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

Professor: Jaclyn Brusso

Date: March 20, 2014

Duration: 80 minutes

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

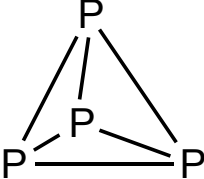
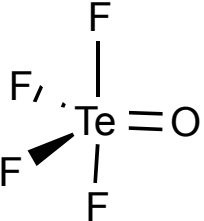
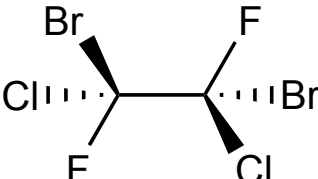
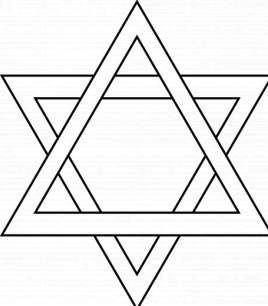
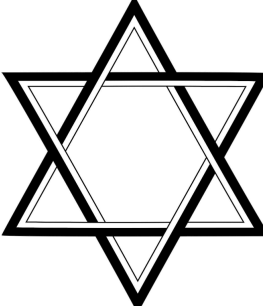

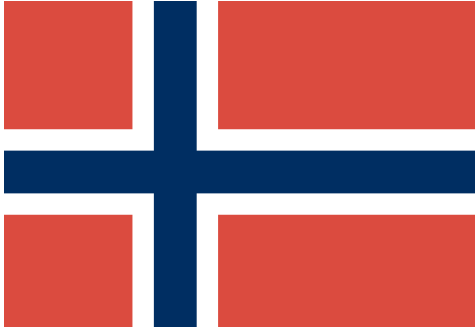
Student Number: \_\_\_\_\_

**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 6 questions. You are expected to answer all 6 questions.
- There are 8 pages. Please make sure you have all 8 pages. NOTE: the last two pages are DATA SHEETS. You may tear them off.
- At the end of the exam, turn in this test booklet and the data sheet.  
GOOD LUCK!

Question	Grade
1	/10
2	/3
3	/13
4	/16
5	/4
6	/6
<b>TOTAL</b>	<b>/18</b>

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

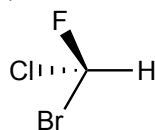
(a)		$T_d$	(f)	$PF_5$	$D_{3h}$
(b)		$C_{2v}$	(g)	$B(OH)_3$	$C_{3h}$
(c)	eclipsed $H_3C-CCl_3$	$C_{3v}$	(h)		$C_i$
(d)		$C_{3v}$	(i)		$D_6$
(e)		$C_{2h}$	(j)		$C_{2v}$

2. Determine whether the following molecules are chiral. Rationalize your response using symmetry/point group arguments. (3 marks)

(a)  $\text{NH}_3$

Answer: achiral

(b)



Answer: chiral

A molecule is chiral if it has *no symmetry operations* (other than E) or if it *only has a proper rotation axis*. Which point groups does this include?

3. Complete the character tables below. (13 marks; ¼ mark per blank)

(a)

$D_{3d}$	E	$2C_3$	$3C_2'$	$i$	$2S_6$	$3\sigma_d$
$A_{2g}$	1	1	-1	1	1	-1
$A_{1u}$	1	1	1	-1	-1	-1

(b)

$C_{2h}$	E	$C_2$	$i$	$\sigma_h$	
$A_g$	1	1	1	1	xy
$B_g$	1	-1	1	-1	xz
$A_u$	1	1	-1	-1	z
$B_u$	1	-1	-1	1	x,y

(c)

$D_4$	E	$2C_4$	$C_2$	$2C_2'$	$2C_2''$	
$A_2$	1	1	1	-1	-1	z
$A_1$	1	1	1	1	1	$z^2$
$B_1$	1	-1	1	1	-1	$x^2-y^2$
E	2	0	-2	0	0	(x,y)

4. (16 marks) Answer the following questions considering the molecule  $IF_5$ .
- What is the point group for this molecule? (1 mark)
  - Assign all symmetry operations associated with this point group. (4 marks)
  - Derive the irreducible representations for the following functions:  $z$ ,  $xy$ ,  $x^2-y^2$  and  $(x,y)$ . (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)

Answer:

- $C_{4v}$
- top row of character table;  $\frac{1}{2}$  mark for each symmetry element listed in the character table
- four 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).
- no because the number of irreducible representations (4) does not equal the number of classes (5).
- $h = 8$

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

5. Consider a hypothetical homonuclear diatomic, which has atomic and molecular orbital energies as shown in the table below.

