Chemistry 1B, Final Exam
May 17, 1999
Professor R.J. Saykally

Name ______________________

TA ______________________

Part A: Carbon Chemistry and Biological Design

I. (25) ____________

II. (25) ____________

III. (25) ____________

IV. (25) ____________

TOTAL (100) ____________

Part B: Cumulative Problems

I. (50) ____________

II. (50) ____________

III. (50) ____________

IV. (50) ____________

TOTAL (200) ____________

TOTAL EXAM SCORE (300) ____________

Rules:
- Work all problems to 3 significant figures
- No lecture notes or books permitted
- No word processing calculators
- Time: 90 minutes
- Show all work to get partial credit
- Periodic Table, Tables of Physical Constants, Conversion Factors, Amino Acids, Genetic Code, Thermodynamic Functions

Inches 1 2 3 4 5 6

Periodic Table of the Elements

Atomic number — Atomic mass

27 58.93 **Co** Cobalt

symbol: Black naturally occurring; White synthetically prepared

name

most stable isotope

Metals

Metalloids

Nonmetals

Noble gases

1 1.01 H Hydrogen																	2 4.003 He Helium
3 6.94 Li Lithium	4 9.01 Be Beryllium											5 10.81 B Boron	6 12.01 C Carbon	7 14.01 N Nitrogen	8 15.999 O Oxygen	9 18.998 F Fluorine	10 20.18 Ne Neon
11 22.99 Na Sodium	12 24.31 Mg Magnesium											13 26.98 Al Aluminum	14 28.09 Si Silicon	15 30.97 P Phosphorus	16 32.06 S Sulfur	17 35.45 Cl Chlorine	18 39.95 Ar Argon
19 39.10 K Potassium	20 40.08 Ca Calcium	21 44.96 Sc Scandium	22 47.90 Ti Titanium	23 50.94 V Vanadium	24 51.996 Cr Chromium	25 54.94 Mn Manganese	26 55.85 Fe Iron	27 58.93 Co Cobalt	28 58.70 Ni Nickel	29 63.55 Cu Copper	30 65.37 Zn Zinc	31 69.72 Ga Gallium	32 72.59 Ge Germanium	33 74.92 As Arsenic	34 78.96 Se Selenium	35 79.90 Br Bromine	36 83.80 Kr Krypton
37 85.47 Rb Rubidium	38 87.62 Sr Strontium	39 88.91 Y Yttrium	40 91.22 Zr Zirconium	41 92.91 Nb Niobium	42 95.94 Mo Molybdenum	43 (98) Tc Technetium	44 101.07 Ru Ruthenium	45 102.91 Rh Rhodium	46 106.40 Pd Palladium	47 107.87 Ag Silver	48 112.41 Cd Cadmium	49 114.82 In Indium	50 118.69 Sn Tin	51 121.75 Sb Antimony	52 127.60 Te Tellurium	53 126.90 I Iodine	54 131.30 Xe Xenon
55 132.91 Cs Cesium	56 137.33 Ba Barium	57 138.91 La Lanthanum	72 178.49 Hf Hafnium	73 180.95 Ta Tantalum	74 183.85 W Tungsten	75 186.21 Re Rhenium	76 190.20 Os Osmium	77 192.22 Ir Iridium	78 195.09 Pt Platinum	79 196.97 Au Gold	80 200.59 Hg Mercury	81 204.37 Tl Thallium	82 207.19 Pb Lead	83 208.98 Bi Bismuth	84 (209) Po Polonium	85 (210) At Astatine	86 (222) Rn Radon
87 (223) Fr Francium	88 226.03 Ra Radium	89 227.03 Ac Actinium	104 (261) Rf Rutherfordium	105 (262) Ha Hahnium	106 (266) Sg Seaborgium	107 (262) Ns Nielsbohrium	108 (265) Hs Hassium	109 (266) Mt Meitnerium	110 (271)	111 (272)	112 (277)	(113)	(114)	(115)	(116)	(117)	(118)

