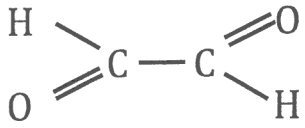
FYS-5206 **OPTICAL SPECTROSCOPY** **EXAM 1-2014**

April 14, 2014

ALLOWED BELONGINGS

- Note sheet, a two-sided A4 written by yourself to memorize details. Return with your exam.
- Simple scientific calculator
- MAOL table book or equivalent

1. Glyoxal (on the right) belongs to C_{2h} point group.



   a) How many normal vibration modes this molecule has?
   b) There is one specific requirement based on molecular symmetry that tells if the vibrational transition is IR absorption active. What is this requirement? And what is the requirement for Raman active vibrational transitions?
   c) Draw one example of normal vibrational modes for each symmetry species in the point group.

C_{2h}	I	C_2	i	σ_h		
A_g	1	1	1	1	R_z	$\alpha_{xx},\alpha_{yy},\alpha_{zz},\alpha_{xy}$
B_g	1	−1	1	−1	R_x,R_y	α_{xz},α_{yz}
A_u	1	1	−1	−1	T_z	
B_u	1	−1	−1	1	T_x,T_y	

2. Explain, how the dissociation energy of two-atom molecule can be determined using
   a) vibrational spectroscopy
   b) electronic spectroscopy
   Which one is more accurate method to determine dissociation energies?

3. NO-molecule in electronic ground state ($^2\Pi$) has $B_e = 1.7046\ \text{cm}^{-1}$, $\alpha = 0.0178\ \text{cm}^{-1}$. The first excited state ($^2\Sigma^+$) has transition energy of $\nu_{00} = 44078.3\ \text{cm}^{-1}$ and at this electronic state $B_e = 1.9952\ \text{cm}^{-1}$, $\alpha = 0.0164\ \text{cm}^{-1}$.
   a) Draw potential curves of these electronic states including few lowest vibrational states and vibronic transitions $\gamma(0,0)$, $\gamma(1,0)$ ja $\gamma(2,0)$ (notation $\gamma(v',v'')$).
   b) Is the band head of $\gamma(0,0)$ -band in P- or R-branch?
   c) Calculate the wavenumber of the band head of the $\gamma(0,0)$ band.

4. Explain shortly the following methods. You can draw pictures to clarify your answer.
   a) Wavelength modulation spectroscopy
   b) Photoacoustic spectroscopy
   c) Laser-induced breakdown spectroscopy
   d) Cavity ring-down spectroscopy

5. A collimated light beam having spectral intensity $I_\nu(0)$ travels through a sample having thickness L and spectral absorption coefficient κ_ν^{ik} related to the specific transition i-k. Beer-Lambert law states that the spectral intensity after the sample is $I_\nu(L) = I_\nu(0)\exp(-\kappa_\nu^{ik}L)$. The width of the absorption line is $\delta\nu$ and the light has spectral bandwidth of $\Delta\nu$. Show, that

   a) if $\Delta\nu \gg \delta\nu$, it yields to $I(L) = I(0)\dfrac{1}{\Delta\nu}\displaystyle\int_{\Delta\nu}\exp(-\kappa_\nu^{ik}L)d\nu$, and

   b) if $\Delta\nu \ll \delta\nu$, it yields to $I(L) = I(0)\exp(-\kappa_0^{ik}L)$,

   where $I \equiv \displaystyle\int_{\Delta\nu} I_\nu d\nu$ is the total light intensity at spectral band of $\Delta\nu$ and κ_0^{ik} is the absorption coefficient at the center of the absorption line. Clarify your solution with pictures.