Mathematical Methods in Chemistry, Part I
Symmetry and Group Theory
Midterm Exam

April 17, 2023

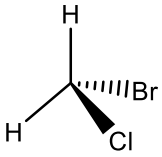
Name:

2 h to complete the exam. Total number of points: 33.

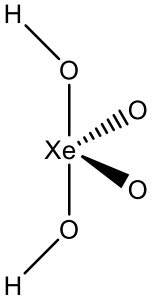
Please note that this is not an open-book exam. Only the material handed out with the exam questions may be used. You are allowed to use a non-programmable calculator, but the calculator will be checked during the exam. Computers or molecular modeling kits are not permitted. Do not write with a pencil or a fountain pen that can be erased. Please have your photo ID ready.

1) Determine the point group of the following molecules and objects. (10 points)

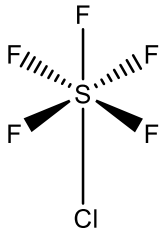
A



B



C



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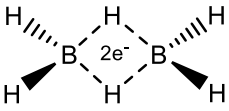

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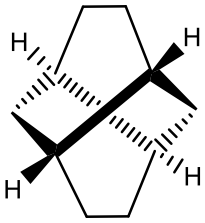
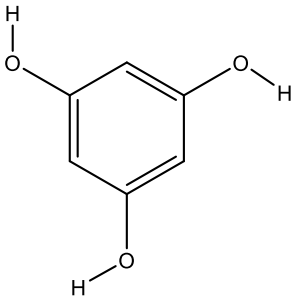
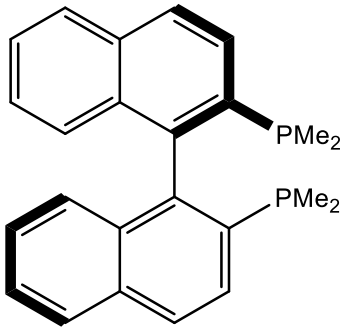


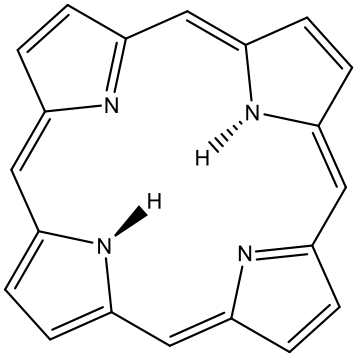
F



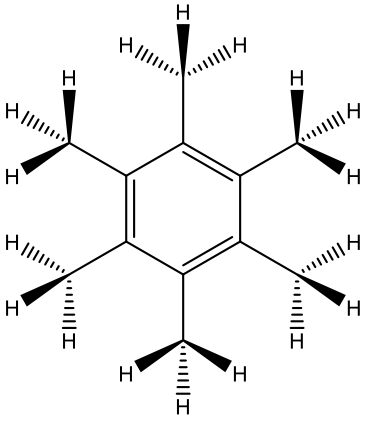
G



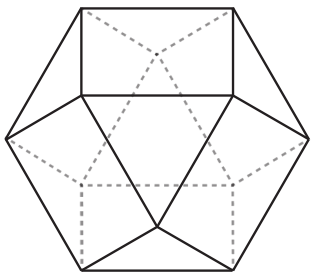
H



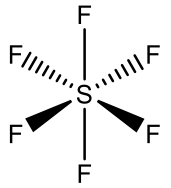
I



J



2) Construct a qualitative molecular orbital diagram for SF_6. (10 points total)



For the basis functions, use the 3s and 3p orbitals of the sulfur atom as well as a 2p orbital on each fluorine atom that is pointing towards the sulfur.

a) Draw the molecular orbital diagram. Make sure to add symmetry labels to each molecular orbital in your diagram and populate the orbitals with electrons. (7 points)

b) Determine the symmetry adapted linear combinations for the six fluorine 2p orbitals that are pointing towards the sulfur and draw them. (3 points)

3) The quaternion group $Q = \{1, -1, a, -a, b, -b, c, -c\}$ is a group with respect to multiplication. (13 points total)

The quaternions, which can be understood as an extension of complex numbers, satisfy the relations

$$a^2 = b^2 = c^2 = -1$$

and

$$abc = -1.$$

a) Write down the group multiplication table of the quaternion group. (4 points)

While multiplication of the quaternions is associative, do not assume that it is commutative.

Hint: If you struggle to figure out the products of the quaternions, you might want to solve problem 3d) first and then use the result to solve this problem. You can also use the information provided in d) to verify your result.

b) Demonstrate that $Q = \{1, -1, a, -a, b, -b, c, -c\}$ is a group with respect to multiplication. Is the group Abelian? (2.5 points)

c) Determine the classes of Q. (2 points)

Hint: You can also use the information provided in d) to solve this problem.

d) The elements a, b, and c of the quaternion group can be represented with the following two-dimensional matrices.

1	-1	a	b	c	-a	-b	-c
…	…	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$	…	…	…

Express the remaining elements of the quaternion group with two-dimensional matrices in order to obtain a two-dimensional representation of the quaternion group. (1 point)

e) The two-dimensional representation obtained in d) is irreducible. Based on this information, construct the character table for the quaternion group. (3.5 points)