Lanthanide series	58 140.12 Ce Cerium	59 140.91 Pr Praseodymium	60 144.24 Nd Neodymium	61 (145) Pm Promethium	62 150.40 Sm Samarium	63 151.96 Eu Europium	64 157.25 Gd Gadolinium	65 158.93 Tb Terbium	66 162.50 Dy Dysprosium	67 164.93 Ho Holmium	68 167.26 Er Erbium	69 168.93 Tm Thulium	70 173.04 Yb Ytterbium	71 174.97 Lu Lutetium
Actinide series	90 232.04 Th Thorium	91 231.04 Pa Protactinium	92 238.03 U Uranium	93 237.05 Np Neptunium	94 (244) Pu Plutonium	95 (243) Am Americium	96 (247) Cm Curium	97 (247) Bk Berkelium	98 (251) Cf Californium	99 (252) Es Einsteinium	100 (257) Fm Fermium	101 (260) Md Mendelevium	102 (259) No Nobelium	103 (262) Lr Lawrencium

Note: Atomic masses shown here are the 1983 IUPAC values (maximum of six significant figures).

Physical Constants

Standard acceleration of terrestrial gravity	$g = 9.80665\ \mathrm{m\ s^{-2}}$ (exactly)
Avogadro's number	$N_0 = 6.022137 \times 10^{23}$
Bohr radius	$a_0 = 0.52917725\ \text{Å} = 5.2917725 \times 10^{-11}\ \mathrm{m}$
Boltzmann's constant	$k_B = 1.38066 \times 10^{-23}\ \mathrm{J\ K^{-1}}$
Electron charge	$e = 1.6021773 \times 10^{-19}\ \mathrm{C}$
Faraday constant	$\mathcal{F} = 96{,}485.31\ \mathrm{C\ mol^{-1}}$
Masses of fundamental particles:	
Electron	$m_e = 9.109390 \times 10^{-31}\ \mathrm{kg}$
Proton	$m_p = 1.672623 \times 10^{-27}\ \mathrm{kg}$
Neutron	$m_n = 1.674929 \times 10^{-27}\ \mathrm{kg}$
Ratio of proton mass to electron mass	$m_p/m_e = 1836.15270$
Permittivity of vacuum	$\epsilon_0 = 8.8541878 \times 10^{-12}\ \mathrm{C^2\ J^{-1}\ m^{-1}}$
Planck's constant	$h = 6.626076 \times 10^{-34}\ \mathrm{J\ s}$
Speed of light in a vacuum	$c = 2.99792458 \times 10^{8}\ \mathrm{m\ s^{-1}}$ (exactly)
Universal gas constant	$R = 8.31451\ \mathrm{J\ mol^{-1}\ K^{-1}}$
	$= 0.0820578\ \mathrm{L\ atm\ mol^{-1}\ K^{-1}}$

Values are taken from "Quantities, Units and Symbols in Physical Chemistry," International Union of Pure and Applied Chemistry, Blackwell Scientific Publications, 1988.

Conversion Factors

Standard atmosphere	1 atm = 1.01325×10^5 Pa = $1.01325 \times 10^5\ \mathrm{kg\ m^{-1}\ s^{-2}}$ (exactly)
Atomic mass unit	1 u = 1.660540×10^{-27} kg
	1 u = 1.492419×10^{-10} J = 931.4943 MeV (energy equivalent from $E = mc^2$)
Calorie	1 cal = 4.184 J (exactly)
Electron volt	1 eV = $1.6021773 \times 10^{-19}$ J = 96.48531 kJ $\mathrm{mol^{-1}}$
Foot	1 ft = 12 in = 0.3048 m (exactly)
Gallon (U.S.)	1 gallon = 4 quarts = 3.78541 L (exactly)
Liter-atmosphere	1 L atm = 101.325 J (exactly)
Metric ton	1 metric ton = 1000 kg (exactly)
Pound	1 lb = 16 oz = 0.45359237 kg (exactly)