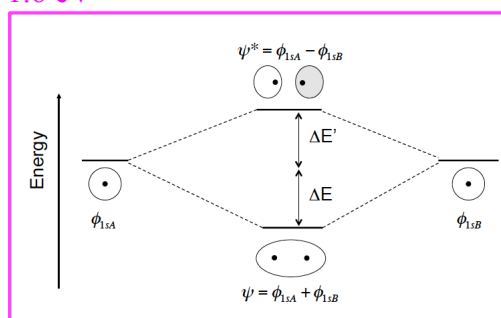
Orbital Energies	
<b>s-orbital</b>	-5.5 eV
<b><math>\sigma</math> MO</b>	-7.3 eV
<b><math>\sigma^*</math> MO</b>	-3.9 eV

- (a) Based on what you know about MO Theory, are the energy levels of the MO's reasonable? Explain. (2 mark)

Answer: No these are not reasonable energy levels for the atomic and molecular orbitals because  $\Delta E' < \Delta E$

$$\Delta E = -5.5 \text{ eV} - (-7.3 \text{ eV}) = 1.8 \text{ eV}$$

$$\Delta E' = -3.9 \text{ eV} - (-5.5 \text{ eV}) = 1.6 \text{ eV}$$

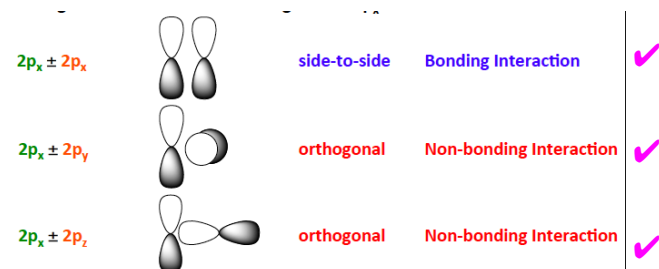


- (b) If the atoms making up the molecule have two electrons in their s-orbitals, would the resulting homonuclear diatomic be stable or unstable? Explain. (2 marks)

Answer: Because  $\Delta E > \Delta E'$  filling with four electrons would result in an overall stabilization of 0.2 eV; thus the molecule would be stable if the orbital energy levels were as outlined in the table.

6. Consider the possible interactions between p-orbitals in O<sub>2</sub>. Using diagrams, demonstrate which interactions lead to bonding and which do not. For the interactions that lead to bonding, what type of molecular orbitals do they result in? (6 marks)

Answer:



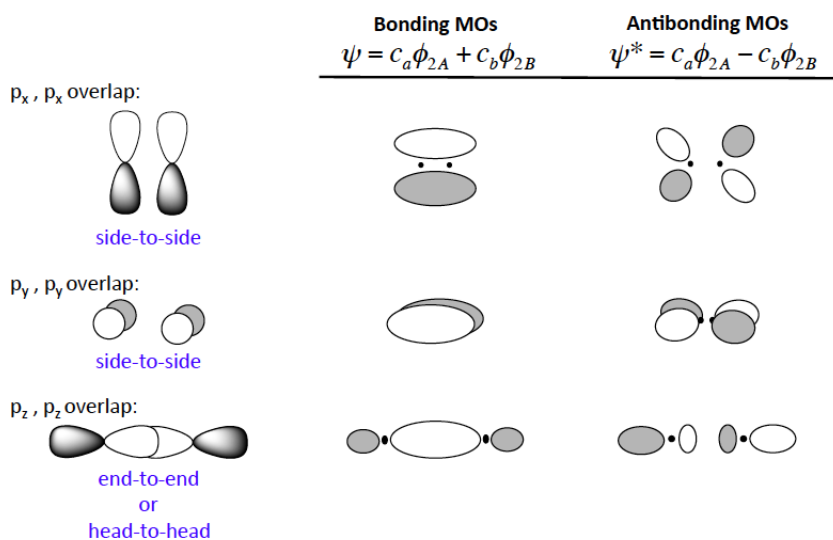
$2p_x \pm 2p_x$  is allowed  
 $2p_y \pm 2p_y$  is allowed  
 $2p_z \pm 2p_z$  is allowed

