

Slater's Rules Answers

Problem 1

Element: N	Slater
Configuration	$1s^2 2s^2 2p^3$
n-value grouping	$(1s)^2 (2s2p)^5$
groupings via Slater.	$(1s)^2 (2s2p)^{5-1=4}$
Slater's shielding value and Z_{eff} .	$1 \times 0.85 + 4 \times 0.35 = 3.1$ $7 - 3.1 = 3.9$

Element: C	Slater
Configuration	$1s^2 2s^2 2p^2$
n-value grouping	$(1s)^2 (2s2p)^4$
groupings via Slater.	$(1s)^2 (2s2p)^{4-1=3}$
Slater's shielding value and Z_{eff} .	$1 \times 0.85 + 3 \times 0.35 = 2.75$ $6 - 2.75 = 3.25$

Element: Mg	Slater
Configuration	$1s^2 2s^2 2p^6 3s^2$
n-value grouping	$(1s)^2 (2s2p)^8 (3s3p)^2$
groupings via Slater.	$(1s)^2 (2s2p)^8 (3s3p)^{2-1=1}$
Slater's shielding value and Z_{eff} .	$12 - 9.15 = 2.85$

Element: Cl	Slater
Configuration	$1s^2 2s^2 2p^6 3s^2 3p^5$
n-value grouping	$(1s)^2 (2s2p)^8 (3s3p)^7$
groupings via Slater.	$(1s)^2 (2s2p)^8 (3s3p)^{7-1=6}$
Slater's shielding value and Z_{eff} .	$17 - 10.9 = 6.1$

Element: Zn	Slater
Configuration	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2$
n-value grouping	$(1s)^2 (2s2p)^8 (3s3p)^8 (3d)^{10} 4s^2$
groupings via Slater.	$(1s)^2 (2s2p)^8 (3s3p)^8 (3d)^{10} 4s^{2-1=1}$
Slater's shielding value and Z_{eff} .	$30 - 25.65 = 4.35$

Element: Te	Slater
Configuration	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 4d^{10} 5s^2 5p^4$ [4f ⁰]
n-value grouping	$(1s)^2 (2s2p)^8 (3s3p)^8 (3d)^{10} (4s4p)^8 (4d)^{10} (4f)^0 (5s5p)^6$
groupings via Slater.	$(1s)^2 (2s2p)^8 (3s3p)^8 (3d)^{10} (4s4p)^8 (4d)^{10} (4f)^0 (5s5p)^{6-1=5}$
Slater's shielding value and	$2 + 8 + 8 + 10 + 18 \times 0.85 + 5 \times 0.35 = 45.05$

Z_{eff}	$52 - 45.05 = 6.95$ (for a 5p electron) What about a 5s electron (not asked for yet-hmmm?) $(1s)^2(2s2p)^8(3s3p)^8(3d)^{10}(4s4p)^8(4d)^{10}(4f)^0(5s5p)^{2-1=1}$ We consider only the 5s electrons, $S = 43.65$ What about a 4d electron? $(1s)^2(2s2p)^8(3s3p)^8(3d)^{10}(4s4p)^8(4d)^{10-1=9}(4f)^0(5s5p)^0$ 5s and 5 p do not shield at all, 4f is empty, $S = 39.15$
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Problem 2

We are interested in the behavior of outer core electrons, but we can use Slater's Rules for any electron. As seen in the rules, electrons that are in orbitals that are after the electron of interest do not contribute to the shielding of that electron. Determine the S and Z_{eff} for each of the following.

Element	Configuration
2s electron in P	$1s^2 2s^2 2p^6 3s^2 3p^3$; If we consider an electron in 3p, $Z_{\text{eff}} = 4.8$; however, we are asked to consider a 2s electron. The other electrons to the right do not shield, and are removed from the calculation ($n_0 = 2$, we start the calculations at $1s^2 2s^{2-1}$ for our grouping ($15 - [2 \times 0.85 + 0.35]$) $Z_{\text{eff}} = 12.95$,
2 p electron in Mg	$12 - 4.15 = 7.85$
2s electron in Cl	$17 - 4.15 = 12.85$ -the other orbitals don't shield. If you are using Calstry, you need to get rid of them in the electron configuration.
1s electron in He	$2 - 0.3 = 1.7$
1s electron in Mg	$12 - 0.3 = 11.7$

Problem 3

Cations and anions: follow the rules!

Element	Configuration
3p electron in Cl^-	$17 - 11.25 = 5.75$
2p electron in Mg^{2+}	$12 - 4.15 = 7.85$
1s electron in Li^+	$3 - 0.3 = 2.7$

Problem 4

Transition elements: reviewing the rules: electrons in the same (nd) group contribute 0.35 towards the overall shielding. Elements in all groups to the left in the Slater configuration format contribute 1.00 towards overall shielding. Electrons in all groups to the right in the Slater configuration contribute nothing towards overall shielding.

