Name **Student Number**

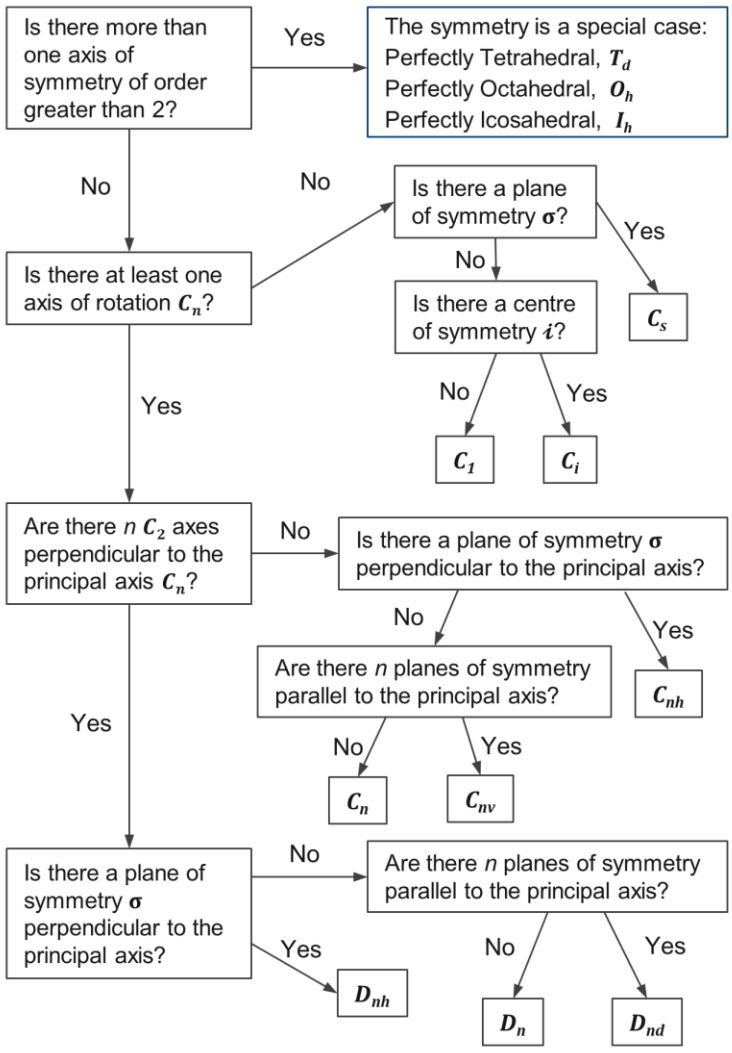
03-59-250 **Midterm 2** **08/11/18 (80 min)**

Note: Exams written in pencil will NOT be re-marked.

Fill out your name on each page. Make sure all pages are handed in at the end.

Hint: There are questions of varying difficulty. Read through the exam and answer the easy ones first!

The distribution of marks for the questions is approximate, and may change. You may use the back of any page for additional space or rough work.



