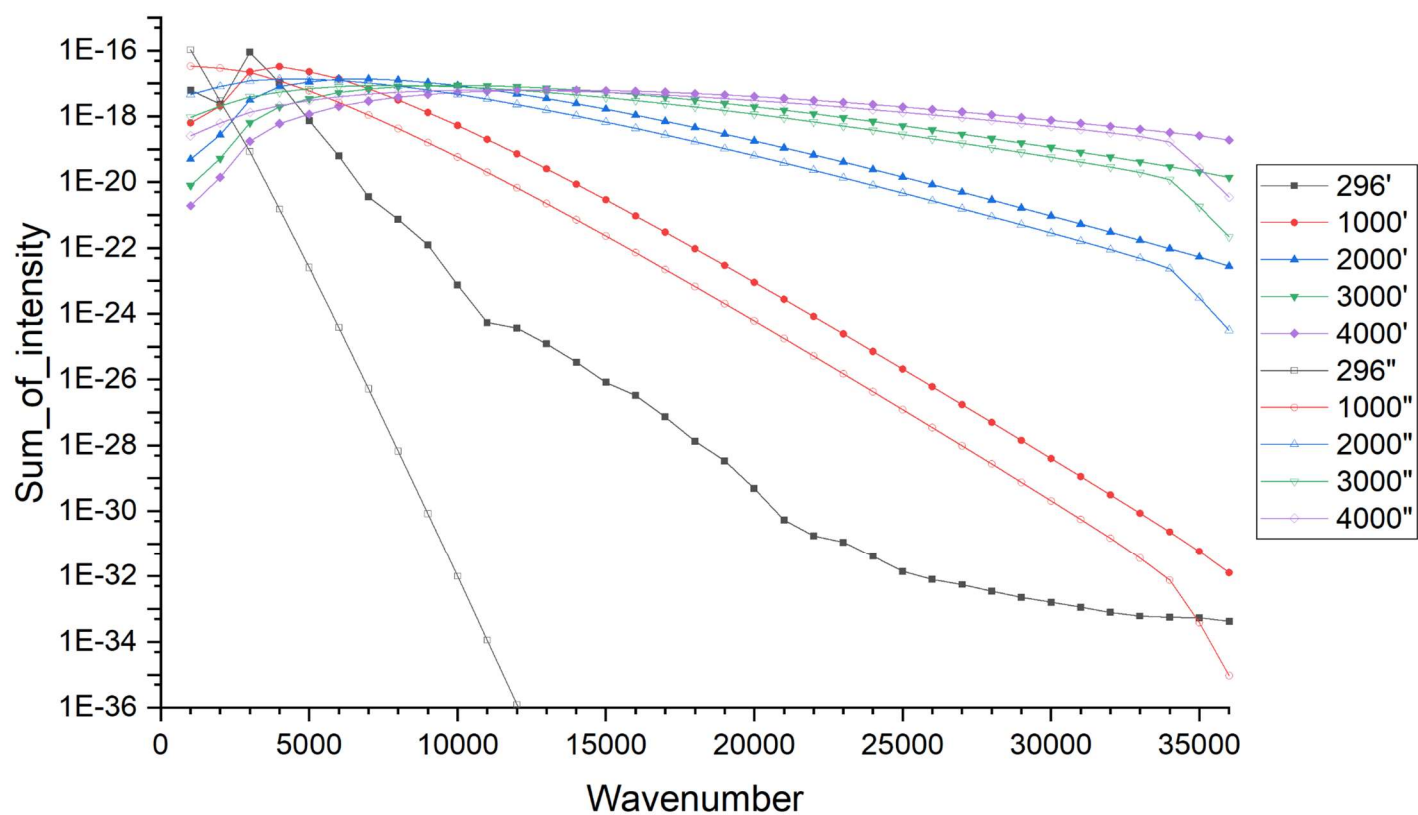




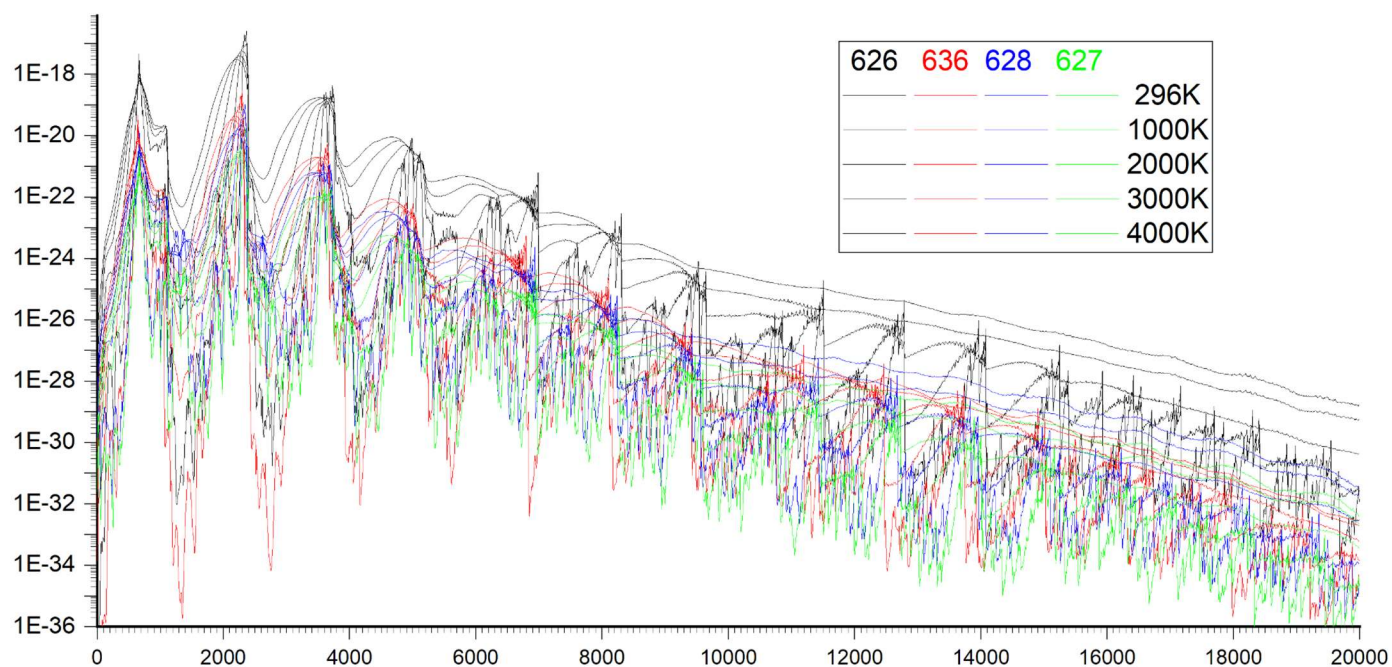
4. CO2 636 list sanity check, the intensity distribution along J' and J''



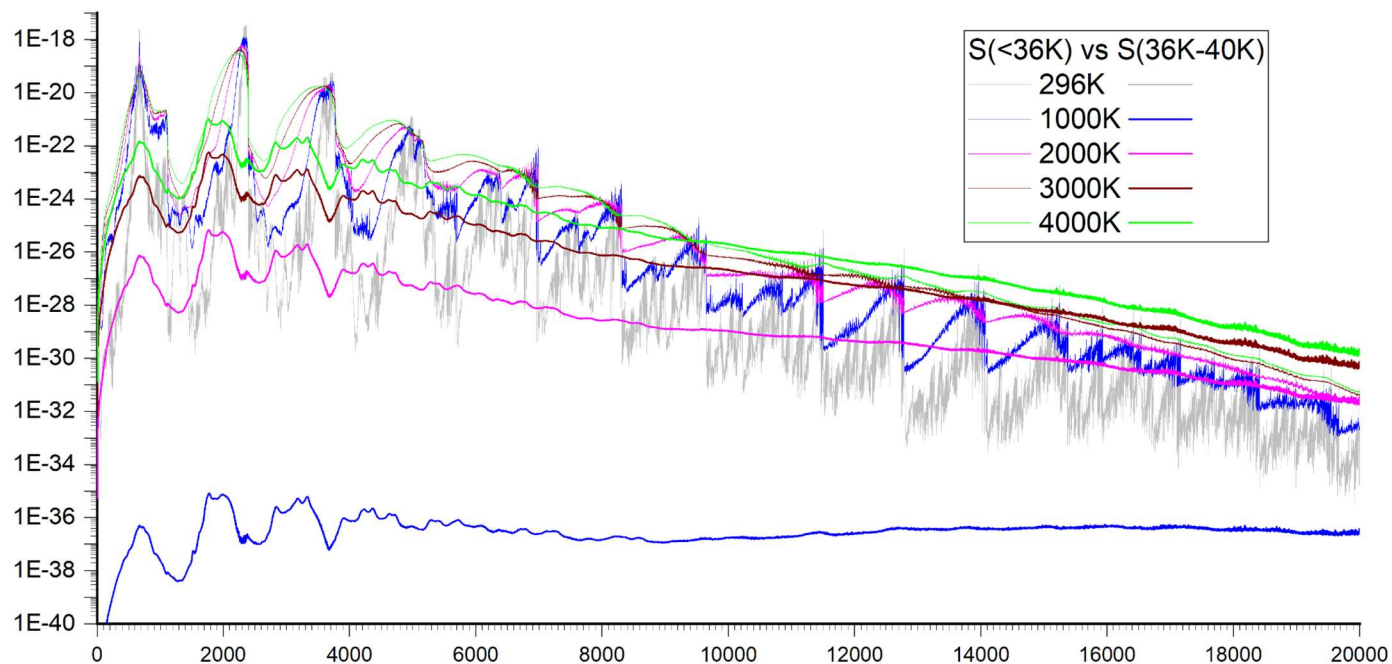
