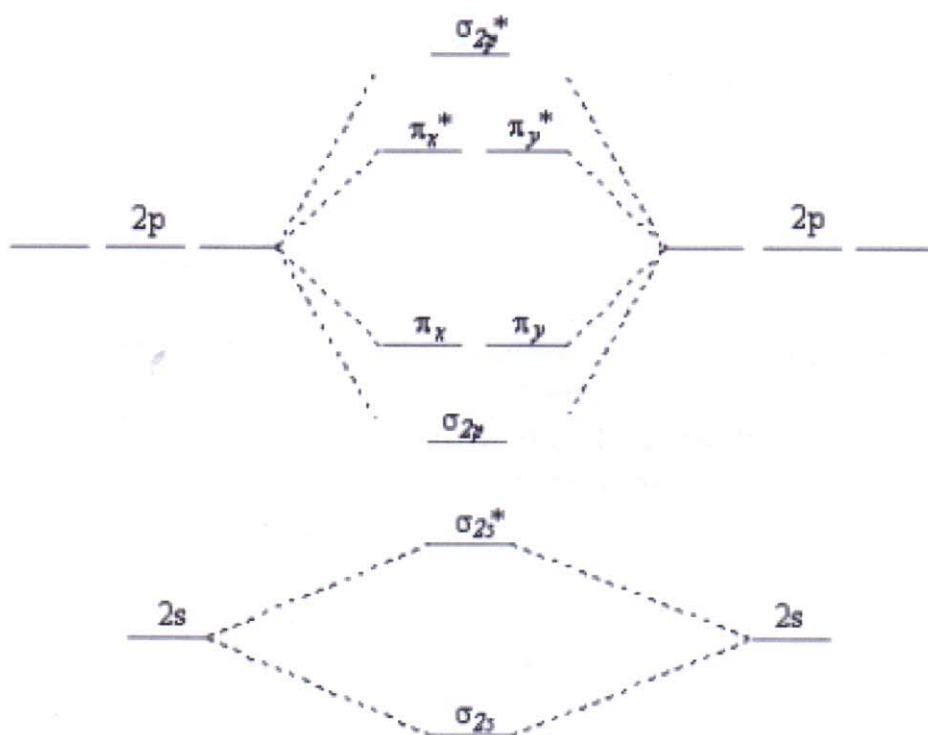


## EXAM

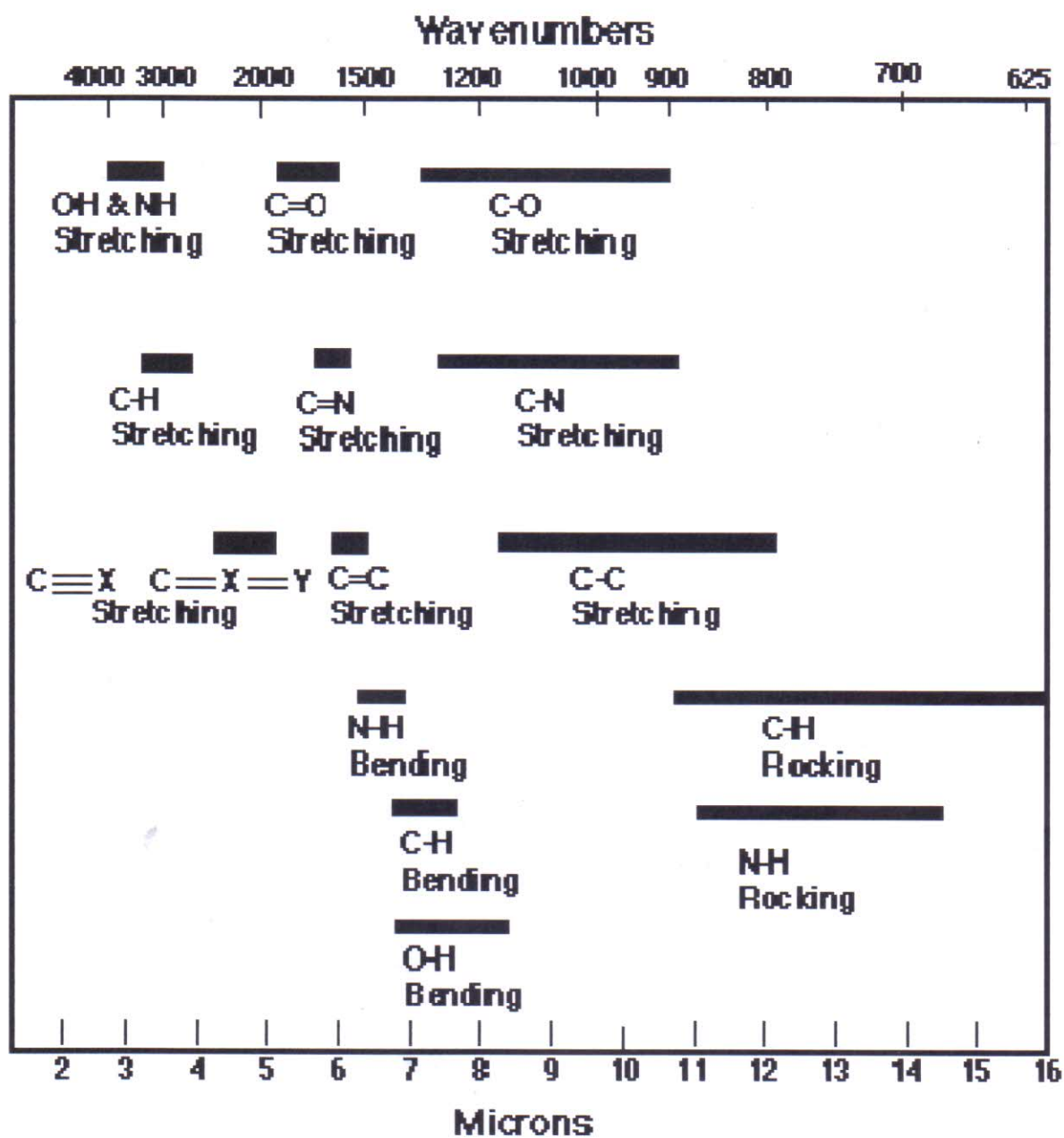
This exam consists out of 4 problems and 3 pages. **Write your name and student number on every page containing answers.** It is not allowed to use your notes, books, mobile phone, etc. The use of a molecular model kit is allowed. Read the questions carefully before you answer them. Answer the question 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) Consider the molecule  $F_2$ .