1	
2	
3	
4	
5	
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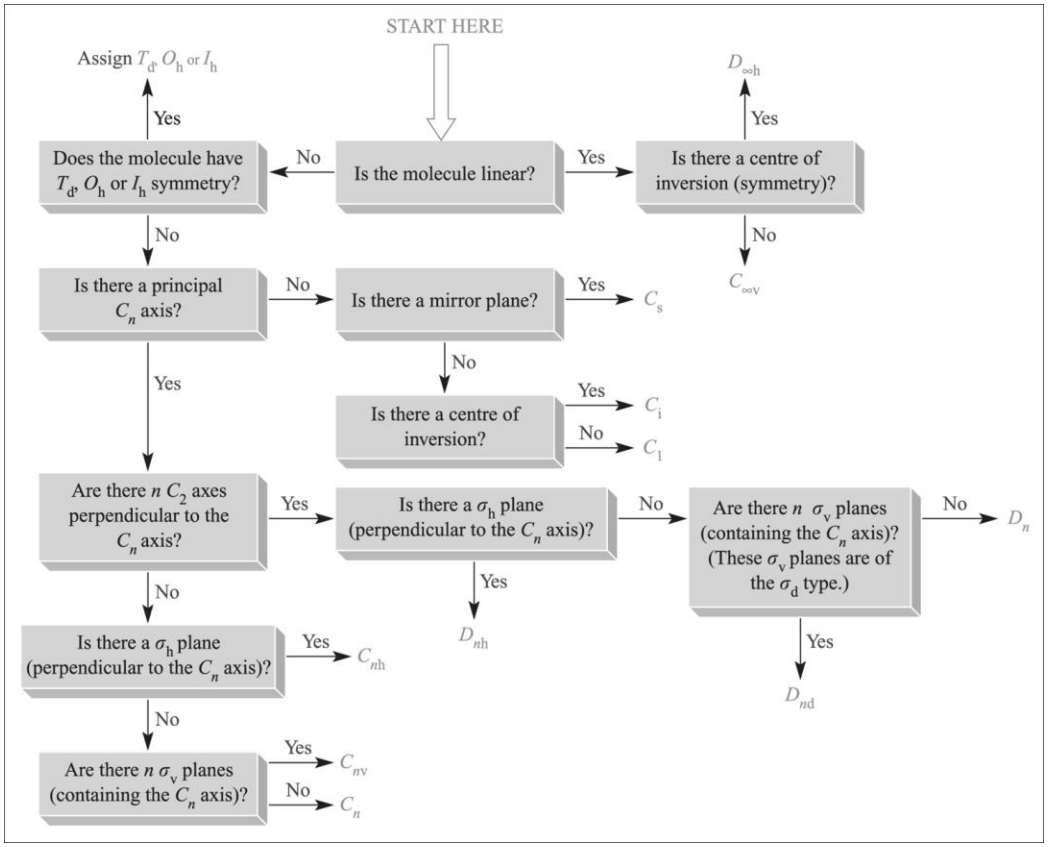
7	
Total	

Group 1	Group 2	Group 3	Group 4	Group 5	Group 6	Group 7	Group 8	Group 9	Group 10	Group 11	Group 12	Group 13	Group 14	Group 15	Group 16	Group 17	Group 18
1 H 1.0078																	2 He 4.0026
3 Li 6.938	4 Be 9.012											5 B 10.806	6 C 12.011	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.180
11 Na 22.990	12 Mg 24.305											13 Al 26.982	14 Si 28.085	15 P 30.974	16 S 32.059	17 Cl 35.45	18 Ar 39.948
19 K 39.098	20 Ca 40.078	21 Sc 44.956	22 Ti 47.867	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.845	27 Co 58.933	28 Ni 58.693	29 Cu 63.546	30 Zn 65.38	31 Ga 69.723	32 Ge 72.630	33 As 74.922	34 Se 78.971	35 Br 79.904	36 Kr 83.798
37 Rb 85.468	38 Sr 87.62	39 Y 88.906	40 Zr 91.224	41 Nb 92.906	42 Mo 95.95	43 *Tc* *(98)*	44 Ru 101.07	45 Rh 102.91	46 Pd 106.42	47 Ag 107.87	48 Cd 112.41	49 In 114.82	50 Sn 118.71	51 Sb 121.76	52 Te 127.60	53 I 126.90	54 Xe 1.008
55 Cs 132.91	56 Ba 137.33		72 Hf 178.49	73 Ta 180.95	74 W 183.84	75 Re 186.21	76 Os 190.23	77 Ir 192.22	78 Pt 195.08	79 Au 196.97	80 Hg 200.59	81 Tl 204.38	82 Pb 207.2	83 Bi 208.98	84 Po –	85 At –	86 Rn –
87 Fr –	88 Ra –		*104 Rf* –	*105 Db* –	*106 Sg* –	*107 Bh* –	*108 Hs* –	*109 Mt* –	*110 Ds* –	*111 Rg* –	*112 Cn* –	*113 Nh* –	*114 Fl* –	*115 Mc* –	*116 Lv* –	*117 Ts* –	*118 Og* –