CO2 636 sanity check, the intensity associated with upper state energy and lower state energy:



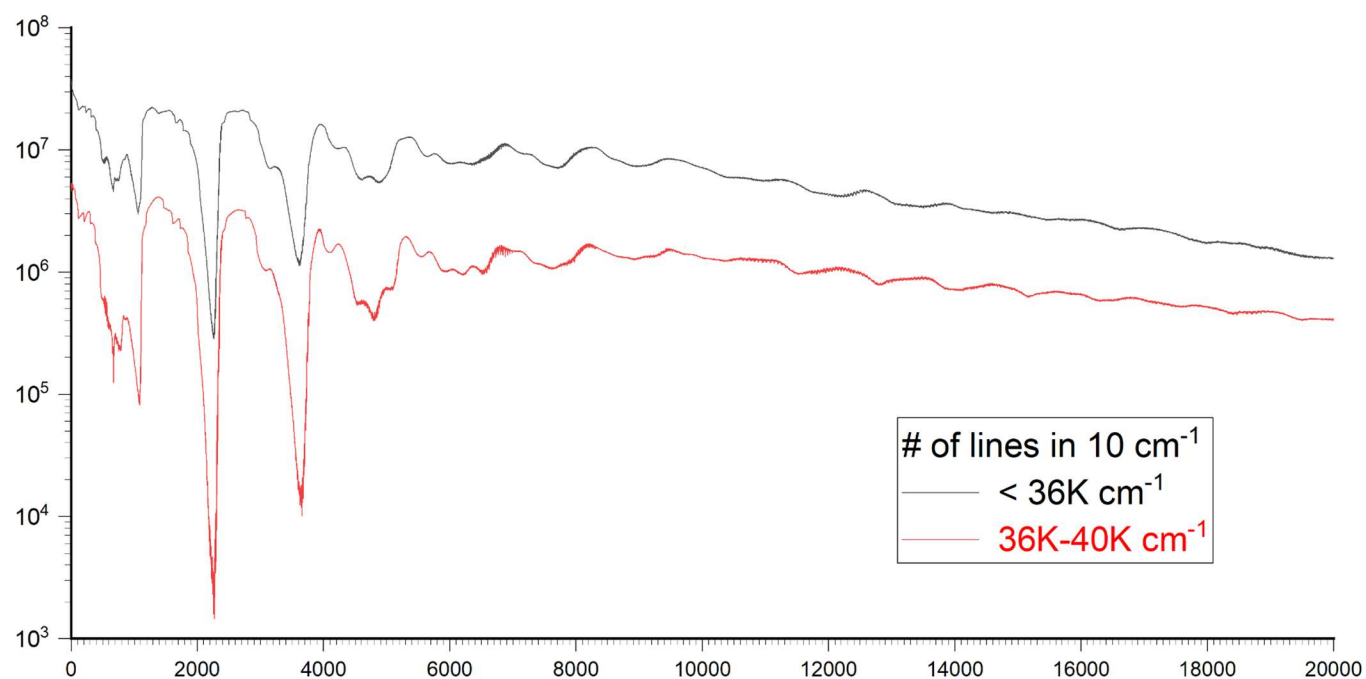
5. Isotopologue contributions to the final iso-mixed