Chemistry 2000 Fall 2013 Test 1
Version A

NAME: ________________________________ Student number: ______________

Time: 90 minutes

Aids permitted: none

Overflow space: If you run out of space to answer a question, there is extra space on pages 8 and 9. Make sure to clearly mark any answers written there with the question number.

Confidentiality agreement: I agree not to discuss (or in any other way divulge) the contents of this exam until **after 5:00 p.m.** Mountain Time on **Wednesday, October 23**. 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.

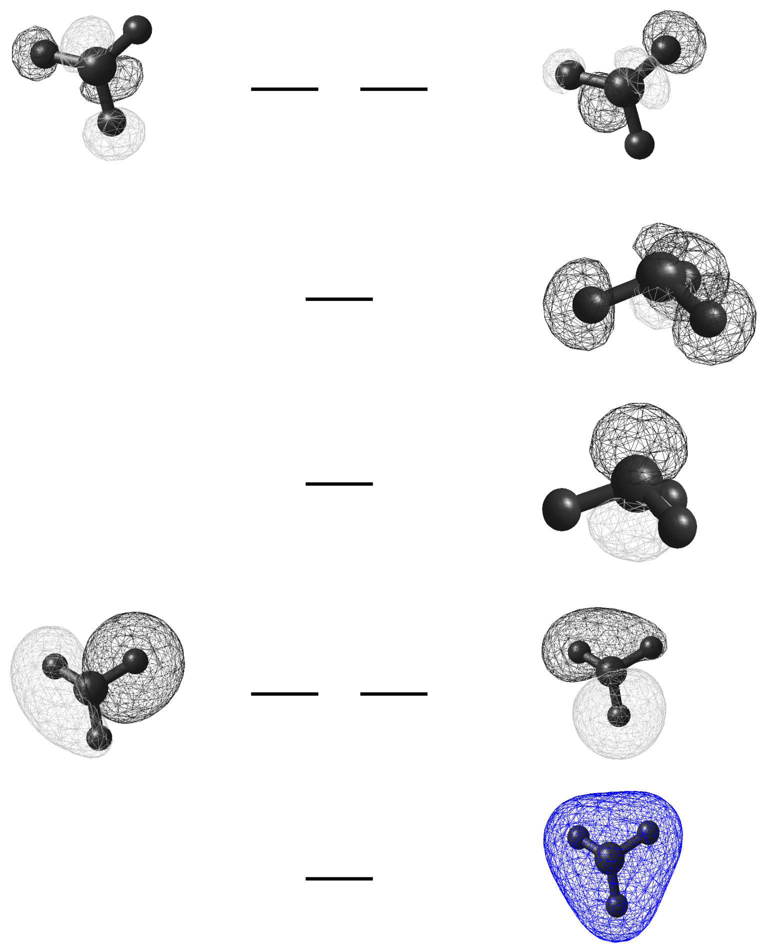
Signature: ________________________________ Date: __________________

Question	Mark
1	/15
2	/8
3	/13
4	/16
Total:	/52
Percentage:	%

NAME:____

/15

1. The valence MO diagram of ammonia is given below, along with drawings of the corresponding orbitals:



The MO diagram is not drawn to scale. The orbitals are either shown looking down onto the molecule (with the nitrogen atom at the top) or from a side view.

(a) Place the valence electrons in the orbitals. [2 marks]

(b) Identify the nonbonding orbital(s) by placing the annotation "nb" next to the appropriate picture(s). [1 mark]

(c) Use an MO argument to determine the N-H bond order. [2 marks]

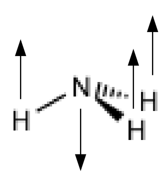
NAME:______________________________

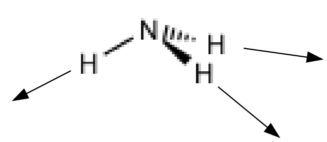
(d) Ammonia is a Lewis base. Which orbital is relevant to this chemical property of ammonia? Does the shape of the orbital agree with the idea that ammonia is a Lewis base? Explain briefly. [4 marks]

(e) Does ammonia have π orbitals? If it does, explain what atomic orbitals would be combined in MO theory to form them. If not, explain why not. [2 marks]

(f) In valence-bond theory, how would we describe the N-H bond in ammonia? [2 marks]

(g) The drawings below illustrate two of the vibrational modes of ammonia. The one on the left is a so-called "umbrella inversion" mode because, if this motion is sufficiently vigorous, the nitrogen can go right through the plane defined by the three hydrogen atoms, much like an umbrella that is inverted in a strong wind. The illustration on the right is a symmetric stretch, in which all the hydrogen atoms move in and out in unison along their respective bonds. State whether each of these modes is or is not IR active. [2 marks]





NAME:______________________________________

/8

2. Explain how a light-emitting diode (LED) works. A diagram may be helpful. What property of the materials used to build the device controls the color of the LED?

/13

3. The superoxide ion, O_2^-, is formed as a byproduct of respiration in living organisms. Superoxides are also formed when some of the alkali metals are burned.

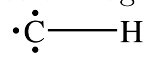
   (a) Draw a Lewis diagram of the superoxide ion. What bond order does your Lewis diagram predict? [4 marks]

NAME:______________________________________

(b) Draw the valence MO diagram for superoxide, label the atomic and molecular orbitals and include tie lines to show the linear combinations that form each MO. Place the valence electrons in your MO diagram. [6 marks]

(c) What bond order does your MO treatment predict? Does it agree with the bond order from the Lewis diagram? [3 marks]

NAME:______________________________

/16 4. Combustion generates many exotic molecular fragments. For example, hydrocarbon combustion generates carbyne radicals:  . The atomic orbital energies of carbon and hydrogen (in Rydbergs) are as follows:

	1s	2s	2p
H	−1.00		
C	−21.6	−1.43	−0.79

(a) By what experimental technique could these atomic orbital energies have been obtained? Explain **briefly** how this experiment is used to determine orbital energies. [5 marks]

(b) How many valence σ and π molecular orbitals can you make from the valence atomic orbitals? [2 marks]

Number of σ orbitals: __________

Number of π orbitals: __________

(c) Sketch a plausible valence MO diagram for the carbyne radical, and place the valence electrons in this diagram. [5 marks]

NAME:____

(d) How many unpaired electrons are there in your MO diagram? How many electrons are in nonbonding orbitals? How do these features compare to the Lewis diagram? [4 marks]

Number of unpaired electrons: __________

Number of electrons in nonbonding orbitals: __________

NAME:____

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 H 1.01																	2 He 4.00
3 Li 6.94	4 Be 9.01											5 B 10.81	6 C 12.01	7 N 14.01	8 O 16.00	9 F 19.00	10 Ne 20.18
11 Na 22.99	12 Mg 24.31											13 Al 26.98	14 Si 28.09	15 P 30.97	16 S 32.07	17 Cl 35.45	18 Ar 39.95
19 K 39.10	20 Ca 40.08	21 Sc 44.96	22 Ti 47.88	23 V 50.94	24 Cr 52.00	25 Mn 54.94	26 Fe 55.85	27 Co 58.93	28 Ni 58.69	29 Cu 63.55	30 Zn 65.41	31 Ga 69.72	32 Ge 72.61	33 As 74.92	34 Se 78.96	35 Br 79.90	36 Kr 83.80
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc	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 131.29
55 Cs 132.91	56 Ba 137.33	57 La 138.91	72 Hf 178.49	73 Ta 180.95	74 W 183.85	75 Re 186.21	76 Os 190.2	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	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg							

58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm	62 Sm 150.36	63 Eu 151.97	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 173.04	71 Lu 174.97
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