Molecular Spectroscopy: Absorption and Laser-induced Fluorescence of I₂

Laboratory protocol
Goals
1. Learn the basics of modern spectroscopic techniques.
2. Measure the molecular constants of I₂ by absorption and laser-induced fluorescence spectroscopy.

Introduction

Light spectroscopy represents an important technique [1] to probe all states of matter and finds many uses in Physics and also all physical and life sciences. In this experimental, we will overview the basics of light spectroscopy, absorption and laser-induced fluorescence, by studying molecular iodine.

Molecular iodine is an ideal case for demonstrating the characteristics of electronic, vibrational, and rotational levels of a diatomic system. By absorption spectroscopy, even with a setup with a modest resolving power, one can record the long series of vibrational levels between the ground and the first excited states and hence extract the molecular constants with a good accuracy. Using laser-induced fluorescence spectroscopy [1-2], and the fortuitous coincidence that the 632.8 nm line of the He-Ne laser lies very close to an absorption band of I₂, the J-selection rules, the anharmonicity of the ground state, and the difference in the molecular bond length between the ground and the excited states are inferred. The combined use of absorption and laser-induced fluorescence spectroscopy shows how complementary results can characterize both the ground and the first excited states of molecular iodine.

Please consult molecular spectroscopy textbooks for more details [3-7].

Equipment (neither exhaustive nor detailed)

- Iodine cell and oven
- Thermocouple and meter
- Acton Research Pro750 monochromator
- W-halogen white light source
- Melles-Griot 3mW He-Ne laser
- Ne calibration source
- Andor 1600x200 CCD detector
- Si PIN light detector
- Light chopper and controller
- Stanford Research lock-in amplifier
- Data acquisition software

Experimental Procedures

Please consult the teaching assistant for detailed experimental procedures.

1. Get yourself familiar with the instruments (monochromator, light detectors, light sources, lock-in amplifier, oven, and software).
2. Record a calibration spectrum (Ne), to get yourself familiar with the equipment. What are the effect of the slit width and the choice of diffraction grating used?
3. Heat the iodine cell (in the oven) in order to get the temperature stabilized around 55°C and get an appropriate vapor pressure.
4. Using the scanning mode (single channel detection) of the monochromator, record an absorption spectrum of the heated iodine gas, from 500 to 650 nm in a forward scattering geometry. You may start with a lower resolution spectrum (fast) before recording a higher resolution one (slow). You
will also need an accurate wavelength calibration provided by the spectrum of a Ne lamp recorded under the same conditions.

5. Using the spectrographic mode (multichannel detection) of the monochromator, record the laser-induced fluorescence from the heated iodine gas, excited by the 632.8 nm line of the He-Ne laser, from 600 to 750 nm in the 90° scattering geometry. You will also need an accurate wavelength calibration provided by the spectrum of a Ne lamp recorded under the same conditions.

Data Analysis
From a proper data analysis, the molecular constants of iodine and the interatomic potential can be extracted.

1. Answer all questions given by the teaching assistant.
2. Find the position of all absorption bands recorded. Assign the appropriate quantum number corresponding to the right vibrational levels corresponding to the excited state.
3. Make a Birge-Sponer plot [1-2] for the ground and excited states of the molecule (B-X system) in units of cm⁻¹.
4. Show the anharmonicity of the molecular potential from a Birge-Sponer plot [1-2].
5. Calculate the dissociation energy from the Birge-Sponer plot.
6. Discuss the implication of an elevated iodine gas temperature on your data.
7. Using the less complicated laser-induced fluorescent spectra of molecular iodine, produce a Birge-Sponer plot, using the vibrational intervals of the ground state (X state) against the largest of the quantum numbers of the intervals.
8. Extract the molecular constants. Compare them with those obtained from the absorption data.
9. Calculate and plot the molecular potential (Morse potential) using the molecular constants calculated from your data. Take into consideration of the range of uncertainty on the molecular constants.

References