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Workshop #10: Quantum Mechanics and Chemical Periodicity

Many important facts and laws in chemistry are experimentally determined, and then rationalized in terms of a theory or artificial concept. The Periodic Law is one of these. It is based on experiment and rationalized in terms of structural concepts. This form of the Periodic Table may be explained on the basis of the order in which the electrons occupy the various energy levels. Actually, the Periodic Table is based on experiment and serves as a guide to the order in which electron-filling of shells takes place.

A relationship between the *s*, *p*, *d*, and *f* orbitals and the Periodic Table may be observed by noting that the long form of the table can be divided into blocks. One of the blocks is two elements wide, another six elements wide, a third ten elements wide, and a fourth is fourteen elements wide, respectively. Specific sections of each period and each period in the table arise from the filling of orbitals of roughly equal energy.

1. For the first problem, complete the following table for the main group elements:

Group Number	IA	IIA	IIIA	IVA	VA	VIA	VIIA	VIIIA
Number of valence electrons				4				
Electronic configuration of valence electrons. Omit principle quantum number.				s^2p^2				
Common oxidation states.				±4				

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2. For the next problem, consider the chart below, which represents the main group (representative elements) portion of the Periodic Table.

   A. Several trends in atomic properties are listed to the sides and below the chart. Convert the lines into arrows by adding arrow heads to each line to indicate the direction of each trend (i.e. → or ←).

   B. In each box, write the electronic configuration of all the valence electrons for that element. Example: see the box containing element 84 (polonium)

IA	IIA	IIIA	IVA	VA	VIA	VIIA	VIIIA or 0
3	4	5	6	7	8	9	10
11	12	13	14	15	16	17	18
19	20	31	32	33	34	35	36
37	38	49	50	51	52	53	54
55	56	81	82	83	84 $6s^2 6p^4$	85	86
87	88						

Nonmetallic Properties Increase

Atomic Radii Increase

Ionization Energy Increases

Electronegativity Increases

Metallic Properties Increase

Atomic Radii Increase

Ionization Energy Increases

Electronegativity Increases

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3. In each square shown below, write the principal quantum number and orbital letter of the expected last electron to enter the atom in its ground state. For this exercise, ignore the exceptions. *(Four of them have been done for you.)*

	I A 1												III A 13	IV A 14	V A 15	VI A 16	VII A 17	VIII A 18
1	1	II A 2																2
2	3	4											5	6	7	8	9	10
3	11	12	III B 3	IV B 4	V B 5	VI B 6	VII B 7	---VIIIB--- 8	9	10	I B 11	II B 12	13	14	15	16	17	18
4	19	20	21	22	23	24	25	26	27	28	29	30 3d	31	32	33	34	35	36
5	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52 5p	53	54
6	55	56 6s	57	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86
7	87	88	89	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118

6	58	59	60	61	62	63	64	65	66 4f	67	68	69	70	71
7	90	91	92	93	93	95	96	97	98	99	100	101	102	103

4. A. Fill in the following table:

Quantum number l	0			3
Orbital Designation		*p*	*d*	

B. What m_l values are possible for the *d* orbitals?

C. What m_s values are possible?

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5. Determine the quantum numbers for all six electrons in the 4*p* sublevel.

Electron	***n***	***l***	m_l	m_s
$4p^1$				
$4p^2$				
$4p^3$				
$4p^4$				
$4p^5$				
$4p^6$				

6. For the sets of quantum numbers below, identify its electron configuration (if possible). If not possible, explain what is wrong.

n	***l***	m_l	m_s	**electron configuration or explanation of problem**
2	0	–1	– ½	_____
4	2	1	–½	_____
2	0	0	+½	_____
5	–1	1	0	_____

7. Determine the maximum number of electrons contained in:

   A. *d* sublevel _____ B. valence (outer) shell _____

   C. a single orbital _____ D. energy level $n = 4$ _____

8. Write FOUR isoelectronic species for the $A1^{+3}$ ion, two cations and two anions.

9. Identify the elements which have no electron with the quantum number $l = 1$.

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10. Consider the bismuth (Bi) atom.

A. Write the complete (start with 1*s*) and shortened (noble gas in brackets) electronic configuration for bismuth. Make certain to place brackets around the closed shell (core) electrons and identify valence electrons and pseudo-core electrons.

B. Draw the orbital diagram for all of the electrons in Bi.

C. Is Bismuth paramagnetic or diamagnetic?

D. Write the set of quantum numbers describing only valence electrons in Bi.

E. Write the shortened electronic configuration for the bismuth ions below:

Bi^{+3} ion _____ Bi^{+5} ion _____

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11. A. Calculate the wavelength (in nm) of light with frequency 2.31×10^{14} Hz.

B. Visible light has wavelengths between 400 to 700 nm. Slightly longer wavelengths are infrared (IR) and shorter are ultraviolet (UV). Is electromagnetic radiation from 2.31×10^{14} Hz found to be IR, Vis, or UV?

12. A. Solve for the wavelength (in nm) caused by a hydrogen electron jumping from $n = 6$ to $n = 3$.

B. Is this photon in the visible, IR, or UV portion of the spectrum?

C. What is the frequency (in s^{-1}) for this photon?

D. Calculate the energy of this photon in both J/photon and in kJ/mol.

13. The compound known as Sunbrella, which is the active ingredient in some sunscreens, absorbs strongly around 266 nm. What is the frequency of the absorption (in MHz)?

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14. For the last problem, fill in the following table for the various chemical species

Species	Short electronic configuration	"Short" Orbital Diagram	Quantum numbers of last e^-	Configuration of valence electrons	Common oxidation state(s)
O	[He] $2s^2 2p^4$	[He] $\underline{\uparrow\downarrow}$ $2s$ $\underline{\uparrow\downarrow}$ $\underline{\uparrow}$ $\underline{\uparrow}$ $2p$	2, 1, –1, ½	$2s^2\ 2p^4$	–2
Si					
K					
Sr					
Cr					Varies
Mn					Varies
Ga					
As					
Mo^{+2}					N/A
Fe^{+3}					N/A
Ag^{+}					N/A