

Chemistry 2000 Fall 2017 Test 1

Version A

NAME: _____

Student number: _____

Time: 90 minutes

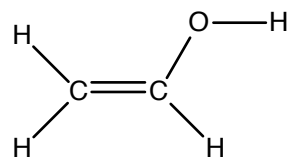
Aids permitted: none. A periodic table is provided on page 7.

Overflow space: There is extra space at the end of this paper. If you need extra space for a question, make sure to give me a clear indication of where I can find the rest of your answer, and label any answers continued in the overflow space with the question number.

Question	Mark
1	/9
2	/5
3	/10
4	/23
5	/5
Total:	/52
Percentage:	%

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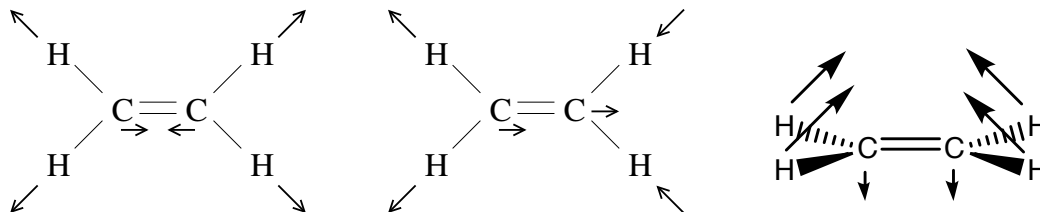
/9 1. The following is a line structure of ethenol:



- (a) Add the missing lone pairs directly to the line structure. [2 marks]
- (b) Indicate the valence-bond theory hybridization of the carbon and oxygen atoms. Write the hybridization near each atom on the line structure. [3 marks]
- (c) In valence-bond theory, how would we describe the π bond between the carbon atoms? What atomic orbitals are involved? [4 marks]

/5 2. (a) How many normal modes does ethene (C_2H_4) have? [2 marks]

- (b) Some of the normal modes of ethene are illustrated below, with arrows indicating the direction of motion of the nuclei during one half of the motion. During the other half, all the arrows are reversed. Circle the one(s) that you expect to be IR active. [3 marks]

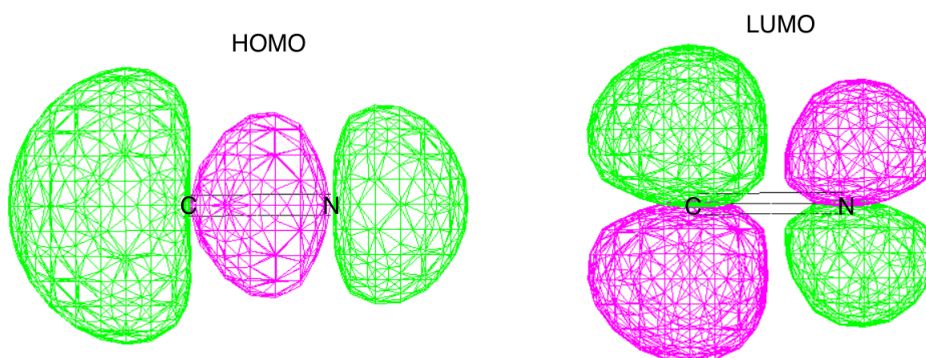


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3. (a) Which orbital, the HOMO or the LUMO, is associated with Lewis **base** reactivity? [1 mark]

(b) The HOMO and LUMO of the cyanide ion (CN^-) are shown below. Nothing is hidden from view in these illustrations. The LUMO is degenerate. In the simple Lewis acid-base reaction of cyanide with a proton, at what end would you predict the proton to attach, and why? Your answer must be based on MO theory. [3 marks]



(c) Classify the HOMO and LUMO as σ or π , and as bonding, nonbonding or antibonding. Write your answers under each illustration. [2 marks]

(d) What is the linear combination of atomic orbitals that would produce each of the orbitals illustrated above? Be specific, and use a sketch of the atomic orbitals in each case. [4 marks]

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4. As mentioned from time to time in class, it is possible to make and study exotic molecules in the gas phase. One such molecule is ArH^+ .

(a) Unlike other exotic molecules we have sometimes discussed, ArH^+ has a Lewis diagram. Draw this diagram, showing where the formal charge is located. [3 marks]

(b) Using the table of orbital energies below, develop the molecular orbital diagram of ArH^+ , and populate your diagram with electrons. Your diagram must be fully labeled with orbital labels and reasonable assignments to bonding, nonbonding (nb), and antibonding (*) categories. What is the predicted bond order? [10 marks]

Hint and note: If you apply the rules we learned in class strictly, you get a relatively simple (and correct) MO diagram.

Atom	Orbital	ϵ/Ry
H	1s	-1.00
Ar	3s	-2.15
	3p	-1.16

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- (c) Discuss the correspondence between the MO diagram and the Lewis diagram. In what ways do they agree and/or disagree? [4 marks]
- (d) Sketch the molecular orbital that is responsible for bonding in ArH^+ . (There is just one.) [2 marks]
- (e) What does MO theory predict about the neutral molecule ArH ? Would this be a stable molecule or not? How does this compare to what you would have predicted based on what you learned in Chem 1000? [4 marks]

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- /5 5. Using band theory, explain why lithium is a conductive metal. A complete answer will consider the number of states available as well as the number of electrons in those states. [5 marks]

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1																		18					
1 H											2								2 He				
1.01											2								4.00				
3 Li	2												13		14		15		16		17		18
6.94	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne						
22.99	9.01											10.81	12.01	14.01	16.00	19.00	20.18						
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar						
22.99	24.31											26.98	28.09	30.97	32.07	35.45	39.95						
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr						
39.10	40.08	44.96	47.88	50.94	52.00	54.94	55.85	58.93	58.69	63.55	65.41	69.72	72.61	74.92	78.96	79.90	83.80						
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe						
85.47	87.62	88.91	91.22	92.91	95.94		101.07	102.91	106.42	107.87	112.41	114.82	118.71	121.76	127.60	126.90	131.29						
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn						
132.91	137.33	138.91	178.49	180.95	183.85	186.21	190.2	192.22	195.08	196.97	200.59	204.38	207.2	208.98									
87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg													

58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
140.12	140.91	144.24		150.36	151.97	157.25	158.93	162.50	164.93	167.26	168.93	173.04	174.97
90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr
232.04	231.04	238.03											