- What term symbol belongs to the ground state of  $F_2$ ? – 2 points
- What term symbols do you get if one electron is moved from a  $\pi^*$  orbital to the  $\sigma_{2p}^*$  orbital? Which of these states can be accessed from the ground state upon absorption of electromagnetic radiation? – 6 points
- For transitions from one electronic state to another electronic state typically many lines are observed in the spectrum as multiple vibrational modes are excited. Explain how and why these modes are excited using an energy diagram. – 7 points

- 2) The typical yellow light that comes from a sodium lamp is due to emission from  $^2P$  states to  $^2S$  states of sodium atoms. In absence of a magnetic field two lines are observed in the spectrum for this particular transition. Explain this. How many lines do you expect to find in the presence of a magnetic field? Use energy diagrams to explain your answers. – 15 points
- 3) There are  $6 \times 5 \times 4 / 3! = 20$  different possibilities to put three electrons into three p orbitals. Give all term symbols that belong to the  $p^3$  configuration. – 15 points
- 4) Consider the molecule cyclopropane and the  $D_{3h}$  character table in the appendix.
- Determine to which irreducible representations the C-C stretching modes belong. – 5 points
  - Determine to which irreducible representations the C-H stretching modes belong. – 5 points
  - Determine the motion that the C-H stretching modes make during vibration. Give your answers in the form of a normalized equation. – 15 points
  - Determine to which irreducible representations the bending modes of cyclopropane belong. – 10 points
  - Give a qualitative sketch of the IR spectrum that you expect on the basis of your answers given in a), b) and d). Assign all peaks that you have drawn in the spectrum. Use the table in the appendix. – 5 points
  - The table in the appendix shows that aliphatic C-H signals can be observed at  $2900 \text{ cm}^{-1}$ . At what frequency do you expect to find C-D signals (D = deuterium). Explain your answer. – 5 points



$D_{3h}$	$E$	$2C_3$	$3C_2$	$\sigma_h$	$2S_3$	$3\sigma_v$	
$A_1'$	1	1	1	1	1	1	$x^2 + y^2, z^2$
$A_2'$	1	1	-1	1	1	-1	
$E'$	2	-1	0	2	-1	0	$(x^2 - y^2, xy)$
$A_1''$	1	1	1	-1	-1	-1	
$A_2''$	1	1	-1	-1	-1	1	
$E''$	2	-1	0	-2	1	0	$(xz, yz)$