

Spectroscopy Exam

Friday November 1st 2019

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Write your name and student number on every page containing answers. It is not allowed to use your notes, books, mobile phone, etc.

This exam consists out of 6 problems and 4 pages. Read the questions carefully before you answer them. Answer the question precisely and clearly indicate how you got to the answer. An explanation how you got to your answer counts at least as many points as the answer itself.

Q1: How many photons are involved in a single scattering event? **3 points**

Q2: What is an improper rotation? **3 points**

Q3: Consider the dioxygen molecule:

a) Determine all term symbols belonging to the ground state configuration of the dioxygen molecule: $(\sigma_{2s})^2(\sigma_{2s}^*)^2(\sigma_{2p})^2(\pi_{2p})^4(\pi_{2p}^*)^2$. **8 points**

b) besides the ground and excited states you found under a) two more excited states with the terms $A^3\Sigma_u^+$ and $B^3\Sigma_u^-$ play an important role in the photochemistry of oxygen. Which absorptions can be observed in the UV-vis spectrum of O_2 at ambient conditions? **8 points**

c) The O_2 molecule with either a $A^3\Sigma_u^+$ Term or a $B^3\Sigma_u^-$ Term easily falls apart into separate atoms. What Term symbols do belong to an oxygen atom with a p^4 configuration? Explain your answer. **8 points**

Q4: The distinct yellow light of a sodium lamp comes from a transition from a 2P Term to a 2S term. In absence of a magnetic field two lines are observed for this transition, while several more lines can be observed in the presence of a magnetic field. Explain these phenomena and indicate how many lines you expect to find for this transition in the presence of a magnetic field. Explain your answer. **8 points**

Q5: Consider the molecule cyclopropane with d_{3h} symmetry:

a) Determine the irreducible representations belonging to the C-H stretches. **8 points**

b) Determine the irreducible representations belonging to the C-C stretches. **8 points**

c) Determine the irreducible representations belonging to the bending modes. **8 points**

d) On the basis of your results in the questions a), b) and c), draw the Raman spectrum of cyclopropane. Include the Stokes, Raleigh and anti-stokes parts of the spectrum. You may assume that the Raman spectrum is recorded in a solution and that rotational features are not visible. Highlight for every peak in your spectrum what it is, and why you drew it in the way you did. **8 points**

Q6: Describe the stretching modes of the molecules below in the form of fully normalized linear equations that represent how the atoms move.

