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P302: Molecular Spectroscopy and Lasers SSPS-315

1. DIATOMIC MOLECULES: Molecular Quantum numbers and classification of electronic states. Molecular orbitals and ground states of  $H_2$ ,  $C_2$ ,  $N_2$  and  $O_2$ . Selection rules. Symmetry properties. Hund's coupling cases 'a' and 'b'. (Ch. 6.2)

2. ROTATIONAL SPECTROSCOPY: Microwave spectrum of a diatomic molecule. Rigid rotator and non-rigid rotator approximations. The effect of isotopic substitution. Moment of Inertia and bond lengths of diatomic and linear triatomic molecule. Quantum theory and mechanism of Raman scattering. Rotational Raman spectra. The Stark effect. Nuclear hyperfine splitting. Vibrational satellites. Symmetry properties of rotational levels. Influence of nuclear spin and statistical weights on pure rotational Raman spectra of  $CO_2$ ,  $O_2$ ,  $H_2$ ,  $N_2$ .

(Ch. 1.3, 4.2, 4.4, 4.8)

3. VIBRATIONAL SPECTROSCOPY: The vibrating-rotating diatomic molecule. Harmonic and anharmonic oscillator energy levels. Evaluation of rotational constants from Infrared spectra. Evaluation of rotational constants from Raman vibration-rotation spectra. Force constants and bond lengths. The influence of nuclear spin on IR and Raman vibration-rotation spectrum of  $CO_2$ . (Ch. 5.1, 5.2.4)

4. MOLECULAR VIBRATIONS: Symmetry operations and  $C_{nv}$  point groups.  $C_{2v}$  and  $C_{3v}$ . Character tables from the properties of irreducible representations. Relationship between reducible and irreducible representations. Selection rules

for IR and Raman spectra. Reducible representation, fundamental vibrational modes and their activity of  $H_2O$ ,  $NH_3$ ,  $CH_3$ ,  $CO_2$ ,  $HCN$  and formaldehyde molecules. Expected vibrational modes for different structures of  $AB_2$  and  $AB_3$  type molecules. Direct product representation and their activity of Overtones, combination tones, hot bands. Forbidden fundamental frequencies from permitted overtones and combination bands. Fermi resonances of  $CO_2$ ,  $H_2O$  and  $CCl_4$  molecules. Group vibrational modes of  $CH_2$  in  $CCl_3-CH_2-CCl_3$  molecule. (Group theory by Raman Ch. 4, 5.2, 6, 7 and 8)

5. ELECTRONIC SPECTROSCOPY OF DIATOMIC MOLECULES: Vibrational analysis of an electronic band system of a diatomic molecule. Progressions and sequences. Deslandres table and vibrational constants. Isotope effect in vibrational spectra and its applications. Dissociation energy and dissociation products. Selection rules and rotational fine structure of vibronic transitions. The Fortrat diagram and the band head. Combination relations and evaluation of rotational constants for bands  ${}^1\Sigma - {}^1\Sigma$  without Q branches. Ch. 6.2.

5. ELECTRONIC SPECTROSCOPY OF POLYATOMIC MOLECULES: Walsh M.O. diagram for  $AH_2$  molecules. Molecular orbitals, electronic configuration and ground states of  $BeH_2$ ,  $BH_2$ ,  $CH_2$ ,  $NH_2$  and  $H_2O$ . The ground states of formaldehyde,  $NH_3$ ,  $CH_3$  and  $CO_2$  molecules. The symmetry type of bonding and non-bonding orbitals in formaldehyde. Allowed  $\pi-\pi^*$  ( $A_1-A_1$ ) and  $n-\sigma^*$  ( $B_2-A_1$ ) electronic transitions and forbidden  $n-\pi^*$  ( $A_2-A_1$ ) vibronic transitions in formaldehyde. Ch. 6.3.1.

7. LASERS: Line broadening (natural, collision, doppler) and its influence on Laser operation. Rate equations for steady state inversions in 3 and 4 level systems. Longitudinal and transverse modes. single mode operation. ABCD ray matrices and cavity stability criteria for stable resonators. Control of Laser output: Q-factor, Q-switching, Laser spiking, self focussing, mode locking, narrow frequency selection. Laser structure and excitation mechanism of  $N_2$  Laser,  $CO_2$  Laser, Excimer Laser and Dye Lasers. (Ch. 8)

8. LASERS IN SPECTROSCOPY: Distinction between Single rovibronic level fluorescence and Resonance Raman Spectroscopy. Hyper Raman spectroscopy, Stimulated Raman and Raman gain spectroscopy. Inverse Raman spectroscopy. CARS and CSRS. (Ch. 8)

Textbooks:

- 1) High resolution Spectroscopy (Butterworths) : J.M.Hollas.
- 2) Laser fundamentals : W.T.Sylvast
- 3) Molecular structure and spectroscopy G.Aruldas (PHI)

Reference:

Molecular spectra and Molecular Structure (van Nostrand) - G. Herzberg