57 La 138.91	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm 144.91	62 Sm 150.36	63 Eu 151.96	64 Gd 157.25	65 Tb 158.93	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.05	71 Lu 174.97
89 Ac –	90 Th 232.04	91 Pa 231.04	92 U 238.03	93 Np –	94 Pu –	*95 Am* –	*96 Cm* –	*97 Bk* –	*98 Cf* –	*99 Es* –	*100 Fm* –	*101 Md* –	*102 No* –	*103 Lr* –

Common VSEPR geometries					
# of objects	**2**	**3**	**4**	**5**	**6**
Base geometry	*linear*	*trigonal planar*	*tetrahedral*	*trigonal bipyramidal*	*octahedral*



Name: _____

1. Quick fire round! Circle or write the correct answer, as appropriate.
   [1 mark each]

   a) Core electrons are too low in energy to be used for bonding

   True **False**

   b) What does LCAO stand for?

   c) What does HOMO stand for?

   d) What does LUMO stand for?

   e) Hybridisation using d-orbitals is a good idea.

   True **False**

   f) x atomic orbitals produce $2x$ molecular orbitals

   True **False**

   g) If the integral of the product of an orbital with itself is equal to 1, then the orbital is referred to as:

   Normal **Orthogonal** **Orthonormal**

   h) What word do we use to describe orbital interactions where $S < 0$?

Name: _____

i) The bonding molecular orbitals of a heteronuclear molecule typically have larger coefficients (c) for the atomic orbital functions (ϕ) of the less electronegative element

True **False**

j) If the nuclear spin quantum number for a nucleus is $\boldsymbol{I}$ = ½, list all the possible nuclear spin values.

k) Which symmetry element do ALL molecules possess? Name and symbol, please.

l) Which symmetry element must a molecule possess in order to label its orbitals g or u?

m) The axis of highest-order rotation (also known as the principal rotation axis) is the….

$\boldsymbol{x}$**-axis** $\boldsymbol{y}$**-axis** $\boldsymbol{z}$**-axis**

Name: _____

2.

a) List three requirements when making molecular orbitals using the LCAO method.
[3 marks]

b) Sketch the following combinations of two d-orbitals (your choice as to which orbital, on two separate atoms!). Label which d-orbitals you choose.
[2 marks each]

i) A σ bonding combination

ii) A π bonding combination

iii) A δ bonding combination

iv) A combination with $\boldsymbol{S}$ = 0.

Name: _____

3. This question is about the homonuclear diatomic B_2.
   a) What are the ground state and first excited state electron configurations for boron? [1 mark]

   B: **B***:

   b) Draw two *different* Lewis structures for B_2. How many bonds are there connecting the boron atoms in each diagram? [1 mark each]
      i) Using the ground state configuration, without promoting to a valence state

      ii) Using the valence state configuration.

   c) Construct and label a molecular orbital diagram for B_2. Don't forget to label the HOMO and LUMO. [5 marks]

d) Based on your molecular orbital diagram, what is the bond order of B_2? [1 mark]

e) Would B_2 be attracted to an externally applied magnetic field (i.e. be paramagnetic)? Explain your answer. [2 marks]

f) Briefly explain why *sp* mixing is seen in B_2 but not in F_2. [2 marks]