a) Sulfate (T_d), SO_4^{2-} **10 points**

b) sulfite (C_{3v}), SO_3^{2-} **10 points**

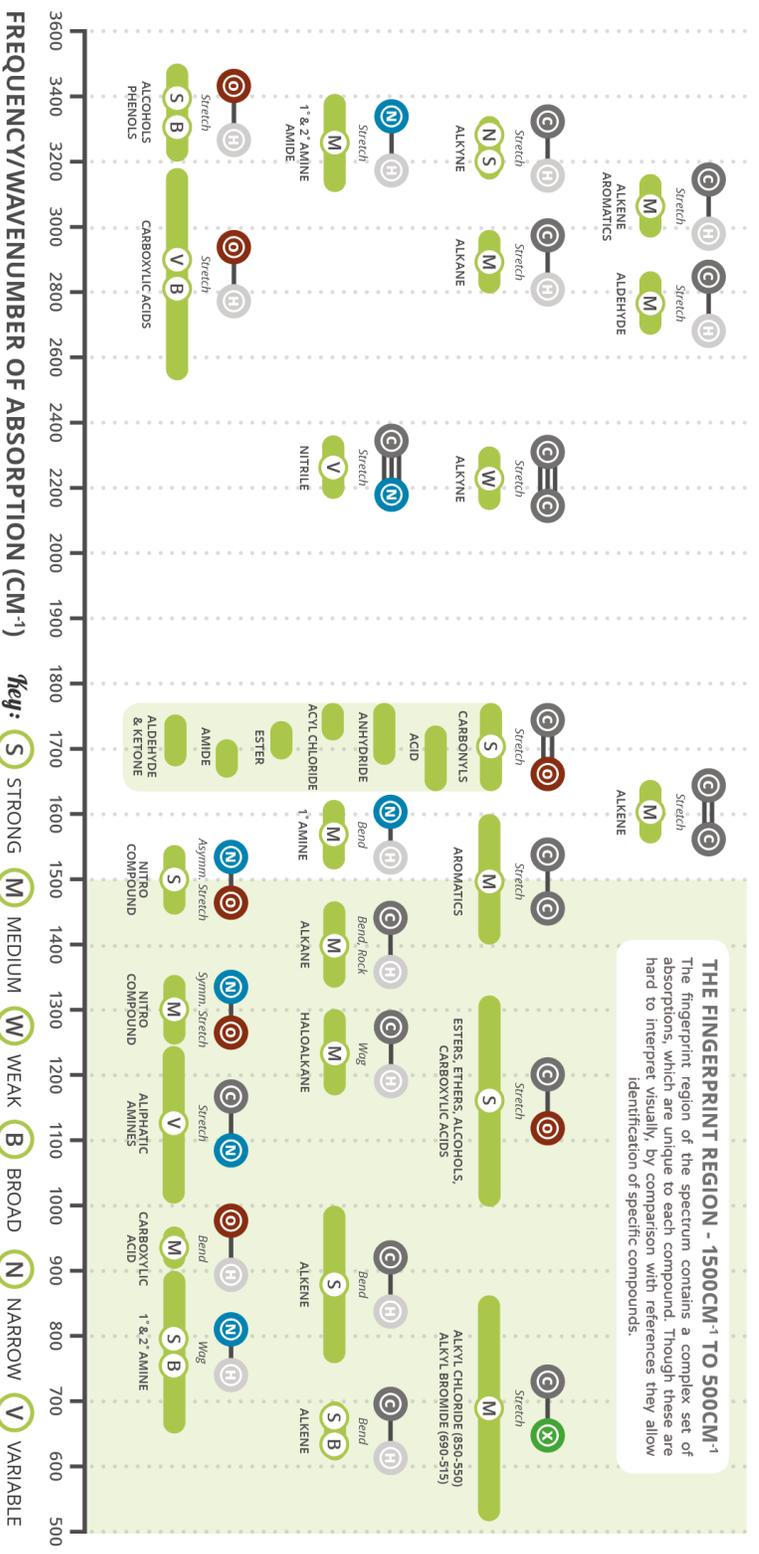
D_{3h}	E	$2C_3$	$3C_2$	σ_h	$2S_3$	$3\sigma_v$		
A'_1	1	1	1	1	1	1		$x^2 + y^2, z^2$
A'_2	1	1	-1	1	1	-1	R_z	
E'	2	-1	0	2	-1	0	(x, y)	$(x^2 - y^2, xy)$
A''_1	1	1	1	-1	-1	-1		
A''_2	1	1	-1	-1	-1	1	z	
E''	2	-1	0	-2	1	0	(R_x, R_y)	(xz, yz)

C_{3v}	E	$2C_3$	$3\sigma_v$		
A_1	1	1	1	z	$x^2 + y^2, z^2$
A_2	1	1	-1	R_z	
E	2	-1	0	$(x, y), (R_x, R_y)$	$(x^2 - y^2, xy), (xz, yz)$

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$		
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)	(xz, yz, xy)

ANALYTICAL CHEMISTRY - INFRARED SPECTROSCOPY

Commonly referred to as IR spectroscopy, this technique allows chemists to identify characteristic groups of atoms (functional groups) present in molecules.



Infrared frequencies make up a portion of the electromagnetic spectrum. If a range of infrared frequencies are shown through an organic compound, some of the frequencies are absorbed by the chemical bonds within the compound. Different chemical bonds absorb different frequencies of infrared radiation. There are a number of characteristic absorptions which allow functional groups (the parts of a compound which give it its particular reactivity) to be identified. This graphic shows a number of these absorptions.



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