Spectrum of Molecular Nitrogen

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Abstract: Using known constants and the vibrational energy, the upper and lower quantum numbers and degradation were assigned to diatomic nitrogen. In order to do this, constant values of energy were used to calculate the total energy of vibration motion for which wavelengths calculated determined quantum numbers. Violet degradation was found in the spectra due to its jagged appearance. However, more research is needed into describing rotational motion in terms of energy. X

0 1 2 4 1 1 2 / 11 = C

Introduction

A single atom can express energy when electrons transitions from one state to another. When two or more atoms exist in a molecule, these transitions can be expressed in nuclear motion, which is made up of both vibrational and rotational motion. Vibrational motion is the periodic changes in distance between nuclei. Rotational motion is the motion of each nucleus moving around each other. For our experiment we focused on the quantitative analysis of vibrational motion, due to its large contribution to the nuclear motion, and the qualitative analysis of rotational motion of diatomic nitrogen in air.

additional not replacement

axis label

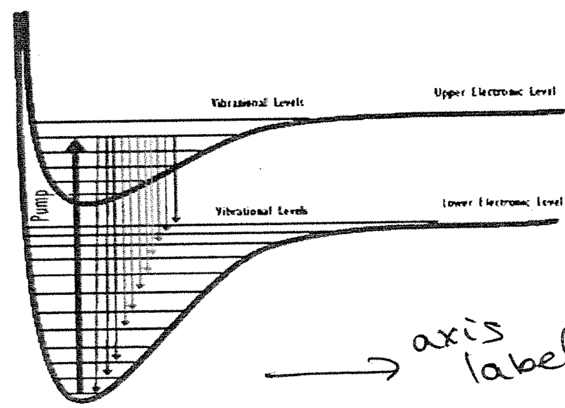

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Figure 1. *The upper level is denoted as Vc while lower level is denoted as Vb.*

Vibrational motion can be expressed in the equation below for which the first three approximations of the two nuclei, that form a harmonic quantum mechanical oscillator, is given by:

$$T = Te + we(v+½) - wexe(v+½)^2 + weye(v+½)^3$$

T-the energy that vibrational motion creates without hbar.

Te-a constant of energy that a non-vibrating, non-rotation molecules would have

we-a constant for a given electronic state, equal to the classical angular frequency of a oscillator

wexe & weye- constants (called the anharmonicity constant) that is the deviation of a system due its harmonic oscillation characteristics

v-the vibrational quantum number where $v \geq 0$

The vibrational motion contributes to the transitions between levels with Vc being the upper level and Vb being the lower level as shown in Figure 1.

Rotational motion can be expressed with the addition of B J(j+1) term for energy. This term represents two nuclei orbiting each other with a constant separation. B is the rotational constant and J is the rotational quantum number. This rotational contribution raises the notion of "violet degradation" and "red degradation." Violet degradation is seen when the bands degrade toward shorter wavelengths, which implies that the internuclear distance in the upper state is smaller than that of the lower. On the other hand, red degradation is the exact opposite.

Method and Experimental apparatus

This is analysis

Given the constants for diatomic Nitrogen, calculations of various changes in energy between states of certain vc and vb values were determined. The energy in cm^{-1} changes for molecular nitrogen can be seen in the following table:

Vc/Vb	0	1	2	3	4	5	6	7	
0	29671	31668	33627	35561	37481	39401	41333	43289	45
1	27966	29963	31922	33856	35776	37696	39628	41584	43
2	26290	28287	30246	32179	34100	36020	37952	39908	41
3	24643	26640	28599	30532	32453	34373	36304	38261	40
4	23025	25022	26981	28915	30835	32755	34687	36643	38
5	21437	23434	25393	27327	29247	31167	33099	35055	37
6	19880	21877	23836	25769	27689	29609	31541	33498	35
7	18352	20349	22308	24242	26162	28082	30014	31970	33

By taking the inverse of the energies above table wavelength were determined for each transition by taking energy and multiplying it by (1/T) in Angstroms as shown below.

Vc/Vb	0	1	2	3	4	5	6	7	8
0	3370	3158	2974	2812	2668	2538	2419	2310	2208
1	3576	3337	3133	2954	2795	2653	2523	2405	2295
2	3804	3535	3306	3108	2933	2776	2635	2506	2387
3	4058	3754	3497	3275	3081	2909	2754	2614	2484
4	4343	3996	3706	3458	3243	3053	2883	2729	2588
5	4665	4267	3938	3659	3419	3209	3021	2853	2699
6	5030	4571	4195	3881	3611	3377	3170	2985	2818
7	5449	4914	4483	4125	3822	3561	3332	3128	2944

Once theoretical calculations were completed, a Monochromator was used. A Monochromator separates and transmits a narrow portion of the optical signal from a wider range of wavelengths available at the input using a photomultiplier. This Monochromator is able to produce identifiable spectra of the light of interest for diatomic nitrogen in an air lamp.

To assign quantum numbers, the chart created was used to see which vc and vb transition wavelengths corresponded to the spectrum. After assigning quantum numbers, degradation assignment could follow.

Analysis

By measuring the air lamp that contained 78% of Nitrogen we were able to produce a spectra that had distinctive lines. Using the theoretical calculations we assign quantum numbers, a change in energy, and degradation. Quantum numbers of the upper state Vc remained at 2 while the lower state Vb changed from 1-7. Change of energy for certain transition is also displayed on the graph. Degradation of the nitrogen is violet because the bands degrade towards a shorter wavelength. This is shown in Figure 2.

should have more than one Vc

Conclusion

Quantum numbers of Vc=2 and Vb= 1-7 and violet degradation were found for diatomic nitrogen. By using the equation for vibrational motion and theoretical approaches of rotational motion, we were able to assign quantum numbers and degradation to spectra. However, like stated before, total energy of the system is created by both vibrational and rotational. Without the mathematical expression of rotational motion, the assigning of quantum numbers could be off by a certain value. More research is needed for this.

Very unlikely. Rot. energies are v small compared to vibrational energy differen

Reference

G. Herzberg: Molecular Spectra and Molecular Structure. 1. Spectra of Diatomic Molecules, 2nd ed. (Van Nostrand, Princeton 1950)

Figure 2. N_2 3000-4500 Å