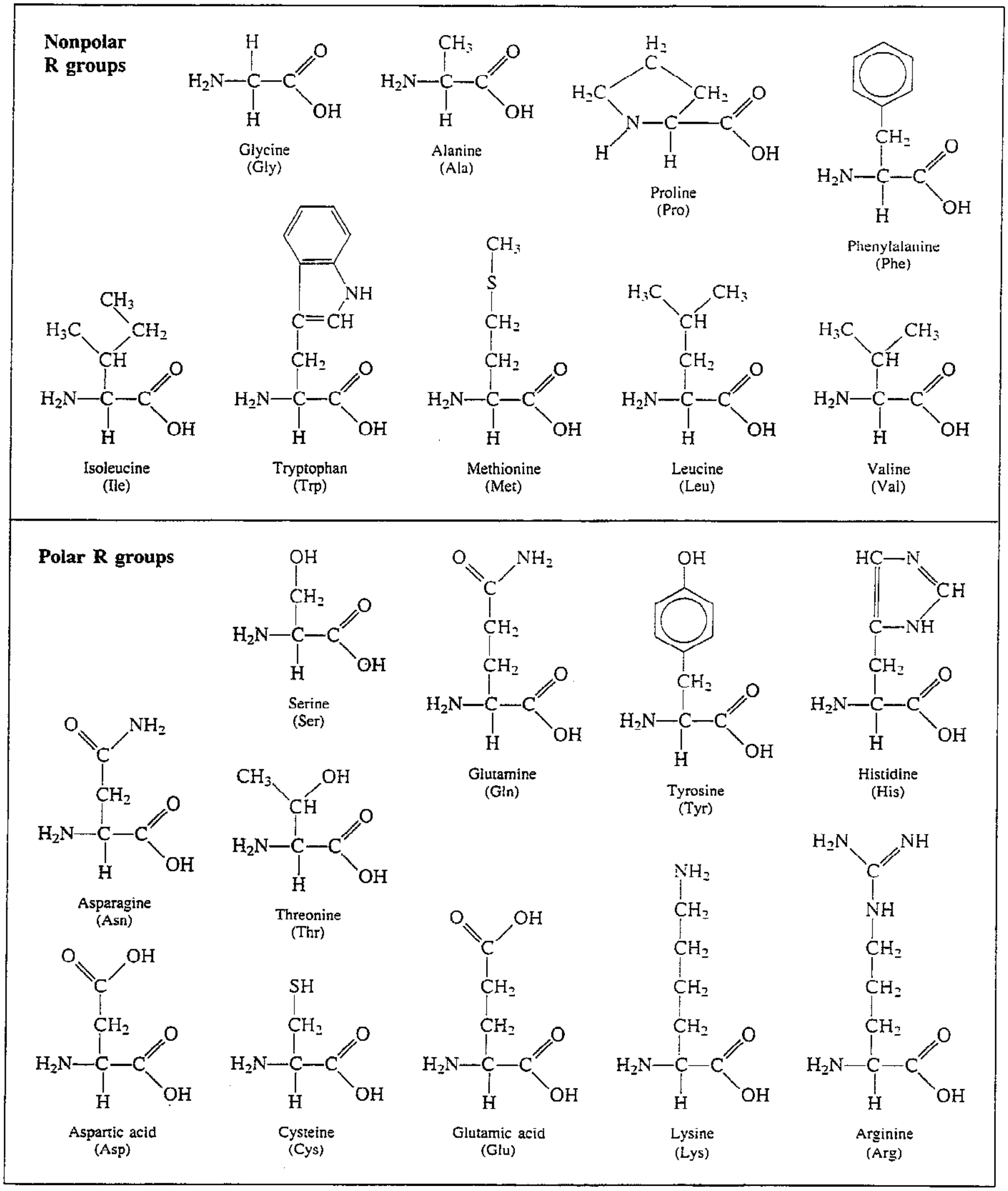

Nonpolar R groups
Glycine (Gly)
Alanine (Ala)
Proline (Pro)
Phenylalanine (Phe)
Isoleucine (Ile)
Tryptophan (Trp)
Methionine (Met)
Leucine (Leu)
Valine (Val)
Polar R groups
Serine (Ser)
Glutamine (Gln)
Tyrosine (Tyr)
Histidine (His)
Asparagine (Asn)
Threonine (Thr)
Aspartic acid (Asp)
Cysteine (Cys)
Glutamic acid (Glu)
Lysine (Lys)
Arginine (Arg)

