ZK C9550: Quantum Chemistry and Molecular Spectroscopy

January 8th, 2015

Used also February 6th, 2017

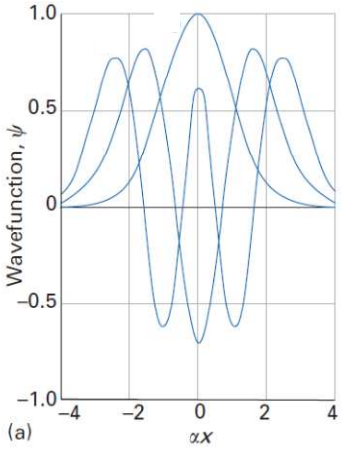
1. Use the energy level scheme for a two-state model to illustrate the origin of the
   (a) Rayleigh scattering
   (b) Raman scattering: Stokes and Anti-Stokes lines

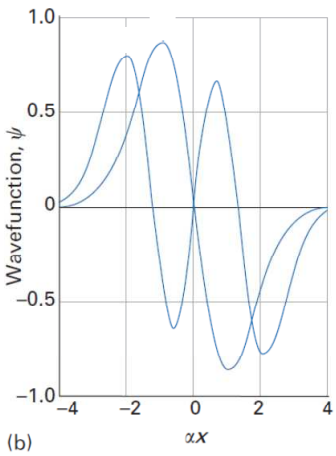
(2 points)

2. A natural linewidth is a result of (1 point)
   (a) disordered movements of molecules in the sample
   (b) intermolecular colissions
   (c) Heisenberg uncertainty relationships

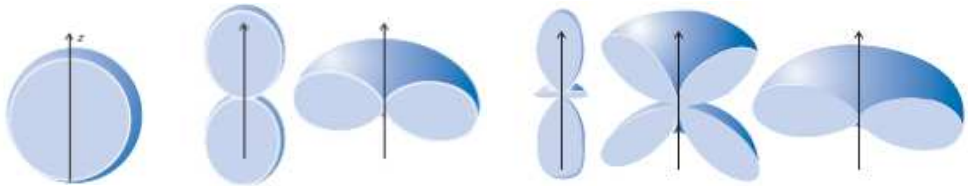
3. Which quantum-mechanical model is represented by the wavefunctions shown below? Fill into the picture the quantum numbers corresponding to the individual wavefunctions.

(3 points)



4. Which quantum-mechanical model is represented by the wavefunctions isosurfaces shown below? Fill into the picture the values of the quantum numbers $l$ and $m_l$ corresponding to the individual wavefunctions. (3 points)



5. Sketch out a qualitative scheme of the electromagnetic spectrum and indicate the arts of molecular excitations typical for the individual regions of the spectrum.

(4 points)

6. Which parameter of the system determines line intensity for a spectroscopic transition between two levels? How is this parameter qualitatively changing, for a constant temperature, from low-energy transitions (NMR) to high-energy transitions (electronic excitations)? (2 points)

7. Write down the general relationship between the energy of a rigid rotor, the angular momentum and the momentum of inertia at the classical and the quantum mechanical levels (constants do not matter).

(2 points)

8. With the help of energy level scheme sketch out the origin of the structure of a vibration-rotational band. Sketch out also the qualitative appearance of the vibration-rotational band in a spectrum (line positions and intensities).

