Lab Checklist: Lab # 7, N_2 molecular spectroscopy

PHYS 272L

(Dated: Fall 2022)

Upload page images of lab notebook as usual. However, pursue the restricted task list items described here. This is a subset of what is described on our public course website. The research questions are these: Task #1: in the range of wavelengths $350 < \lambda < 500nm$, what are the transitions observable between the electronic states designated $C^3\Pi_u \longrightarrow B^3\Pi_g$, **solely** for $\upsilon' = 1 \longrightarrow \upsilon''$ transitions, and how do they compare with the known values (taking values in the research literature, from Lofthus and Krupenie (table 29)? Task #2: the confining potentials look very like that of the simple harmonic oscillator, and such potentials are sometimes called harmonic potentials. Yet they are slightly distorted, or anharmonic. From measurements of transitions observed in the first task, find the effective fundamental frequency of oscillation (*in weird energy units:* cm^{-1}), and the 'strength' of its anharmonicity (that is, the value of its first order correction), also in cm^{-1}. How do our experimental values compare with values published in the literature, from table 1 of Laher and Gilmore.

I. DELIVERABLES

☐ Task #1 stuff.

  - ☐ Produce an *annotated* plot of the received N_2 spectrum, **identifying as many transitions stemming from the $\upsilon' = 1$ vibrational states of the $C^3\Pi_u$ electronic state as you can.** This is a plot of Intensity (arb. units) vs. wavelength. Make sure the units of the abscissa (independent variable) are correct.

  - ☐ *As a check on progress*, directly measure the energy gaps that give rise to the annotated lines, and exhibit calculations of the wavelengths for two of the annotated spectral lines of the measured spectrum. From the attached figure (and Fig. 2 from "Molecular Spectroscopy of N2 version 2.0", Lab #7 on our public course web site), including an estimate of their uncertainty through error propagation and estimates of the measurement uncertainties. Discuss the rationale for those uncertainties, that is, justify the choice made for the estimates of uncertainty. Show intermediate steps, with units and conversion factors. Notes on using adobe acrobat tools for making measurements of objects in figures in a pdf files are found below. Comment on this check on progress, briefly.

  - ☐ Produce a table of results with (at least) 7 columns, identifying 1) the $\upsilon' - \upsilon''$ transition scheme (as is done in table 29 in Lofthus and Krupenie), 2) the accepted wavelength from table 29 (described in the lab handout), 3) the observed value (from the plotted spectrum), 4) discrepancy ($\Delta\lambda_D$?), 5) experimental uncertainty, ($\Delta\lambda_U$?), 6) the measured energy gap itself **for two of the observed lines**, noting that the energy of the transition is referred to as $T_{\upsilon',\upsilon''}$ on our public course web site, and 7) the calculated value of the wavelength from the gap energies (see calculation in the checklist item above. Recall that all column headings must include a meaningful descriptor, and units.

☐ Task #2 stuff.

  - ☐ Produce a table of the energy differences ($T_{\upsilon',\upsilon''}$), and the difference of the energy differences ($\Delta T_{\upsilon''} \equiv T_{\upsilon',\upsilon''} - T_{\upsilon',(\upsilon''+1)}$) for the $C^3\Pi_u \longrightarrow B^3\Pi_g$ system, for $\upsilon' = 1 \longrightarrow \upsilon''$, as many as could be found in the observed spectrum (350 - 500 nm), with the following columns: 1) the $\upsilon' - \upsilon''$ values as in table 1, 2) $T_{\upsilon',\upsilon''}$ (in cm^{-1}, *gotten directly from the figure showing the potential wells for each electronic state, attached to this document, and Fig. 2 from, etc. just two of them taken from first table...*, 3) $T_{\upsilon',\upsilon''}$, *this time calculated directly from the standard lines from table 29 in Lofthus*, (exhibit a calculation below the table in the uploaded document), 4) $\Delta T_{\upsilon''}$ (refer to discussion in lab handout, near Eq. (3), with this clarification: please use the $\Delta T_{\upsilon''}$ resulting from the $T_{\upsilon',\upsilon''}$ entries calculated from the standard wavelength found in table 29 in Lofthus. 5) uncertainty in $\Delta T_{\upsilon''}$ (use suitable notation).

  - ☐ Record algebraic modeling work. From an approximate formula for the energy of each vibrational state, good to second order in $(\upsilon + \frac{1}{2})$,

$$T_\upsilon \approx T_e + \omega_e(\upsilon + \frac{1}{2}) - \omega_e x_e(\upsilon + \frac{1}{2})^2 \tag{1}$$

prove to yourself, given this approximation, that the energy *gap* is given by

$$\begin{aligned}\Delta T_{\upsilon''} &\equiv T_{\upsilon',\upsilon''} - T_{\upsilon',(\upsilon''+1)} \\ &= \omega_e - 2\omega_e x_e(\upsilon'' + 1),\end{aligned} \tag{2}$$

which is the physical, or theoretical model we will use in connection a computational model to obtain ω_e and $\omega_e x_e$ by fitting model to data.

- ☐ Use the second data table values as input to Fitteia, along with a suitable computational model derived from above, and obtain (with uncertainty) the values for the parameters ω_e and $\omega_e x_e$, expressed in cm^{-1}. Include the image of the fitting plot showing the header information. Annotate the figure with your best fit values for ω_e and $\omega_e x_e$.
- ☐ Write a 'How-To' for the modeling work in the checklist item above, that includes an estimate of the uncertainties in ω_e and $\omega_e x_e$.
- ☐ write a paragraph evaluating the goodness of the agreement of a) measured wavelengths, and b) measured ω_e and $\omega_e x_e$ parameters with accepted values (found in Laher & Gilmore), and c) Considering the *shapes* of the potential curves for the ground ($X^1\Sigma_g^+$), and excited ($B^3\Pi_g$) electronic states, comment on whether the measured value of ω_e for the $B^3\Pi_g$ electronic state is plausible by virtue of those shapes. This will of course require quantitative comparisons between discrepancies and uncertainties, and the correct use of significant figures.