Table 25-4
The genetic code

First position (5′ end)	*Second position*				*Third position (3′ end)*
	U	C	A	G	
U	Phe	Ser	Tyr	Cys	U
	Phe	Ser	Tyr	Cys	C
	Leu	Ser	Stop	Stop	A
	Leu	Ser	Stop	Trp	G
C	Leu	Pro	His	Arg	U
	Leu	Pro	His	Arg	C
	Leu	Pro	Gln	Arg	A
	Leu	Pro	Gln	Arg	G
A	Ile	Thr	Asn	Ser	U
	Ile	Thr	Asn	Ser	C
	Ile	Thr	Lys	Arg	A
	Met	Thr	Lys	Arg	G
G	Val	Ala	Asp	Gly	U
	Val	Ala	Asp	Gly	C
	Val	Ala	Glu	Gly	A
	Val	Ala	Glu	Gly	G

APPENDIX D

Standard Chemical Thermodynamic Properties

	Substance	ΔH_f° (25°C) kJ mol^{-1}	S° (25°C) J K^{-1} mol^{-1}	ΔG_f° (25°C) kJ mol^{-1}	c_P (25°C) J K^{-1} mol^{-1}
	$H(g)$	217.96	114.60	203.26	20.78
	$H_2(g)$	0	130.57	0	28.82
	$H^+(aq)$	0	0	0	0
	$H_3O^+(aq)$	−285.83	69.91	−237.18	75.29
IV	$C(s$, graphite$)$	0	5.74	0	8.53
	$C(s$, diamond$)$	1.895	2.377	2.900	6.11
	$C(g)$	716.682	157.99	671.29	20.84
	$CH_4(g)$	−74.81	186.15	−50.75	35.31
	$C_2H_2(g)$	226.73	200.83	209.20	43.93
	$C_2H_4(g)$	52.26	219.45	68.12	43.56
	$C_2H_6(g)$	−84.68	229.49	−32.89	52.63
	$C_3H_8(g)$	−103.85	269.91	−23.49	73.0
	n-$C_4H_{10}(g)$	−124.73	310.03	−15.71	97.5
	$C_4H_{10}(g$, isobutane$)$	−131.60	294.64	−17.97	96.8
	n-$C_5H_{12}(g)$	−146.44	348.40	−8.20	120
	$C_6H_6(g)$	82.93	269.2	129.66	81.6
	$C_6H_6(\ell)$	49.03	172.8	124.50	136
	$CO(g)$	−110.52	197.56	−137.15	29.14
	$CO_2(g)$	−393.51	213.63	−394.36	37.11
	$CO_2(aq)$	−413.80	117.6	−385.98	—
	$CS_2(\ell)$	89.70	151.34	65.27	75.7
	$CS_2(g)$	117.36	237.73	67.15	45.40
	$H_2CO_3(aq)$	−699.65	187.4	−623.08	—
	$HCO_3^-(aq)$	−691.99	91.2	−586.77	—
	$CO_3^{2-}(aq)$	−677.14	−56.9	−527.81	—
	$HCOOH(\ell)$	−424.72	128.95	−361.42	99.04
	$HCOOH(aq)$	−425.43	163	−372.3	—
	$COOH^-(aq)$	−425.55	92	−351.0	−87.9
	$CH_2O(g)$	−108.57	218.66	−102.55	35.40
	$CH_3OH(\ell)$	−238.66	126.8	−166.35	81.6
	$CH_3OH(g)$	−200.66	239.70	−162.01	43.89
	$CH_3OH(aq)$	−245.93	133.1	−175.31	—
	$H_2C_2O_4(s)$	−827.2	—	—	117
	$HC_2O_4^-(aq)$	−818.4	149.4	−698.34	—
	$C_2O_4^{2-}(aq)$	−825.1	45.6	−673.9	—
	$CH_3COOH(\ell)$	−484.5	159.8	−390.0	124.3
	$CH_3COOH(g)$	−432.25	282.4	−374.1	66.5
	$CH_3COOH(aq)$	−485.76	178.7	−396.46	—
	$CH_3COO^-(aq)$	−486.01	86.6	−369.31	−6.3

