

Chemistry 2000 Fall 2017 Test 1

Version B

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 bottom of page 3 and 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.

Confidentiality agreement: I agree not to discuss (or in any other way divulge) the contents of this exam until **after 8:30 p.m.** Mountain Time on **Tuesday, October 17**. I understand that breaking this agreement would constitute academic misconduct, a serious offense with serious consequences. The minimum punishment would be a mark of zero 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.

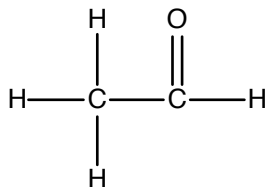
Signature: _____

Date: _____

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

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



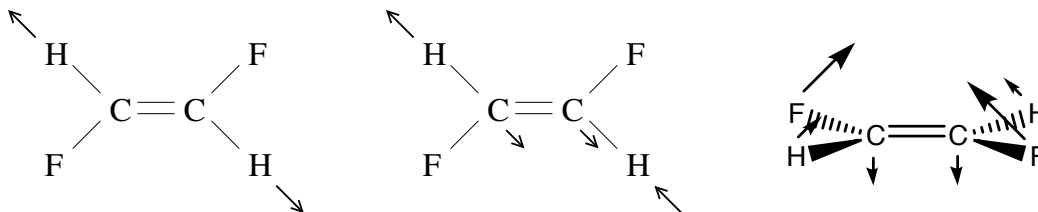
- (a) Add the missing lone pairs directly to the line structure. [2 marks]
- (b) Indicate the valence-bond theory hybridization of the carbon atoms. Write the hybridization near each atom on the line structure. [2 marks]
- (c) In valence-bond theory, which oxygen orbital would be used to make the σ bond between the oxygen and carbon? [1 mark]
- (d) In valence-bond theory, how would we describe the π bond between one carbon atom and the oxygen? What atomic orbitals are involved? [4 marks]

/5 2. Using band theory, explain why potassium 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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/5 3. (a) How many normal modes does trans-1,2-difluoroethene ($C_2F_2H_2$) have? [2 marks]

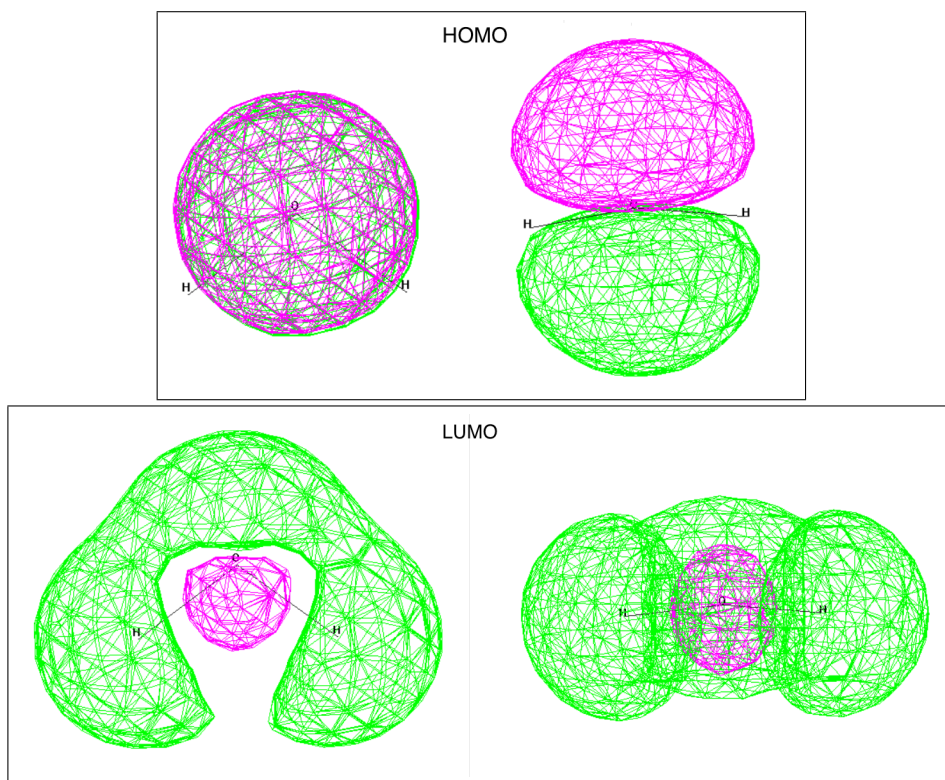
(b) Some of the normal modes of trans-1,2-difluoroethene are illustrated below, with arrows indicating the direction of motion of the nuclei during one half of the motion. During the other half, all the arrows are reversed. Circle the one(s) that you expect to be IR active. [3 marks]



/10 4. (a) Which orbital, the HOMO or the LUMO, is associated with Lewis **base** reactivity? [1 mark]

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- (b) Water often reacts as a Lewis base. The HOMO and LUMO of water are shown below. In both cases, the top (left) and side (right) view of each orbital are provided. In a Lewis acid-base reaction of water with a metal ion, where would the metal ion bind 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 inside the boxes containing the illustrations. [2 marks]

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- (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. Note: one of the sketches may be very simple. [4 marks]

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5. 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]

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- (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]

1																		18				
1 H											2								2 He			
1.01											2								4.00			
3 Li	4 Be											13		14		15		16		17		10 Ne
6.94	9.01											5 B	6 C	7 N	8 O	9 F	10 Ne					
11 Na	12 Mg											10.81	12.01	14.01	16.00	19.00	20.18					
22.99	24.31											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar					
		3	4	5	6	7	8	9	10	11	12	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											