NAME:	Section: Student Number:
Spring 2017	Chemistry 2000 Practice Midterm #1C/ 50 marks
INSTRUCTIONS:	 Please read over the test carefully before beginning. You should have 6 pages of questions, a blank "overflow" page and a periodic table page. If your work is not legible, it will be given a mark of zero. Marks will be deducted for incorrect information added to an otherwise correct answer. Calculators are not permitted. You have 90 minutes to complete this test.

Confidentiality Agreement:

I agree not to discuss (or in any other way divulge) the contents of this exam until after 8:00 pm Mountain Time on <u>Thursday</u>, February 9th, 2017. I understand that breaking this agreement would constitute academic misconduct, a serious offense with serious consequences. The minimum punishment would be a mark of 0/50 on this exam and removal of the "overwrite midterm mark with final exam mark" option for my grade in this course; the maximum punishment would include expulsion from this university.

Signature: _____ Course: CHEM 2000 (General Chemistry II) Semester: Spring 2017 The University of Lethbridge Date: _____

Question Breakdown							
Q1	/ 18						
Q2	/ 8						
Q3	/ 3						
Q4	/ 3						
Q5	/ 18						

Total	/ 50
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NAN	ME: Section: Student Number:	
1.	Consider the NO^+ cation according to molecular orbital (MO) theory.	[18 marks]
(a)	Provide a molecular formula for one neutral diatomic molecule that is isoelectronic with	NO ⁺ . [1 mark]
(b)	Draw the Lewis structure for NO ⁺ . Include all non-zero formal charges.	[1 mark]
(c)	What N–O bond order does your Lewis diagram predict for <i>NO</i> ⁺ ?	[1 mark]

(d) The unlabeled valence MO energy level diagram for NO^+ is shown below. [7 marks]

- i. Label all atomic and molecular orbitals on this diagram.
- ii. Place the correct number of valence electrons into the atomic orbitals.
- iii. Place the correct number of valence electrons into the molecular orbitals.



- 1. continued...
- (e) Write the valence orbital occupancy (i.e. electron configuration) in line notation for NO^+ . [1 mark]
- (f) On the MO energy level diagram on the previous page, clearly label the highest occupied molecular orbital(s) of *NO*⁺ as the "HOMO"(s). [1 mark]
- (g) In the space below, draw a picture of the orbital(s) you labeled as HOMO. Clearly indicate relative phase as well as the location of each nucleus. [1 mark]

- (g) What bond order does your MO treatment predict for *NO*⁺? Does it agree with the bond order from your Lewis diagram? [2 marks]
- (h) What is the bond order if an electron is added to NO⁺? In other words, what is the bond order in NO? [1 mark]
- (i) What will happen to the potential energy curve of the N-O bond if you remove an electron from NO^+ ? Be specific. You may find it helpful to sketch the potential energy curve before and after the electron is removed. [2 marks]

2.

[8 marks]

Shown below is the valence MO energy level diagram for the *linear* HCO⁺ cation, also known as the acylium cation. Below that, pictures of the nine valence molecular orbitals are given, each labeled with a letter (A-I). All the pictures have HCO⁺ in the same orientation (H at the left; O at the right).

- (a) None of the MOs on this diagram have been labeled as bonding, nonbonding or antibonding. Mark the antibonding MOs with a * and mark the nonbonding MOs with the subscript 'nb'.
- (b) <u>In the box next to each energy level</u> on the MO diagram, use the letters provided to identify the picture(s) corresponding to each energy level. *There should be one letter per box.*





3.

[3 marks]

In band theory, compounds with a band gap smaller than or close to k_BT , (which is very small) can be considered metallic conductors. Briefly explain the band structure of metals and why metals are considered electric conductors. *You may find it helpful to include a diagram in your answer*.

4.

[3 marks]

Fentanyl (a synthetic opioid pain medication) was originally developed in 1960s, but more recently the combination of its extreme potency and use/distribution as a recreational drug has resulted in a significant increase in deaths by overdose to the general public. Consider the fentanyl molecule in accordance with valence bond theory:



Parts of the structure above are drawn using the "line-bond" method meaning that not all carbon atoms are explicitly represented by a C.