continued

	Substance	ΔH_f° (25°C) kJ mol^{-1}	S° (25°C) J K^{-1} mol^{-1}	ΔG_f° (25°C) kJ mol^{-1}	C_P (25°C) J K^{-1} mol^{-1}
VI	$O_2(g)$	0	205.03	0	29.36
	$O(g)$	249.17	160.95	231.76	21.91
	$O_3(g)$	142.7	238.82	163.2	39.20
	$OH^-(aq)$	−229.99	−10.75	−157.24	−148.5
	$H_2O(\ell)$	−285.83	69.91	−237.18	75.29
	$H_2O(g)$	−241.82	188.72	−228.59	35.58
	$H_2O_2(\ell)$	−187.78	109.6	−120.42	89.1
	$H_2O_2(aq)$	−191.17	143.9	−134.03	—
	$S(s$, rhombic)	0	31.80	0	22.64
	$S(s$, monoclinic)	0.30	32.6	0.096	—
	$S(g)$	278.80	167.71	238.28	23.67
	$S_8(g)$	102.30	430.87	49.66	156.44
	$H_2S(g)$	−20.63	205.68	−33.56	34.23
	$H_2S(aq)$	−39.7	121	−27.83	—
	$HS^-(aq)$	−17.6	62.8	12.08	—
	$SO(g)$	6.26	221.84	−19.87	30.17
	$SO_2(g)$	−296.83	248.11	−300.19	39.87
	$SO_3(g)$	−395.72	256.65	−371.08	50.67
	$H_2SO_3(aq)$	−608.81	232.2	−537.81	—
	$HSO_3^-(aq)$	−626.22	139.7	−527.73	—
	$SO_3^{2-}(aq)$	−635.5	−29	−486.5	—
	$I_2(s)$	0	116.14	0	54.44
	$I_2(g)$	62.44	260.58	19.36	36.90
	$I_2(aq)$	22.6	137.2	16.40	—
	$I(g)$	106.84	180.68	70.28	20.79
	$I^-(aq)$	−55.19	111.3	−51.57	−142.3
	$I_3^-(aq)$	−51.5	239.3	−51.4	—
	$HI(g)$	26.48	206.48	1.72	29.16
	$ICl(g)$	17.78	247.44	−5.44	35.56
	$IBr(g)$	40.84	258.66	3.71	36.44

Part A: Carbon Chemistry and Biological Design

I. (5 points each)

1. List four proposed allotropic forms of carbon, their hybridization and their geometries.

______	______	______
______	______	______
______	______	______
______	______	______

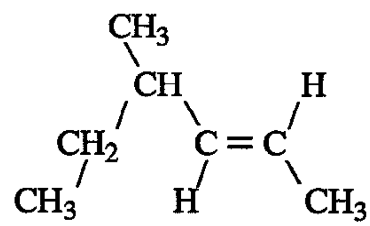
2. Draw the structure of C_5 confirmed in the Saykally labs, explicitly showing the approximate bond lengths and angles and the hybridization.

3. Should cyclic C_6 or C_{10} be more stable? Explain.

4. (3+2 points)
A. Describe (in words) the crystal structure of diamond.

