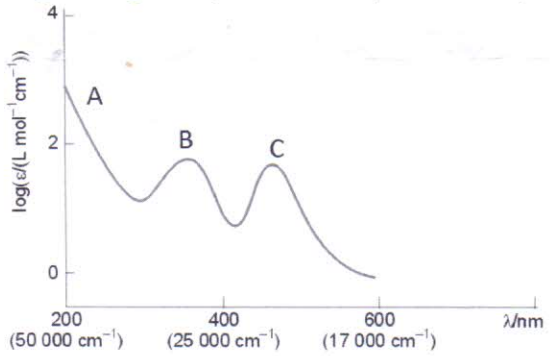
Exam 2016-2017 (ii)

This exam consists out of 4 problems and 2 pages. ***Write your name and student number on every page containing answers****. It is not allowed to use your notes, books, mobile phone, etc. The use of a molecular model kit is allowed. Read the questions carefully before you answer them. Answer the question precisely and clearly indicate how you got to the answer. When a justification is asked, it counts as least as many points as the answer itself. The number of points (total = 90) is indicative and may be re-evaluated.*

1) The typical yellow light that comes from a sodium lamp is due to emission of light from a ^2P state to ^2S state in sodium. In absence of a magnetic field two sharp peaks can be observed in the emission spectrum. Explain this. How many signals do you expect to find for this ^2P to ^2S emission of in case sodium is placed in a magnetic field. - *20 points*

2) Consider an octahedral d^2 complex.
   a. Give all term symbols belonging to octahedral d^2 complex and indicate which of these term(s) is/are the ground state. - *5 points*
   b. In the Figure below is given the absorption spectrum. Which three d-d transitions are most important to explain this spectrum? - *5 points*
   c. Assume that Δ (the energy difference between the t_{2g} and e_g orbitals) is relatively large. Assign the peaks in the spectrum. Explain your answer. - *10 points*



3) Give the irreducible representations of the C-H stretching modes of the compounds below. Determine how the H atoms move during the C-H stretching modes. Give your answer in the form of normalized linear combinations. - *30 points*
   a. Methane (T_d)
   b. Ethene (D_{2h})
   c. 1,3,5-trichlorobenzene (D_{3h})

4) Give the irreducible representations belonging to the IR active bending modes of chloroform ($CHCl_3$, C_{3v}). - *20 points*

Free-ion Term	Terms in O_h
S	A_{1g}
P	T_{1g}
D	$E_g + T_{2g}$
F	$A_{2g} + T_{1g} + T_{2g}$
G	$A_{1g} + E_g + T_{1g} + T_{2g}$
H	$E_g + 2T_{1g} + T_{2g}$
I	$A_{1g} + A_{2g} + E_g + T_{1g} + 2T_{2g}$

Electronic Configuration	**Term Symbol**
s^1	^{2}S
p^1, p^5	^{2}P
p^2, p^4	^{1}S, ^{1}D, ^{3}P
p^3	^{2}P, ^{2}D, ^{4}S
d^1, d^9	^{2}D
d^2, d^8	^{1}S, ^{1}D, ^{1}G, ^{3}P, ^{3}F
d^3, d^7	^{4}F, ^{4}P, ^{2}H, ^{2}G, ^{2}F, ^{2}D (2), ^{2}P
d^4, d^6	^{5}D, ^{3}H, ^{3}G, ^{3}F (2), ^{3}D, ^{3}P(2), ^{1}I, ^{1}G(2), ^{1}F, ^{1}D(2), ^{1}S(2)
d^5	^{6}S, ^{4}G, ^{4}F, ^{4}D, ^{4}P, ^{2}I, ^{2}H, ^{2}G(2), ^{2}F(2), ^{2}D(3), ^{2}P, ^{2}S

Character table for T_d point group

	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$	linear, rotations	quadratic
A_1	1	1	1	1	1		$x^2+y^2+z^2$
A_2	1	1	1	-1	-1		
E	2	-1	2	0	0		$(2z^2-x^2-y^2, x^2-y^2)$
T_1	3	0	-1	1	-1	(R_x, R_y, R_z)	
T_2	3	0	-1	-1	1	(x, y, z)	(xy, xz, yz)

Character table for D_{2h} point group

	E	C_2 (z)	C_2 (y)	C_2 (x)	i	σ (xy)	σ (xz)	σ (yz)	linear, rotations	quadratic
A_g	1	1	1	1	1	1	1	1		x^2, y^2, z^2
B_{1g}	1	1	-1	-1	1	1	-1	-1	R_z	xy
B_{2g}	1	-1	1	-1	1	-1	1	-1	R_y	xz
B_{3g}	1	-1	-1	1	1	-1	-1	1	R_x	yz
A_u	1	1	1	1	-1	-1	-1	-1		
B_{1u}	1	1	-1	-1	-1	-1	1	1	z	
B_{2u}	1	-1	1	-1	-1	1	-1	1	y	
B_{3u}	1	-1	-1	1	-1	1	1	-1	x	

Character table for D_{3h} point group

	E	$2C_3$	$3C'_2$	σ_h	$2S_3$	$3\sigma_v$	linear, rotations	quadratic
A'_1	1	1	1	1	1	1		x^2+y^2, z^2
A'_2	1	1	-1	1	1	-1	R_z	
E'	2	-1	0	2	-1	0	(x, y)	(x^2-y^2, xy)
A''_1	1	1	1	-1	-1	-1		
A''_2	1	1	-1	-1	-1	1	z	
E''	2	-1	0	-2	1	0	(R_x, R_y)	(xz, yz)

Character table for C_{3v} point group

	E	$2C_3$ (z)	$3\sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0