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## **MIDTERM 2: CHM 2311 – Introduction to Structure and Bonding**

Professor: Jaclyn Brusso

Date: March 17, 2016

Duration: 75 minutes

Name: \_\_\_\_\_

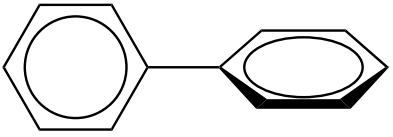
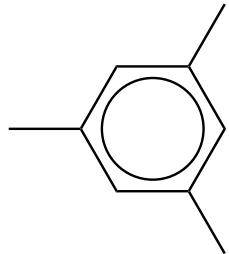


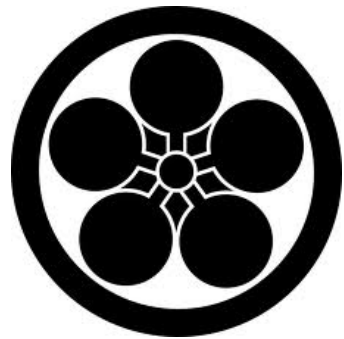


Student Number: \_\_\_\_\_

### **Instructions:**

- Be sure to print your name and ID number clearly on this test booklet.
- This is a closed book examination.
- Please write legibly and show your work to receive credit for your answers. Partial marks *in some cases* may be awarded for partially correct work.
- For remarking, the exam *must* be written in pen.
- There are 4 questions. You are expected to answer all 4 questions.
- There are 6 pages. Please make sure you have all 6 pages. NOTE: the last page is a DATA SHEET. You may tear it off.
- At the end of the exam, turn in this test booklet and the data sheet.  
GOOD LUCK!

<b>Question</b>	<b>Grade</b>
<b>1</b>	<b>/10</b>
<b>2</b>	<b>/29</b>
<b>3</b>	<b>/4</b>
<b>4</b>	<b>/11</b>
<b>TOTAL</b>	<b>/54</b>

1. Determine the point group for each of the following molecules/shapes. (1 mark each; *no partial marks*).

(a)	$[\text{SbF}_6]^-$	$O_h$	(f)	<i>trans</i> - $[\text{SbBr}_2\text{F}_4]^-$	$D_{4h}$
(b)		$D_{2d}$	(g)		$D_{3h}$
(c)	$\text{IF}_5$	$C_{4v}$	(h)		$C_s$
(d)		$C_{4h}$	(i)		$D_{5h}$
(e)		$D_{2h}$	(j)		$C_{2v}$

2. Complete the following character tables. (29 marks; ½ mark each)

(a)

$D_4$	E	$2C_4$	$C_2$	$C_2'$	$C_2''$	
$A_1$	1	1	1	1	1	$z^2$
$B_2$	1	-1	1	-1	1	xy
$B_1$	1	-1	1	1	-1	$x^2-y^2$
$A_2$	1	1	1	-1	-1	z

(b)

$C_{4v}$	E	$2C_4$	$C_2$	$2\sigma_v$	$2\sigma_d$	
$A_1$	1	1	1	1	1	z
$A_2$	1	1	1	-1	-1	$R_z$
$B_1$	1	-1	1	1	-1	$x^2-y^2$
$B_2$	1	-1	1	-1	1	xy
<b>E</b>	2	0	-2	0	0	(x,y)

(c)

$D_{4h}$	E	$2C_4$	$C_2$	$2C_2'$	$2C_2''$	$i$	$S_4$	$\sigma_h$	$2\sigma_v$	$2\sigma_d$	
$A_{1g}'$	1	1	1	1	1	1	1	1	1	1	$z^2$
$B_{2g}'$	1	-1	1	-1	1	1	-1	1	-1	1	xy
$B_{1g}'$	1	-1	1	1	-1	1	-1	1	1	-1	$x^2-y^2$
$A_{2u}''$	1	1	1	-1	-1	-1	-1	-1	1	1	z

3. (4 marks) Using the properties of character tables and the rules for assigning irreducible representations, find the errors in the character tables below. Explain your answers.

(a)

$D_{3d}$	E	$2C_3$	$3C_2'$	$i$	$2S_6$	$3\sigma_d$	
$A_{2u}$	1	1	-1	-1	-1	1	z
$E_u$	2	-1	0	-2	-1	0	(x,y)

The sum of the products of the characters, multiplied together for each class and multiplied by the number of operations in the class for this pair of irreducible representations does not equal zero; therefore does not satisfy the requirement for irreducible representations to be orthogonal to one another.

$$\hookrightarrow A_{2u} * E_u = (1 \times 2) + 2(1 \times -1) + 3(-1 \times 0) + (-1 \times -2) + 2(-1 \times -1) + 3(1 \times 0) = 4 \neq 0$$

$A_{2u}$  is a correct irreducible rep;  $E_u$  is incorrect

(b)

$D_{3h}$	E	$2C_3$	$3C_2$	$\sigma_h$	$2S_3$	$3\sigma_v$	
$A_2''$	1	1	-1	-1	-1	1	z
$A_1'$	1	1	1	1	1	1	$z^2$
T	2	-1	0	2	-1	0	(x,y)

The label T should be E because the character for the identity is 2

$A_2''$  and  $A_1'$  are acceptable irreducible representation

(c)

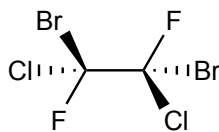
$C_{3v}$	E	$2C_3$	$3\sigma_v$	
$A_1$	1	1	1	$z^2$
$B_2$	-1	1	-1	z
E	2	-1	0	x,y

$B_2$  is incorrect because cannot have a negative character for the identity; incorrect function

The function for E is incorrect, must have parentheses around the (x,y)

$A_1$  is an acceptable irreducible representation

4. (11 marks) Answer the following questions considering the molecule 1,2-dibromo-1,2-dichloro-1,2-difluoroethane (shown below).



