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

April 17, 2024

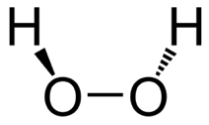
Name:

2 h to complete the exam. Total number of points: 38.

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.

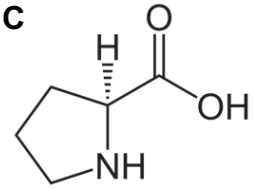
1) Determine the point group of the following molecules and objects. (12 points)

A



B

C



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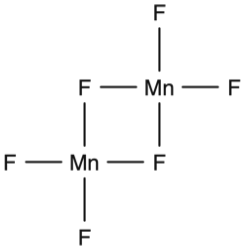

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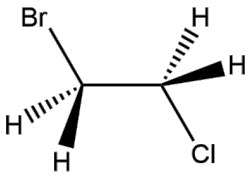
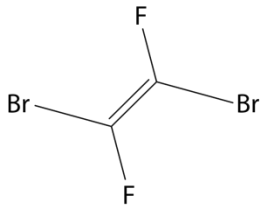
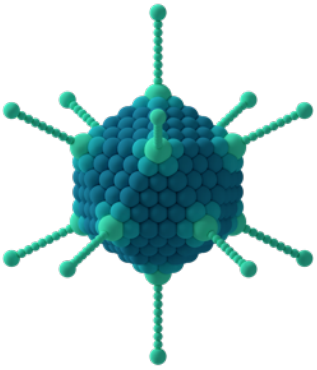


F

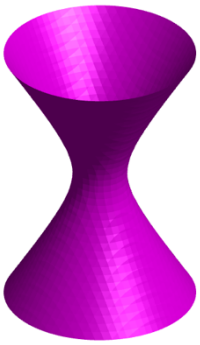


G



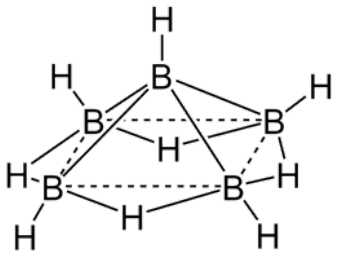
Adenovirus

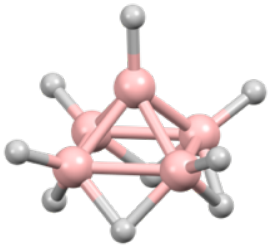
H



$$\frac{x^2}{a^2} + \frac{y^2}{b^2} - \frac{z^2}{c^2} = 1$$

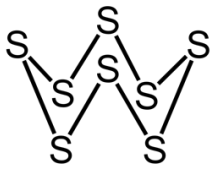
I

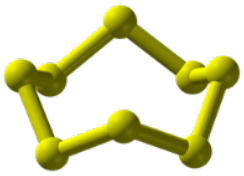




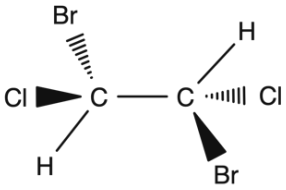
Pentaborane(9)

J

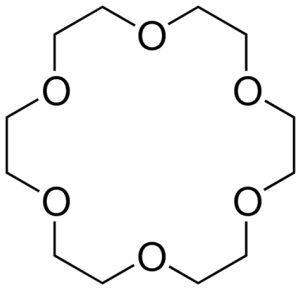


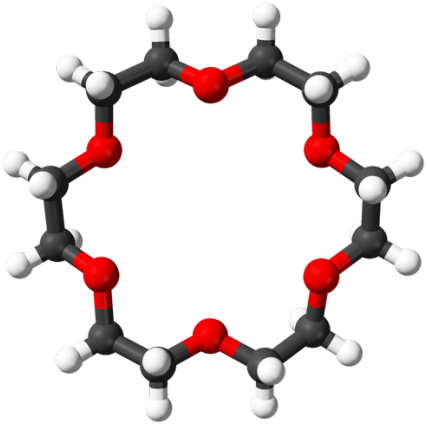


K



L





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2) Determine all subgroups of the points groups C_{4v}, C_i, C_{2h}, D_{2h}. (2 points)

3) BrF_5 has a square pyramidal geometry. How many peaks do you expect to find in the IR and Raman spectrum? (10 points)

4) Assume that $\{\psi_1, \psi_2\}$ is a basis of a representation Γ of the group G and consider the direct product $\Gamma \otimes \Gamma$. The symmetrized part of the direct product contains the following three functions

$$\left\{\psi_1\psi_1, \frac{1}{2}(\psi_1\psi_2 + \psi_2\psi_1), \psi_2\psi_2\right\},$$

which form a basis for another representation Γ_s.

Note that in this notation $\psi_1\psi_2 = \psi_1(r_1)\psi_2(r_2)$ and $\psi_2\psi_1 = \psi_2(r_1)\psi_1(r_2)$, where r_1 and r_2 are coordinates in three-dimensional space.

Show that the character χ_{Γ_s} of this representation for an operation R is given by the following formula

$$\chi_{\Gamma_s}(R) = \frac{1}{2}[\chi_\Gamma(R)^2 + \chi_\Gamma(R^2)],$$

where χ_Γ represents the character of the representation Γ. (7 points)

5) In class, we have used symmetry to construct a qualitative MO diagram of CH_4. For the minimal basis, we used the 2s and 2p orbitals on the carbon atom. Show that we would have obtained the same result if we had instead used four sp^3 hybridized orbitals on the carbon.

To this end, show that the sp^3 orbitals give rise to SALCs of the same symmetry species as the 2s and 2p orbitals. Determine the SALCs of the sp^3 orbitals. Finally, show that these SALCs are identical to the 2s and the 2p orbitals. (7 points total)