line list at 5 temperatures:



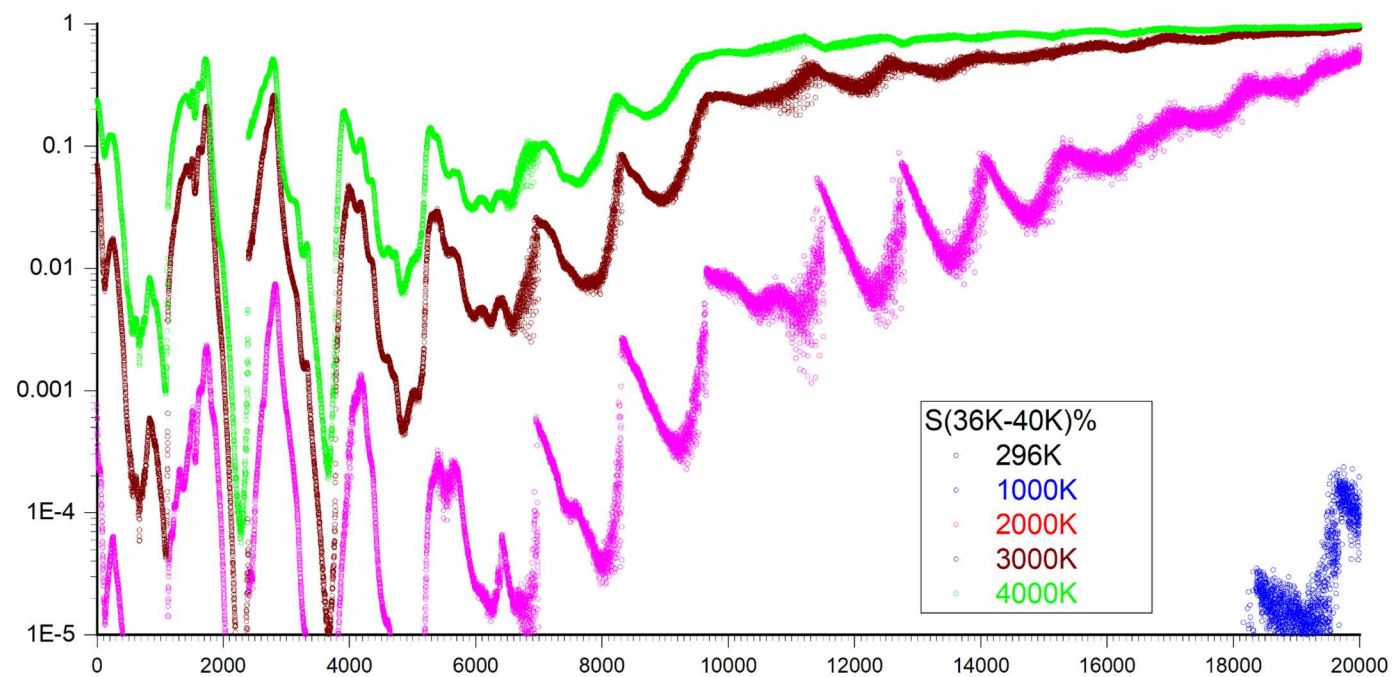
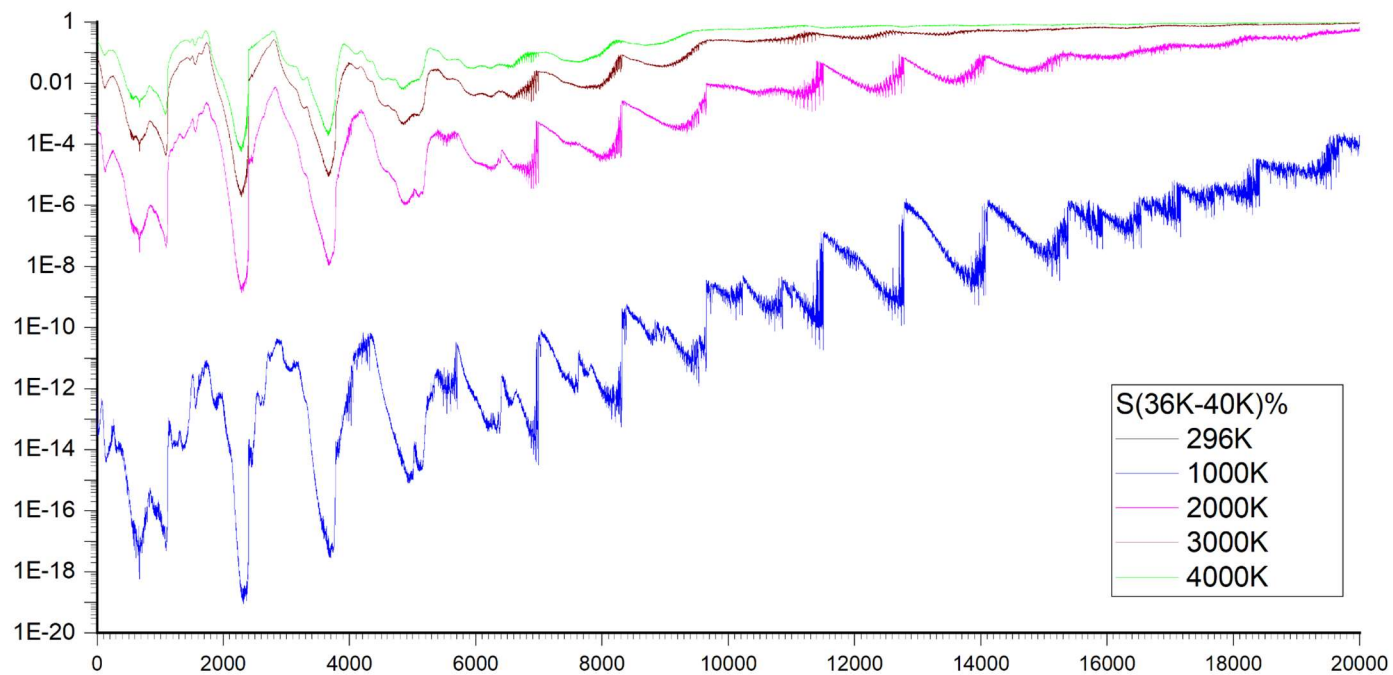
6. In final list, <36K cm⁻¹ vs 36K-40K cm⁻¹, statistics by 1 cm⁻¹ : (a) associated intensities



