

NAME OF PRACTICAL

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Category

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Atul Singh Arora: *Name of Practical*, Category,

*Every honest researcher I know admits he's just a professional amateur.
He's doing whatever he's doing for the first time. That makes him an
amateur. He has sense enough to know that he's going to have a lot of
trouble, so that makes him a professional.*

— Charles F. Kettering (1876-1958) (Holder of 186 patents)

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CHEMISTRY NOTES

October 19, 2012

1.1 PEAK BROADENING

1.1.1 *Natural (Lifetime)*

$$\Delta E \tau = h/2\pi$$

$$h\Delta \nu \tau = h/2\pi$$

1.1.1.1 *Collisions*

Collisions can cause the lifetime to reduce. Some gasses will collide and go away, but in some, as you increase the pressure, the width will increase, and the intensity will decrease simply because a lot of electrons are unable to emit. It's the area under the peak that's constant, not the peak. Not only is the width increase, also there's a loss of intensity for reasons stated earlier.

But the average lifetime decreases. So remove other gasses and reduce the pressure, you're suppressing collisional broadening.

Every other broadening mechanism when removed, then you're left with the natural width of the peak. Collisions are inelastic, because its not just change of kinetic energy, because there's a change in potential energy (How?)

Its not dropping the intensity, there's no physical way you can understand that, but you need to understand FT. Increase in energy, causes increase in temperature also (Biplob Question)

Temperature rise is not like you can boil water on it. That class of spectroscopy is called photo thermal spectroscopy. Also called thermal lensing, photo acoustic. What they do is measure the heat (not certain about this..)

1.1.1.2 *Doppler*

Molecular motion that's always happening. By maxwell boltzman distribution, you have the nice bell shaped curve. When you increase the temperature, the same thing just becomes wider. Then there's a greater distribution of speeds. Classic example of the fact that frequencies observed are different (speed in this case) for a moving observer (or source), is a train sound (car sound). If the sodium is moving towards a source of 590 nm, then the sodium atom would not absorb because for the sodium atom, the wavelength is less than 590

nm. So if the source emits various wavelengths, then the sodium atom would absorb at different wavelengths because of doppler effects and this causes peak broadening called doppler broadening.

If I make liquid sodium or solid sodium, then that will add to complications. So you must cool it without solidifying or liquefying it. 10 K everything is solid, except helium etc., but you must cool these without them interacting with each other.

Need to know mean free path, pressure etc. to calculate things.

Doppler shift you know quantitatively. If you put it in the Maxwell Boltzman distribution, you get the width of the doppler broadening (don't memorize this) is given by $\Delta\nu_D = 7 \times 10^{-7} \nu \sqrt{\frac{T}{M}}$. This explains why Raman has a huge doppler, therefore the peaks are so very broad. Plus you have a root of T. Higher the molecular weight, the distribution gets smaller, therefore the doppler width becomes smaller. (not certain)

When you're stuck with doppler broadening, you've to cool the guy (because for a given technique your frequency is fixed), without freezing.

One method is to put the water in an Argon matrix (Biplob question) and this will be cooled. Also you can use the super cooling thing sir had talked about in one of his talks (figure out the precise name of the technique). Adsorption (Prashansa Question), the doppler's then gone, but the interaction with solid mustn't be strong otherwise pointless. But it could be used, take graphite its not that bad. But others like magnesium etc. can NOT be used.

1.1.1.3 Others

Electric Field, perturbation Time of Flight Pressure Broadening

REMOVING DEGENERACY

November 2, 2012

2.1 INTRODUCTION

2.1.1 *Nuclear Spin*

Electron has a spin half. If $s = 1/2$, then length of the vector would be $\sqrt{1/2(1/2 + 1)}\hbar/2\pi$. Electron spins, thus it generates a magnetic moment. Thus you can relate the magnetic moment, to its angular momentum. μ is proportional to S . So for a proton, everything would be the same, except the charge. Now μ is related to I , the angular momentum of the charged particle. (μ is the angular momentum). $\mu = g\beta_N I \text{ JT}^{-1}$, g depends on the nucleus. There's no need to remember that number, where $\beta_n = \frac{e\hbar}{4\pi m_p}$. It defines the magnetic moment the angular momentum will produce. The g value is different for Carbon and Hydrogen. Very characteristic of the nucleus you're looking at. That's important because it tells you where it'll lie in the spectrum.

To make the plus half

$$E = B_z \cdot \mu_z$$

$$E = -B_z g \beta_n I_z$$

$$\Delta E = g B_z \beta_n$$

The population difference will be as small as 10 in 2 million. When would a molecule absorb? Detour: Lets consider a system in which all atoms are in ground state. When you give energy, the first will go up. So say initially there were ten, now there are nine ground, one excited. Now as the population becomes small, the probability of stimulated emission becomes the same as probability of stimulated absorption and a dynamic equilibrium is reached. Now here, if the population of the excited state becomes high enough, then it will relax back due to quenching and thus the experiment can go on. However, the point anyway is the population difference is very small. When you go to higher fields, then you can more sensitively see better. 9 Tesla for a 400 MHz. In solids, the spectra will get extremely broadened (because life time will become extremely small). Therefore we don't use solids, and don't use gasses because they don't have any quenching. In liquids it's ideal and that's what we used. In gasses, first getting the experiment to work will be more difficult since the number density will be very low.

You can always express, ΔE in Herts, so if B_z is 9, then for Hydrogen, $\nu = 400$ MHz. You had to wait for superconductors for getting 9 Tesla. Even today, people who sell us 60 MHz machine, had come.

Suppose there's a bare proton, this is what I see (400 MHz). But supposing I take CH_4 , but it's a proton with electrons surrounding it, and they will change the ΔE . The electrons also have their own intrinsic spin (when the magnetic field is applied), then these two spins will start to cancel, then the number of electrons will decide how much of the magnetic field reaches the proton. So if you apply 9 Tesla, then it'll probably see less field. So they won't absorb at 400 MHz, but it'll instead absorb at less than 400 MHz. Now if you take CH_3OH , then the oxygen will take away most of the electrons, thus the H in OH will get a field closer to what you've applied. This is the electrons shielding. Thus NMR is so powerful as it can tell you about the environment around it. (Srijit: Wouldn't the protons of other atoms in the molecule interfere?) You have two absorptions, thus you can tell the molecule in many cases. With infra-red, it's hard even for the expets to tell which molecule it is. If you pin it to the wall and tell him to figure out the exact molecule, he'll say shoot me. So even with a molecular formula, you should be able to tell the structure, using NMR. It's almost always unambiguous. Of course then why aren't we just doing NMR? Well it can't tell you how strong the bond is, the forces etc., that's why you need other techniques

It's always easy to change the magnetic field, so you start with 9 Tesla, and keep dropping. So the first guy that hits, would be OH's H and then the CH_3 's H.

Today we of course don't do it this way. FT is used today. Nobody today does sweeping magnetic fields.

Only if $I \neq 0$ do you get something. It's like a closed shell system giving you a singlet sigma system. If you take carbon 12, 6 proton, 6 neutron, thus its NMR inactive. If Odd + Even = $1/2$ integral spins.

COLOPHON

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https://github.com/toAtulArora/IISER_repo