UNIVERSITY of WISCONSIN
GREEN BAY

Chemistry | 2016-2017 Assessment Report

1. Please give a brief overview of the assessment data you collected this year.

The assessment data that was collected this year was in the form of exam questions designed to determine if students understood a key concept in quantum mechanics and spectroscopy (this is learning objective #4 on the chemistry's learning outcome list: Have knowledge of atomic and molecular structure, thermodynamics, kinetics, quantum mechanics and spectroscopy.)

The key concepts evaluated was the idea that energy levels for many systems are discrete (rather than continuous) and that an absorption or emission peak in a spectrum (IR, Raman, photoelectron, UV-Vis absorption, microwave,…) corresponds not a particular energy level, but rather a transition between energy levels. This is a concept that is often misunderstood in the lower level chemistry courses CHEM 211/212.

The students were tested through exam questions (see report below) to test their knowledge. The first exam (Feb. 21, 2017) had a question concerning the calculation of an absorption peak once the students calculate the value of the individual energy levels. The second exam (March 28, 2017) had a question were the student were given a vibrational spectrum and were asked to calculate the fundamental frequency and anharmonicity vibrational constants.

I. Introduction

<u>Outcome #4</u>
Have knowledge of quantum mechanics and spectroscopy.

<u>Course Assessed</u>
CHEM 321 Structure of Matter. This is an upper level course designed to teach how molecular structure relates to spectroscopic properties. This is the equivalent of physical chemistry II at most universities. This is a challenging course that is very math intensive and at times abstract (due to the quantum mechanical concepts involved).

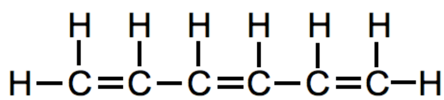
<u>Nature of Assessment</u>
One of the important aspects of quantum chemistry and spectroscopy is the idea that many systems have discrete energy levels. We study the standard systems such as particle-in-a-box, harmonic oscillator, rigid rotor, and the hydrogen atom. It is emphasized that spectroscopy (the interaction of light with matter) can give use detailed information (bond length, ionization energies, …) about molecule under study. It is critical that students understand that an absorption peak in a spectrum corresponds to a jump between two energy levels. Many undergraduates make the mistake of equating the peak with a single energy level. I wanted to make sure this concept was understood firmly by the students.

Assessment of this knowledge took place over the semester as both homework assignments as well as exam questions.

II. Assessment

Exam questions

Exam #1 Question7. What is the wavelength of light required to induce a transition from the ground state to the first excited state (lowest energy excited state) in 1,3,5-hexatriene, C_6H_8. Assume that the molecule is linear with bond lengths of 154pm for C-C single bonds and 135pm for C=C double bonds (10^{-12} m = 1 pm).

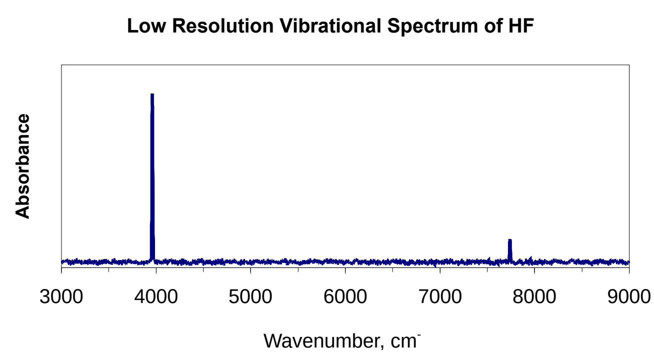


This question requires the students to understand the particle-in-a-box energy levels and that the energy of light needed to induce this transition has to be equal to the difference between two energy levels. By counting the number of pi electrons and filling up the energy levels in the aufbua order (fill up lowest energies first and two electrons per energy level) the students can calculate the levels involved in this transition.

Exam #2 Question 12. A low-resolution spectrum of the IR spectrum of HF shows a strong fundamental peak at 3959 cm^{-1} and another much weaker peak due to the first overtone at 7738 cm^{-1}. Ignoring the rotational contributions and taking the vibrational energy levels as anharmonic,

$$\tilde{E} = \left(n + \frac{1}{2}\right)\widetilde{\nu_e} - \left(n + \frac{1}{2}\right)^2 \widetilde{\chi\nu_e}$$

determine the values of $\tilde{\nu}_e$ and $\chi\tilde{\nu}_e$ from the spectrum.



This question requires the students to understand the concept that the two peaks correspond to a fundamental peak between vibrational levels n=0 and n=1, while the overtone peak corresponds to a transition between the vibrational levels n=0 and n=2. Knowing this they can use the given vibrational energy equation to calculate the vibrational constants (2 equations/2 unknowns).

Rubric

Criterion	0 = unacceptable / not answered	1 = acceptable	2 = above expectations
Exam 1:	Did not understand concept that a peak on	Understand that a difference in energy levels were	Able to apply the PIB model to the problem and correctly

	a spectrum is a difference between two energy levels	involved but didn't know which levels. Everything else calculated correctly	calculate the proper energy levels involved. Get the answer correct.
Exam 2:	Did not understand concept that a peaks on a spectrum correspond to a transition between two energy levels	Could identify only one peak but not the other	Identified both peaks and were able to determine the vibrational constants asked for

III. Results

Student	Exam 1 score	Exam 2 score	Average
1	1	2	1.5
2*	0	0	0
3**	2	0	1
4	0	2	1
5	1	2	1.5
6	2	2	2
7	1	0	0.5
Average	**1 (1.2)**	**1.1 (1.3)**	**1.1 (1.25)**

* Student was having personal issues throughout semester and missed many classes (ultimately received an F).

** This was my best student. When I talked to him about this problem, he said he knew how to do it and that he was confusing this problem with another concept.

IV. Discussion

The impact that student 2 (who rarely attended lectures due to personal issues) is a concern, so the numbers we re-calculated without this student and corresponding results are the parenthetical values. The data seem to indicate that by exam 2 there was more comprehension of the connection between spectral peaks and quantum energy levels. Overall, the exam scores were above acceptable. I don't think any major changes are suggested by the data, but I do plan to provide more homework problems in future offerings emphasizing this concept.

2. How will you use what you've learned from the data that was collected?

The data collected will be assessed to determine if the students are understanding this connection between absorption spectrum and molecular properties. The data will tell us two things, one if the students in the upper level structure of matter class (CHEM 321) have a clear and correct concept of spectroscopy. Two, the data could be used to determine if we should possibly emphasize this topic when it is first introduced to the students in CHEM 211/212 during their freshman/sophomore years.