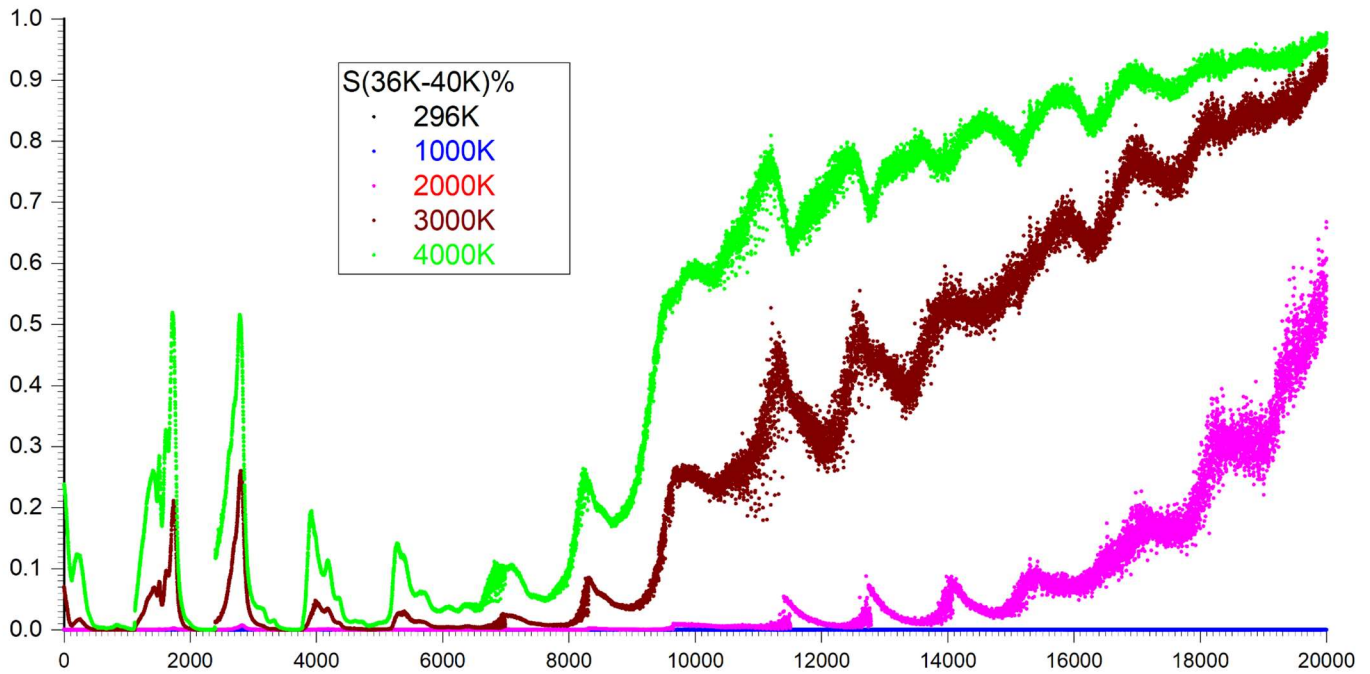
(b) associated number of lines



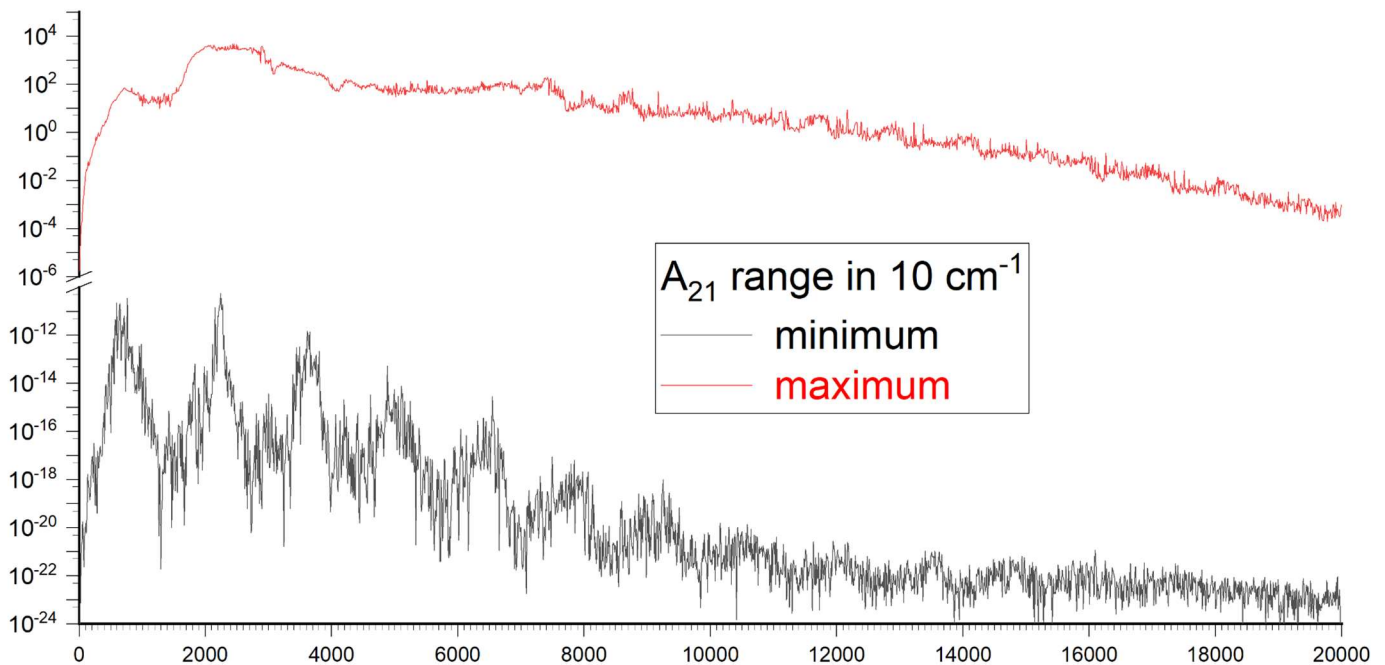
(c) the intensity ratio in total intensity sum = $S(<36K) + S(36K-40K)$