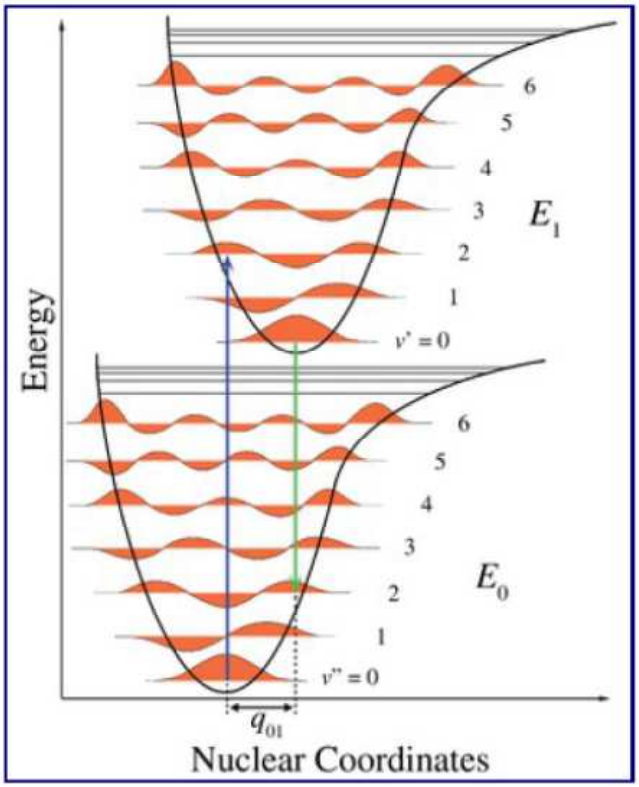
(3 points)

9. The Franck-Condon factor is equal to
   (a) $\int \Psi^*_{vibr,e}(R)\, \Psi_{vibr,g}(R)\, dR$
   (b) $\int \Psi^*_{vibr,e}(R)\, \hat{\boldsymbol{\mu}}\, \Psi_{vibr,g}(R)\, dR$
   (c) $\int \Psi^*_{rot,e}(R)\, \Psi_{rot,g}(R)\, dR$

(1 point)

10. Sketch out a qualitative electron spectrum for a system of energy levels in the following figure. What determines the intensity of a particular spectral line?

(3 points)

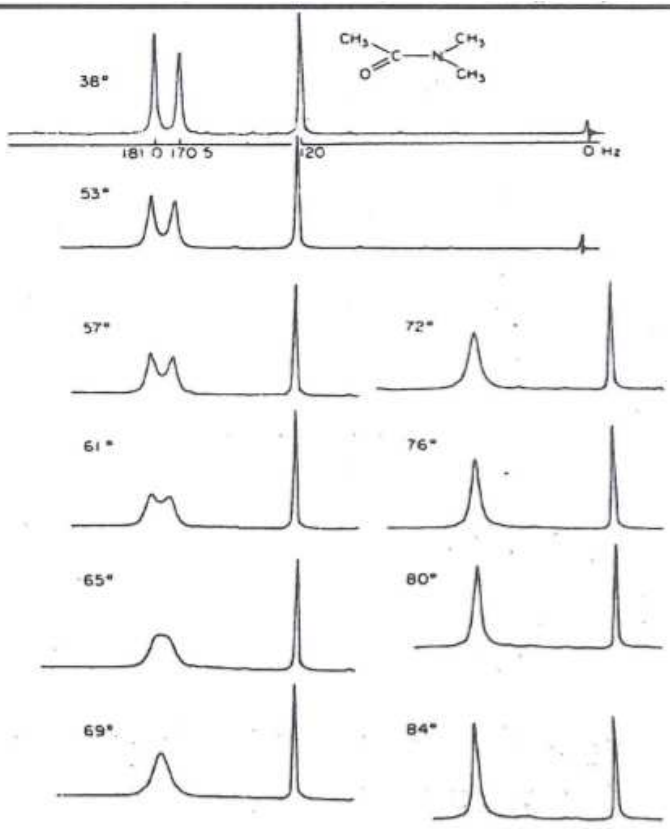


11. With the help of energy level scheme, sketch out the transitions observed during an EPR experiment.

(3 body)

12. (Voluntary) Explain, why in an NMR spectrum of N,N dimethylacetamid the temperature influences the number of signals of interacting protons.

( 3 points)




The 60 MHz $^1$H spectrum of *N*, *N*-dimethylaldehyde at the temperatures indicated.