B. Why is diamond a better heat conductor than graphite?

5. (5 points) Name the molecule



II. (5 points each) Consider the Fullerene C_{72}:

A. The number of pentagons is ______________________.

B. The number of hexagons is ______________________.

C. The number of dangling bonds is ______________________.

D. The hybridization of each carbon is ______________________.

E. Compare the stability of C_{72} with that of C_{70}.

III. (5 points each)

1. The 3 components of DNA are (be specific):

   ______________ ______________ ______________

2. Specify 3 ways in which DNA differs from RNA:

   ____

   ____

   ____

3. What role does NAD^+ play in biology?

4. The purine base ______________________ interacts with the pyrimidine base

   ______________________ to form a Watson-Crick pair with 3 hydrogen bonds.

5. In RNA, the ______________ position of a pyrimidine or the ______________

   position of a purine attaches at the ______________ position of the ribose, while the

   phosphates attach to the ______________ and ______________ positions.

IV. (10+5+5+5 points)

1. Write the polypeptide coded by the m-RNA sequence GUC GGA GAC UCA UUU GCG.

2. Write the DNA sequence that is transcribed to the RNA.

3. To which residue would valine hydrogen bond in an α-helix?

4. Which of the residues in the sequence above are most likely to be found in a β-sheet?

Part B: Cumulative Problems

I. (10+10+20+5+5 points)

1. In the presence of a large excess of H_2, the reaction $H_2(g) + I_2(g) \xrightarrow{k_f} 2\,HI(g)$, k_f (1000K) = 240 L Mol^{-1} S^{-1} appears to be first order. Calculate the half-life for this pseudo-first order forward reaction at 1000K in this limit for $[H_2]$ = 200 moles/liter.

2. If the activation energy for the above reaction is 165 kJ/mol, calculate the pseudo-first order rate constant at 2000K.

3. Calculate the activation energy for the reverse reaction at 1000K.

4. Calculate the <u>initial</u> rate at which heat is released by the reaction at 1000K in the bimolecular limit with $[H_2] = 0.081$ mol L^{-1} and $[I_2] = 0.036$ mol L^{-1}.

5. List and label the important steps in the mechanism for the H_2/O_2 explosion.

II. (10 points each) Consider the combustion of propane (C_3H_8) as a source of energy.

1. Suppose that a fuel cell is used to generate electrical power from this reaction. Calculate the maximum electrical work that can be extracted at 800K if all gases are maintained at 2.00 atmospheres.

2. Calculate the maximum total work that can be extracted at 800K from this reaction in the ideal gas approximation.

3. Calculate the efficiency of this fuel cell at 800K. What assumption must be made?

4. Calculate the cylinder temperature required for an internal combustion engine to have an efficiency of 80% (exhaust temperature = 1200K).

5. What is the maximum voltage this fuel cell could generate at 800K, if 12 electrons are transferred per mole of reaction?

III. (10 points each)

1. Sketch and <u>label</u> the energy bands for diamond and graphite. Indicate the location of the Fermi level.

2. Calculate the wavelength (nm) of the lowest energy transition of an electron confined in a 1.00 nm quantum dot $\left(E_n = \frac{h^2n^2}{8mL^2}\right)$.

3. Graph the probability for finding the electron in the quantum dot for n=2 state. Compare with the result expected from classical physics.

4. Use the Uncertainty Principle to calculate the uncertainty in the total energy (ΔE) for an electron confined in this quantum dot (hint: $E = \frac{P^2}{2M}$).

5. State the conditions under which one expects to observe dramatic quantum effects, and describe the effects.

IV. (10 points each) Consider the aromatic heterocyclic molecule C_5H_5N.

1. Draw a MO energy level diagram for the pi electrons, labelling the frontier orbitals, and showing the occupancy.

2. Sketch the shape(s) of the HOMO of this molecule.

3. Sketch the shape of one of the hybrid orbitals on the carbons. What is the hybridization?

4. Describe the factors affecting the stability of the above molecule relative to the analogous $C_5H_5^-$ anion.

5. List four universal (or nearly so) characteristics of known living systems.