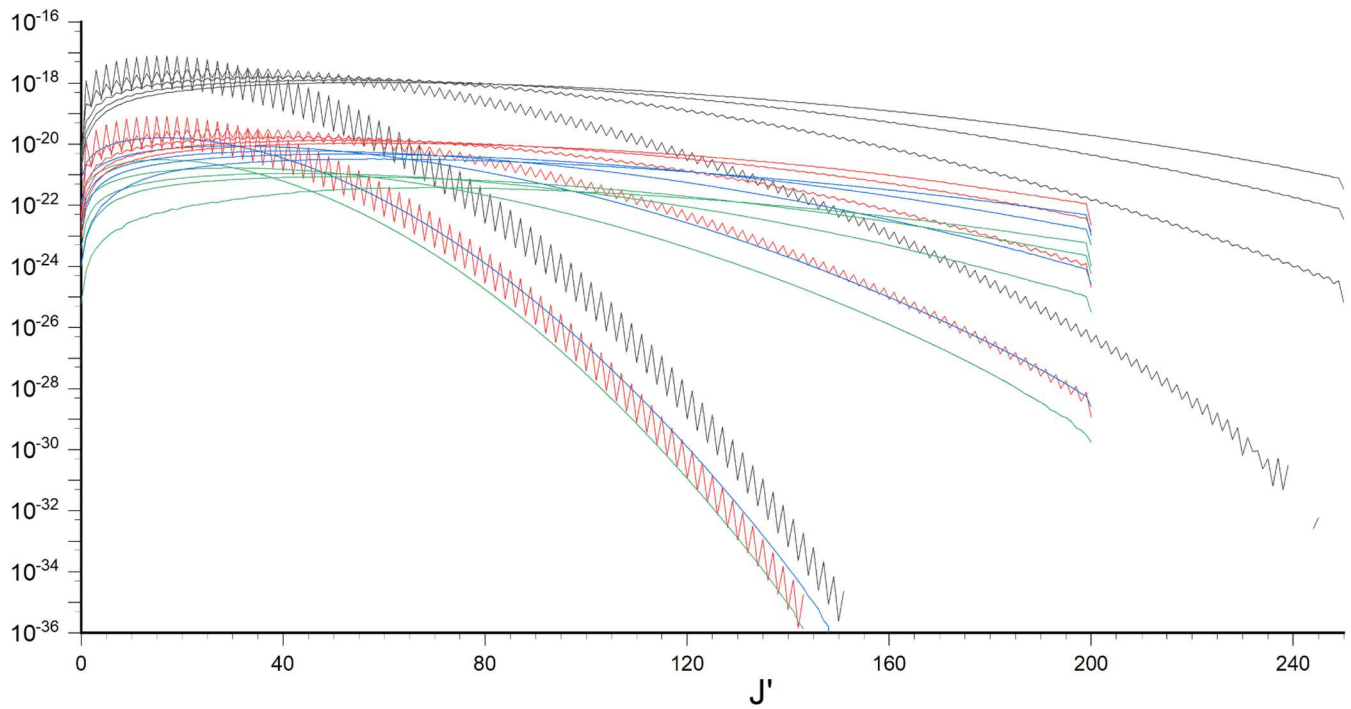
or



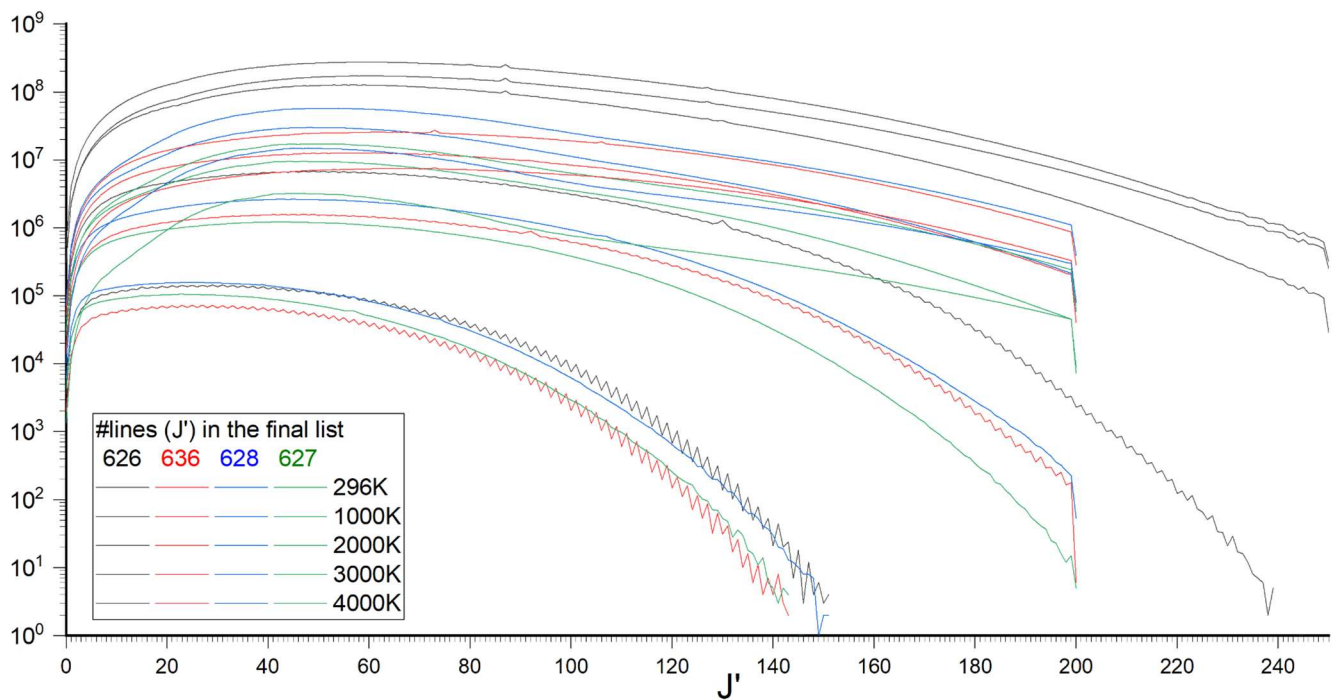
7. In final list, the range of A_{21} coefficients in each 10 cm^{-1}