(a) What is the hybridization for each of the four labeled carbon atoms in this molecule? [2 marks]

Carbon #	Hybridization
C_1	
C_2	
C ₃	
C_4	

(b) How many π bonds are there in this molecule?

[1 mark]

5.

[18 marks]

- (a) Consider the **linear** neutral H_3 molecule. It has one central hydrogen atom and two terminal hydrogen atoms. [9 marks]
 - i. Draw a molecular orbital energy level diagram for H_3 .
 - ii. Label all atomic and molecular orbitals on your diagram, clearly indicating if each MO is bonding, nonbonding or antibonding.
 - iii. Populate the atomic orbitals with the correct number of electrons.
 - iv. Populate the molecular orbitals with the correct number of electrons.

- (b) Draw a picture of each molecular orbital next to your MO energy level diagram. Clearly indicate relative phase as well as the location of each nucleus. [3 marks]
- (c) Calculate the H–H bond order for the H_3 molecule.
- (d) What are the H–H bond orders for H_3^+ and for H_3^- ?

 H_3^+ bond order =

 H_3^- bond order =

[1 mark]

[2 marks]

- 5. continued...
- What are the magnetic properties of H_3 , H_3^+ , and H_3^- ? (paramagnetic or diamagnetic) [1 mark] (e)

*H*₃ is _____

- *H*⁺₃ is _____
- *H*₃⁻ is _____
- Sketch a UV-photoelectron spectrum for the H_3 molecule. Label the bands with the labels of the appropriate MOs. *You do not need to provide numerical values for the energies.* [2 marks] (f)

Overflow Page

If you use this page for any answers, please clearly indicate which question is being answered and make sure you note on the page for the question itself that the answer continues here.

1	Chem 1000 Standard Periodic Table												18				
1.0079																	4.0026
H																	He
1	2											13	14	15	16	17	2
6.941	9.0122	1										10.811	12.011	14.0067	15.9994	18.9984	20.1797
Li	Be											В	С	Ν	0	F	Ne
3	4											5	6	7	8	9	10
22.9898	24.3050											26.9815	28.0855	30.9738	32.066	35.4527	39.948
Na	Mg	_	-	_	_	_	_	_				Al	Si	Р	S	Cl	Ar
11	12	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
39.0983	40.078	44.9559	47.88	50.9415	51.9961	54.9380	55.847	58.9332	58.693	63.546	65.39	69.723	72.61	74.9216	78.96	79.904	83.80
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Со	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
85.4678	87.62	88.9059	91.224	92.9064	95.94	(98)	101.07	102.906	106.42	107.868	112.411	114.82	118.710	121.757	127.60	126.905	131.29
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Те	Ι	Xe
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54
132.905	137.327		178.49	180.948	183.85	186.207	190.2	192.22	195.08	196.967	200.59	204.383	207.19	208.980	(210)	(210)	(222)
Cs	Ba	La-Lu	Hf	Та	W	Re	Os	Ir	Pt	Au	Hg	TI	Pb	Bi	Po	At	Rn
55	56		72	73	74	75	76	77	78	79	80	81	82	83	84	85	86
(223)	226.025		(265)	(268)	(271)	(270)	(277)	(276)	(281)	(280)	(285)	(284)	(289)	(288)	(293)	(294)	(294)
Fr	Ra	Ac-Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og
87	88		104	105	106	107	108	109	110	111	112	113	114	115	116	117	118
		138.906	140.115	140.908	144.24	(145)	150.36	151.965	157.25	158.925	162.50	164.930	167.26	168.934	173.04	174.967	
		La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Но	Er	Tm	Yb	Lu	
		57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	
		227.028	232.038	231.036	238.029	237.048	(240)	(243)	(247)	(247)	(251)	(252)	(257)	(258)	(259)	(262)	
		Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	
		89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	

Developed by Prof. R. T. Boeré (updated 2016)