Chemistry 6330
Winter Quarter 2018

Midterm Exam

Name: _____

Question 1: _____ pts / 15 pts

Question 2: _____ pts / 10 pts

Question 3: _____ pts / 20 pts

Question 4: _____ pts / 15 pts

Question 5: _____ pts / 25 pts

Question 6: _____ pts / 15 pts

TOTAL: _____ **PTS / 100 PTS**

(1) [15 pts] Consider a mathematical group.

(a) [8 pts] List the properties that define a group.

(b) [3 pts] What is a subgroup?

(c) [4 pts] What is a class?

(2) [10 pts] Suppose that a S_4 rotation about the y-axis operates on a general Cartesian point (a,b,c).

(a) [7 pts] What is the Cartesian coordinate of the transformed point? Show your work.

(b) [3 pts] What is the general 3x3 matrix for a reflection through a plane that contains the z-axis and the line x=y?

(3) [20 pts] For the following products of symmetry operations, determine (i) a single symmetry operation that is equal to the product and (ii) if the symmetry operations commute.

(a) [10 pts] $C_2^z \bullet \sigma_{x=y}$

(i) _____   (ii) Commute? _____

(b) [10 pts] $C_4^x \bullet i$

(i) _____   (ii) Commute? _____

(4) [15 pts] A blank character table for the D_{2d} symmetry point group is shown below. Use your knowledge of the properties of groups and representations to generate the five irreducible representations A_1, A_2, B_1, B_2, and E. Show your work (i.e. explain how you arrived at answers)!

D_{2d}	E	$2S_4$	C_2	$2C_2'$	$2\sigma_d$		
A_1							x^2+y^2, z^2
A_2						R_z	
B_1							x^2-y^2
B_2						z	xy
E						$(x,y)\ (R_x,R_y)$	(xz,yz)

(5) [25 pts] Consider ethene drawn below.

$$\underset{H}{\overset{H}{\diagdown}}C=C\underset{H}{\overset{H}{\diagup}}$$
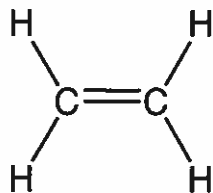
(a) [6 pts] Identify all the symmetry elements and symmetry operations of the molecule (it may help to draw them on the molecule)

(b) [4 pts] What is the point group of ethene? _____

(c) [10 pts] Write the representation for transposing the four H atoms in ethene.

(d) [5 pts] Is the representation in part (c) reducible or irreducible? Explain your answer.

(6) [15 pts] The following questions pertain the D_{4h} point group (character table included).

   (a) [10 pts] Find the direct product $E_u \bullet E_u$ and reduce to a sum of irreducible representations.

(b) [5 pts] Show that the irreducible representations B_{2g} and E_g are orthogonal to one another.

Selected Character Tables

C_{2h}	E	C_2	i	σ_h		
A_g	1	1	1	1	R_z	x^2, y^2, z^2, xy
B_g	1	-1	1	-1	R_x, R_y	xz, yz
A_u	1	1	-1	-1	z	
B_u	1	-1	-1	1	x, y	

D_2	E	$C_2(z)$	$C_2(y)$	$C_2(x)$		
A	1	1	1	1		x^2, y^2, z^2
B_1	1	1	-1	-1	z, R_z	xy
B_2	1	-1	1	-1	y, R_y	xz
B_3	1	-1	-1	1	x, R_x	yz

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$		
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	

D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1	1	1		x^2+y^2, z^2
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1	R_z	
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1		x^2+y^2
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1		xy
E_g	2	0	-2	0	0	2	0	-2	0	0	(R_x, R_y)	(xz, yz)
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1		
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1	z	
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1		
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1		
E_u	2	0	-2	0	0	-2	0	2	0	0	(x,y)	

ADDITIONAL BLANK PAPER FOR WORK - Do not turn in final answers on this sheet.