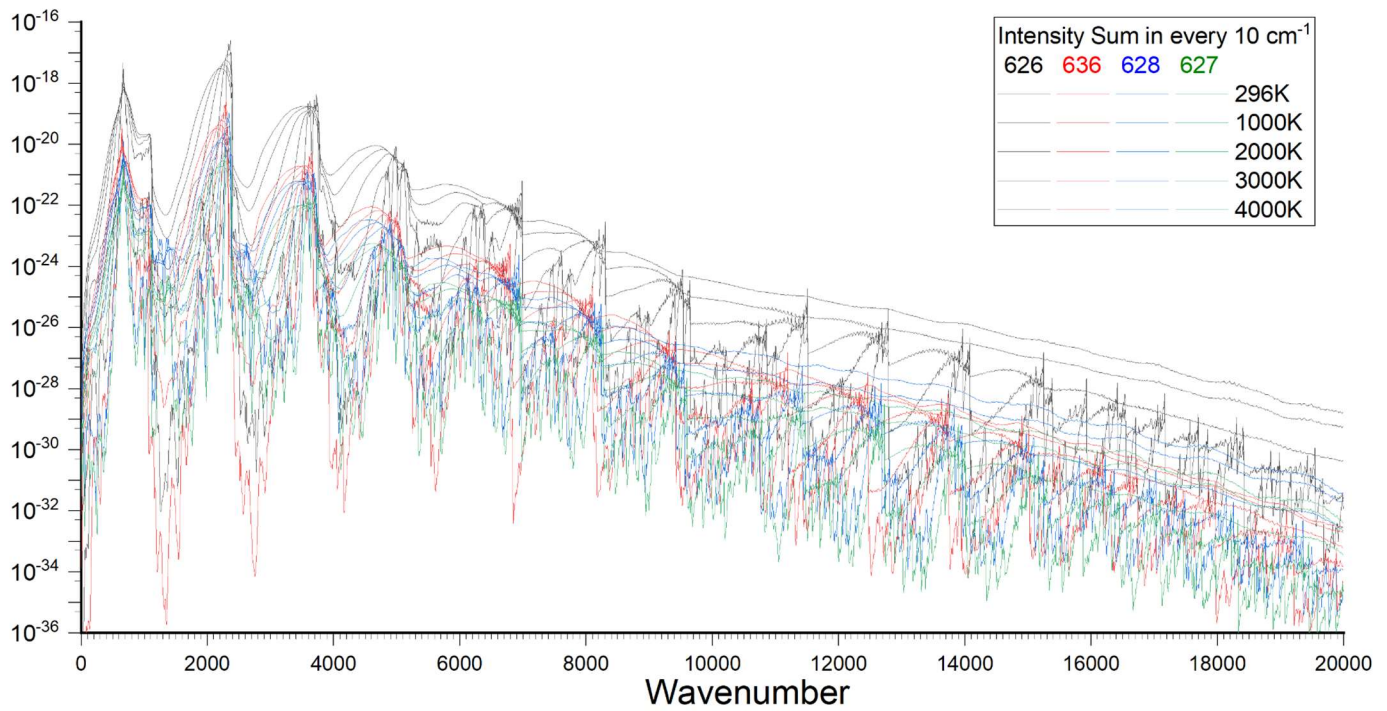
8. In final list, the intensity distribution along J' [626 black, 636 red, 628 blue, 627 olive/green]



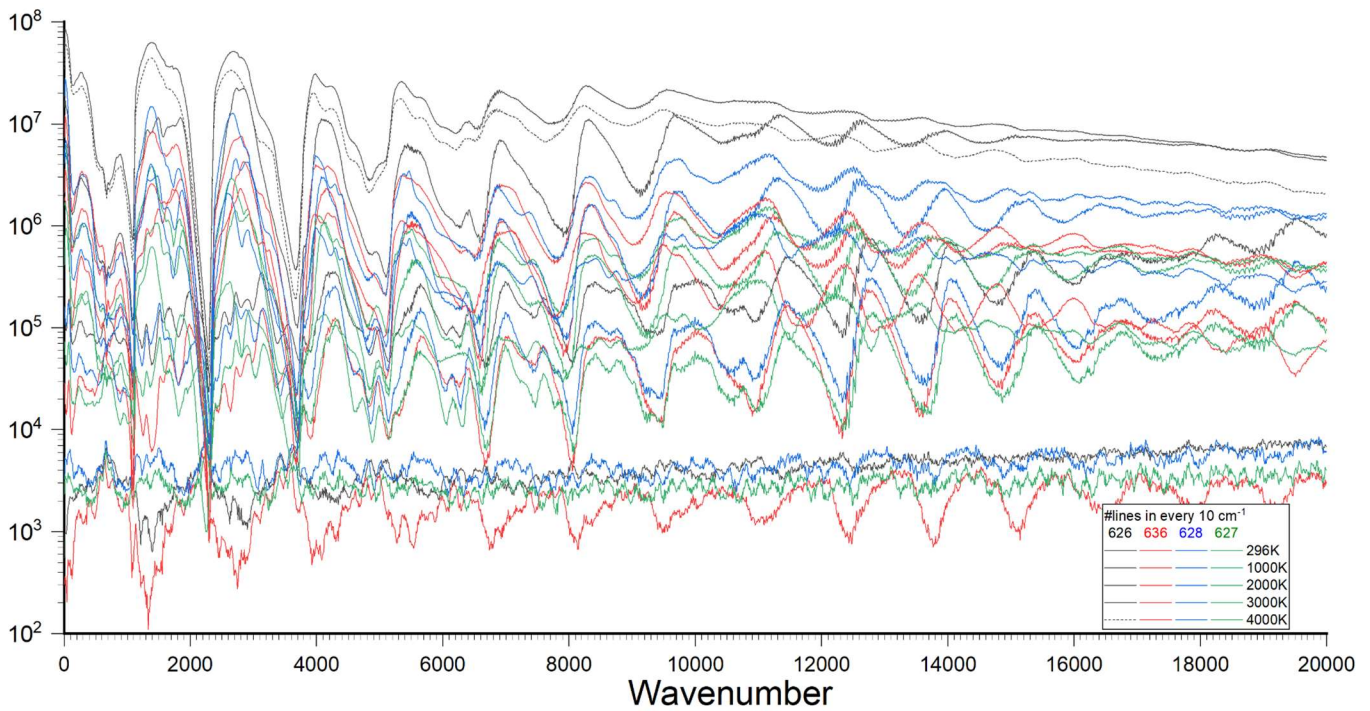
The number of lines distribution along J' – We see small bumps at a few J' 's, which are iso & temperature dependent, but we do not know how much irregular intensities are there, or if they did cause any detectable noises.