all other combinations lead to orthogonal overlap and therefore result in non bonding MO's ✓

1) End-to-end → forms  $\sigma$  bonds ✓



2) Side-to-side → forms  $\pi$  bonds ✓



# DATASHEET

Key																																			
11	Atomic number																																		
Na	Element symbol																																		
Sodium	Element name																																		
22.99	Average atomic mass*																																		
1	1A	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18																	
1	H	2															10	Ne																	
Hydrogen	1.01	Helium															4.00																		
3	Li	4															5	B	6	7	8	9	10												
Lithium	6.94	Beryllium															Boron	10.81	Carbon	12.01	Nitrogen	14.01	Oxygen	16.00	Fluorine	19.00	Neon	20.18							
11	Na	12	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18																	
Sodium	22.99	Magnesium	3B	4B	5B	6B	7B	8B	9B	10B	11B	12B	Al	Si	P	S	Cl	Ar																	
Aluminum	26.98	Silicon	28.09	Phosphorus	30.97	Sulfur	32.07	Chlorine	35.45	Argon	39.95																								
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36																		
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr																		
Potassium	39.10	Calcium	40.08	Scandium	44.96	Titanium	47.87	Vanadium	50.94	Chromium	52.00	Manganese	54.94	Iron	55.85	Cobalt	58.93	Nickel	58.69	Copper	63.55	Zinc	65.39	Gallium	69.72	Germanium	72.61	Arsenic	74.92	Selenium	78.96	Bromine	79.90	Krypton	83.80
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54																		
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe																		
Rubidium	85.47	Strontium	87.62	Yttrium	88.91	Zirconium	91.22	Niobium	92.91	Molybdenum	95.94	Technetium	(98)	Ruthenium	101.07	Rhodium	102.91	Palladium	106.42	Silver	107.87	Cadmium	112.41	Indium	114.82	Tin	118.71	Antimony	121.76	Tellurium	127.60	Iodine	126.90	Xenon	131.29
55	56	57	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86																		
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn																		
Cesium	132.91	Barium	137.33	Lanthanum	138.91	Hafnium	178.49	Tantalum	180.95	Tungsten	183.84	Rhenium	186.21	Osmium	190.23	Iridium	192.22	Platinum	195.08	Gold	196.97	Mercury	200.59	Thallium	204.38	Lead	207.2	Bismuth	208.98	Polonium	(209)	Astatine	(210)	Radon	(222)
87	88	89	104	105	106	107	108	109																											
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt																											
Francium	(223)	Radium	(226)	Actinium	(227)	Rutherfordium	(261)	Dubnium	(262)	Seaborgium	(266)	Bohrium	(264)	Hassium	(269)	Mitlerium	(268)																		
* If this number is in parentheses, then it refers to the atomic mass of the most stable isotope.																																			
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	140.12	Praseodymium	140.91	Neodymium	144.24	Promethium	(145)	Samarium	150.36	Europium	151.96	Gadolinium	157.25	Terbium	158.93	Dysprosium	162.50	Holmium	164.93	Erbium	167.26	Thulium	168.93	Ytterbium	173.04	Lutetium	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	232.04	Protactinium	231.04	Uranium	238.03	Neptunium	(237)	Plutonium	(244)	Americium	(243)	Curium	(247)	Berkelium	(247)	Californium	(251)	Einsteinium	(252)	Fermium	(257)	Mendelevium	(258)	Nobelium	(259)	Lawrencium	(262)								

