Advanced Atomic and Molecular Physics | 2017-06-12 | Prof. Heyne, 7. assignment

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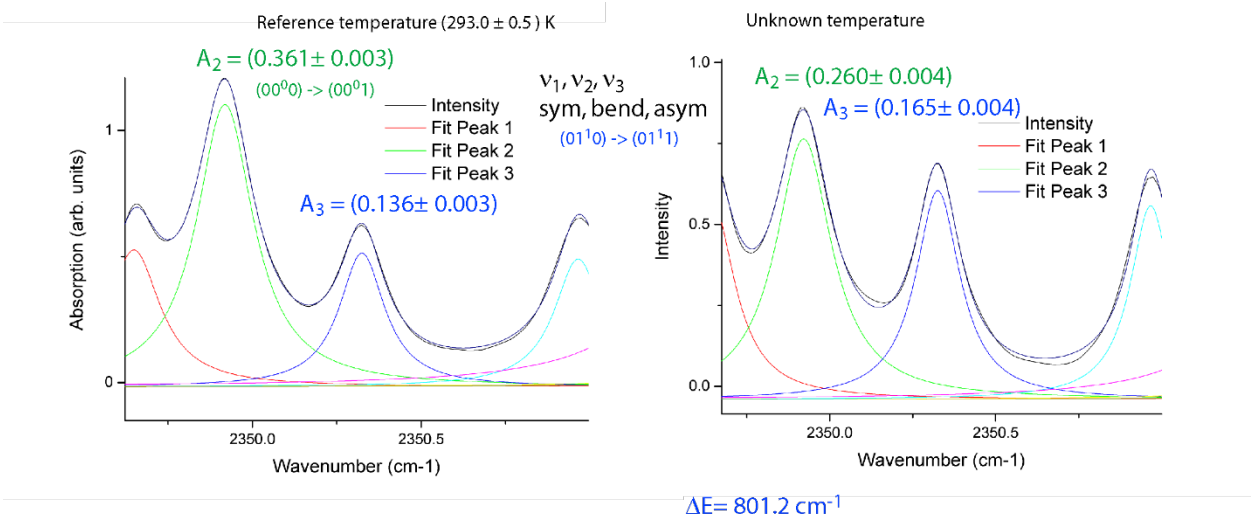
Deadline: lecture Thursday (2017-06-22)

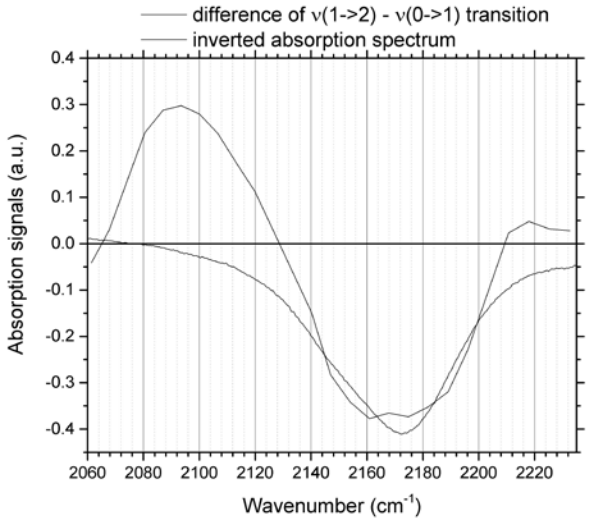
1. The rotational-vibrational transitions of $^{12}C^{16}O_2$ give rise to a multitude of IR-absorption bands. In the figures below, a zoom into the spectral window of the P-branch is given: Simple asymmetric stretching vibrations $(00^00) \rightarrow (00^01)$ together with hot band transitions (with excited bending vibrations) $(01^10) \rightarrow (01^11)$ are visible in the graphs. The ro-vib transition $(00^00) \rightarrow (00^01)$ is found at 2349.917 cm^{-1} (K=2 → K=0), and the hot ro-vib transition $(01^10) \rightarrow (01^11)$ is found at 2350.332 cm^{-1} (K=19 → K=18). The frequency of both transitions is nearly identical, but with a difference in total energy of ΔE=801.2 cm^{-1} due to the excited bending vibration (additional internal energy) for the hot ro-vib transition.
   (a) (2 points) Show that the absorption of peak A2 and A3 show different behavior upon increasing the temperature from 293 K to 393 K (use the formula from the lecture).
   (b) (3 points) The absorption A of a single band changes with temperature. By comparing the ratio R(T) of two absorption bands $R(T)=A_2/A_3$ at different temperatures (R(T) and $R_{ref}(T)$), the unknown temperature T can be determined.

$$R(T) = R(T_{ref})e^{-\frac{\Delta E}{kT}\left(\frac{-1}{T}+\frac{1}{T_{ref}}\right)}$$

   Determine the unknown temperature T with errors given by the errors of the areas of the absorption bands. The unknown temperature T was measured with an alternative and slow method to be (343.0 ± 0.5) K. Discuss your results with this value.



2. The anharmonicity β of a vibration is experimentally measured. Using the model of a Morse potential, one can estimate the following parameters: D_0, D_e, and ν_{max}.
   (a) (1 point) Determine the anharmonicity constant from the figure below. Presented are two vibrational transition bands, the negative ν=0→1, and the positive ν=1→2 transition. In comparison, the inverted absorption spectrum is shown.



   (b) (1 point) Determine D_0, D_e, and ν_{max} from the anharmonicity constant.