Name: _____

4. HO^- and HF are two isoelectronic species.
   a) Briefly define the term *isoelectronic*. [1 mark]

   b) Draw and label a molecular orbital diagram for the hydroxide ion, HO^-. Don't forget to label the HOMO and LUMO. [4 marks]

   c) Based on your molecular orbital diagram for hydroxide, explain why HF is an acid. Think: how would the two diagrams compare? [2 marks]

d) The HOMOs of water (H_2O) and hydroxide are both non-bonding atomic p-orbitals on the oxygen atom. Why is hydroxide considered a base, but H_2O is considered neutral? [2 marks]

Name: _____

5. Nitric oxide (NO) is an important intercellular signalling molecule that is involved in blood pressure regulation and neurotransmission.
   a) Draw and label a molecular orbital diagram for NO. You may assume there is no sp mixing in NO. [4 marks]

   b) Which orbitals are used to make the π-symmetry orbitals? Sketch <u>one</u> of each of the π-bonding and π^* antibonding orbitals for NO, clearly showing whether there is a greater contribution from N or O in each. [2 marks each]

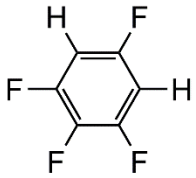
Name: _____

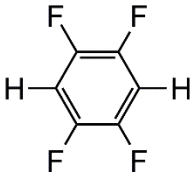
6.

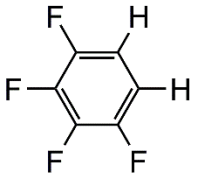
a) The interaction of matter with light results in the transition between two quantised molecular energy states. Indicate which regions of the electromagnetic spectrum are associated with which transitions. [2 marks]

Infrared	Electronic transitions
Microwave	Nuclear spin transitions
Radio frequency	Rotational transitions
Ultraviolet	Vibrational transitions

b) How many signals would you observe in the ^{13}C NMR spectra of each of these isomers of tetrafluorobenzene? [1 mark each]







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Name: _____

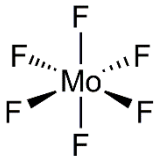
c) Predict the shape of the following 4 compounds and hence the number and relative intensity of peaks in the ^{19}F spectrum: [3 marks each]

i) SF_6	iii) SF_5^-
ii) SF_4	iv) SO_2F_2

Name: _____

7.

a) What is the point group of MoF_6? List all of the symmetry elements found in this molecule. (I only require the type of element, not the number of each one). [5 marks]



Point group?

Symmetry Elements?

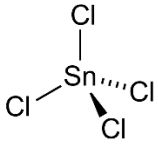
b) Assign the point group to each of the following species. [1 mark each]

N_2

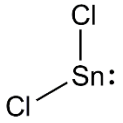
Point group:

CO

Point group:



Point group:



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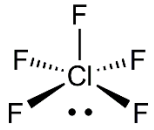
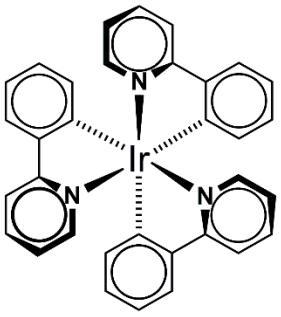


Point group:

BONUS! Can you assign the point group to these iridium complexes? [1 mark each]



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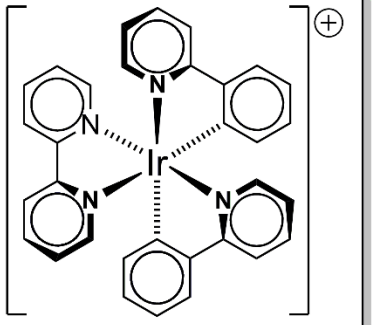

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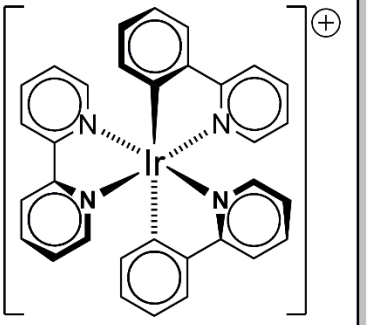

Point group:

End of exam