- What is the point group for this molecule? (1 mark)
- Assign all symmetry operations associated with this point group. (1 mark each)
- Derive the irreducible representations for the following functions: z, xy. (1 mark each; *no partial marks*)
- Assign symmetry labels to each of the irreducible representations from (c). (1 mark each; *no partial marks*)
- Build a character table including the information from parts a-c. (1 mark; *no partial marks*)
- Is this a complete character table? Why? (1 mark)
- What is the order of this point group? (1 mark)
- Is this molecule chiral? Explain why or why not based on symmetry arguments. (1 mark)

Answer:

- $C_i$
- top row of character table; 1 mark for each symmetry element listed in the character table
- two rows in the character table; 1 mark for each irreducible representation, no partial marks
- left hand column of character table; 1 mark each, no partial marks
- 1 mark for correctly drawing the table including the point group and symmetry elements, functions and symmetry labels (order of symmetry elements and functions does not matter).
- yes because the number of irreducible representations (2) is equal to the number of classes (2).
- $h = 2$
- No, this molecule is not chiral. A molecule is chiral if it has *no symmetry operations* (other than E) or if it *only has a proper rotation axis*.

$C_i$	E	i	
$A_g$	1	1	xy
$A_u$	1	-1	z

# DATASHEET

1																		18																																																																																																															
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* If this number is in parentheses, then it refers to the atomic mass of the most stable isotope.																																																																																																																																	
<table border="1"> <tr> <td>58</td><td>59</td><td>60</td><td>61</td><td>62</td><td>63</td><td>64</td><td>65</td><td>66</td><td>67</td><td>68</td><td>69</td><td>70</td><td>71</td> </tr> <tr> <td>Ce</td><td>Pr</td><td>Nd</td><td>Pm</td><td>Sm</td><td>Eu</td><td>Gd</td><td>Tb</td><td>Dy</td><td>Ho</td><td>Er</td><td>Tm</td><td>Yb</td><td>Lu</td> </tr> <tr> <td>Cerium</td><td>Praseodymium</td><td>Neodymium</td><td>Promethium</td><td>Samarium</td><td>Europium</td><td>Gadolinium</td><td>Terbium</td><td>Dysprosium</td><td>Holmium</td><td>Erbium</td><td>Thulium</td><td>Ytterbium</td><td>Lutetium</td> </tr> <tr> <td>140.12</td><td>140.91</td><td>144.24</td><td>(145)</td><td>150.36</td><td>151.96</td><td>157.25</td><td>158.93</td><td>162.50</td><td>164.93</td><td>167.26</td><td>168.93</td><td>173.04</td><td>174.97</td> </tr> <tr> <td>90</td><td>91</td><td>92</td><td>93</td><td>94</td><td>95</td><td>96</td><td>97</td><td>98</td><td>99</td><td>100</td><td>101</td><td>102</td><td>103</td> </tr> <tr> <td>Th</td><td>Pa</td><td>U</td><td>Np</td><td>Pu</td><td>Am</td><td>Cm</td><td>Bk</td><td>Cf</td><td>Es</td><td>Fm</td><td>Md</td><td>No</td><td>Lr</td> </tr> <tr> <td>Thorium</td><td>Protactinium</td><td>Uranium</td><td>Neptunium</td><td>Plutonium</td><td>Americium</td><td>Curium</td><td>Berkelium</td><td>Californium</td><td>Einsteinium</td><td>Fermium</td><td>Mendelevium</td><td>Nobelium</td><td>Lawrencium</td> </tr> <tr> <td>232.04</td><td>231.04</td><td>238.03</td><td>(237)</td><td>(244)</td><td>(243)</td><td>(247)</td><td>(247)</td><td>(251)</td><td>(252)</td><td>(257)</td><td>(258)</td><td>(259)</td><td>(262)</td> </tr> </table>																		58	59	60	61	62	63	64	65	66	67	68	69	70	71	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Cerium	Praseodymium	Neodymium	Promethium	Samarium	Europium	Gadolinium	Terbium	Dysprosium	Holmium	Erbium	Thulium	Ytterbium	Lutetium	140.12	140.91	144.24	(145)	150.36	151.96	157.25	158.93	162.50	164.93	167.26	168.93	173.04	174.97	90	91	92	93	94	95	96	97	98	99	100	101	102	103	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	Thorium	Protactinium	Uranium	Neptunium	Plutonium	Americium	Curium	Berkelium	Californium	Einsteinium	Fermium	Mendelevium	Nobelium	Lawrencium	232.04	231.04	238.03	(237)	(244)	(243)	(247)	(247)	(251)	(252)	(257)	(258)	(259)	(262)
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