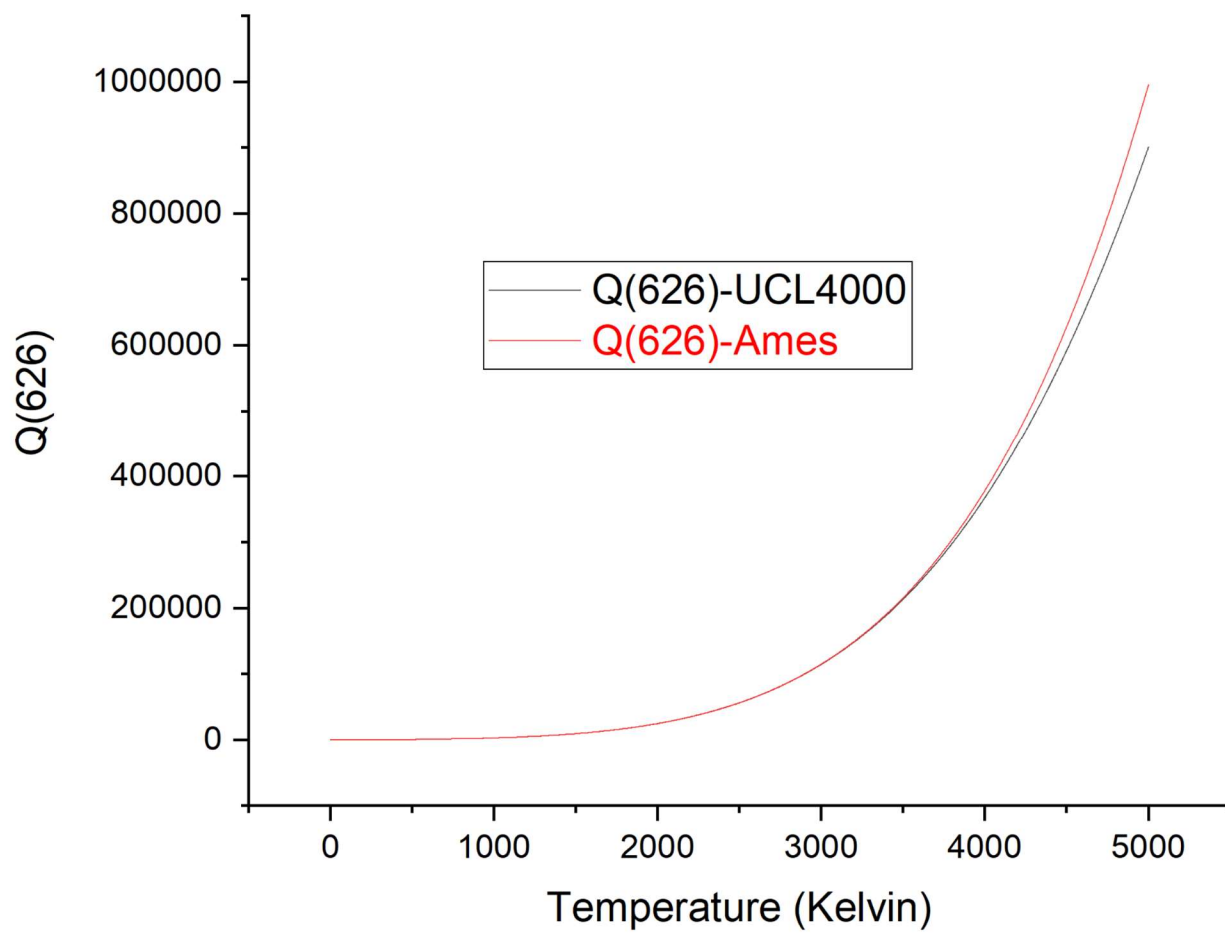
9. In final list, the intensity sum of each isotopologue in 10 cm^{-1} interval, same plot as #5.



The number of isotopologue lines in each 10cm-1 interval. Note the 2nd highest black (626) curve below 10000 cm-1 is the short-dashed line for the 4000K list, which is less than the 3000K list (the highest curve), due to the 99% intensity cutoff we adopted for 4000K.



-----Above was prepared on 05/18/2022-----



Partition function comparison plot is added on 09/01/2022