Element	Configuration
A 3d electron in Ni	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^8 4p^2; (1s)^2 (2s 2p)^8 (3s 3p)^8 (3d)^{8-1} (4s)^2;$ $S = 18 \times 1.00 + 7 \times 0.35 = 20.45; 28 - 20.45 = 7.55$
3d electron in Mn	$25 - 19.4 = 5.6$
4d electron in Ru	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^7 5s^1 44 - X = 5.9$

Problem 5

Going through the calculations, I wrote the electron configurations for the atoms, and then removed the outer most electrons. Notice that I still kept the empty shell to help me with the math. Then I grouped the shells, and totaled the electrons in each shell, and did the math. I also looked at the atom vs the ion.

Cadmium has a larger Z_{eff} than strontium. This is true for both the atom and the ion, of course with the $Z_{\text{eff(cation)}} > Z_{\text{eff(atom)}}$. The size of atoms and ions depends on the attractive force of the cloud to the nucleus. The outermost electron is less shielded for the strontium ion than for the cadmium ion, but the $Z_{\text{Cd}} > Z_{\text{Sr}}$ so $Z_{\text{eff(Cd)}} > Z_{\text{eff(Sr)}}$. A smaller Z_{eff} means the attraction between the nucleus and the outer most electron is also small. The electron of interest is able to “move” further away from the nucleus, creating a larger radius. Also, take note-when we are starting with the ion. There are no electrons in 5s; our first electrons come out of the 4d shell.

I also picked for comparison an inner orbital that both atoms have in their configuration, 3s. The Z_{eff} for the 3s orbital should be bigger for the atom or ion with the larger nuclear charge, and it turns out it does not matter if it is the ion or the atom, because it is an inner orbital.

Element: Cd	Slater
Configuration	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10}$
n-value grouping	$(1s)^2 (2s, 2p)^8 (3s, 3p)^8 (3d)^{10} (4s, 4p)^8 (4d)^{10} (5s, 5p)^2$
groupings via Slater.	$(1s)^2 (2s, 2p)^8 (3s, 3p)^8 (3d)^{10} (4s, 4p)^8 (4d)^{10} (5s, 5p)^{2-1=1}$
3s for Cd atom	$(1s)^2 (2s, 2p)^8 (3s, 3p)^{2-1=1}$

Element: Cd ²⁺	Slater
Configuration	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10}$
n-value grouping	$(1s)^2 (2s, 2p)^8 (3s, 3p)^8 (3d)^{10} (4s, 4p)^8 (4d)^{10} (5s, 5p)^0$
groupings via Slater.	$(1s)^2 (2s, 2p)^8 (3s, 3p)^8 (3d)^{10} (4s, 4p)^8 (4d)^{10-1} (5s, 5p)^0$
	The 3s will be the same for the atom and the ion

Element: Sr	Slater
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Configuration	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2$
n-value grouping	$(1s)^2 (2s, 2p)^8 (3s, 3p)^8 (3d)^{10} (4s, 4p)^8 (5s, 5p)^2$
groupings via Slater.	$(1s)^2 (2s, 2p)^8 (3s, 3p)^8 (3d)^{10} (4s, 4p)^8 (5s, 5p)^{2-1=1}$
3s for Sr atom	$(1s)^2 (2s, 2p)^8 (3s, 3p)^{2-1=1}$

Element: Sr^{2+}	Slater
Configuration	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^0$
n-value grouping	$(1s)^2 (2s, 2p)^8 (3s, 3p)^8 (3d)^{10} (4s, 4p)^8 (5s, 5p)^0$
groupings via Slater.	$(1s)^2 (2s, 2p)^8 (3s, 3p)^8 (3d)^{10} (4s, 4p)^{8-1=7} (5s, 5p)^0$
	The 3s will be the same for the atom and the ion

Calculations

$$S = 0.35 n_0 + 0.85 n_{n-1} + 1.00 n_{n-2}$$

$$S_{Cd} = 1 \times 0.35 + 10 \times 0.85 + 8 \times 0.85 + 10 \times 1.00 + 8 \times 1.00 + 8 \times 1.00 + 2 \times 1.00 = 43.65; Z_{eff_{5s \text{ in Cd}}} = 48 - 43.65 = 4.35$$

$$S_{Cd}^{2+} = 0 \times 0.35 + 9 \times 0.35 + 8 \times 1.00 + 10 \times 1.00 + 8 \times 1.00 + 8 \times 1.00 + 2 \times 1.00 = 39.15; Z_{eff_{4d \text{ in Cd}}} = 48 - 39.15 = 8.85$$

$$S_{5s} = 1 \times 0.35 + 8 \times 0.85 + 10 \times 1.00 + 8 \times 1.00 + 8 \times 1.00 + 2 \times 1.00 = 35.15$$

$$Z_{eff_{5s \text{ in Sr}}} = 38 - 35.15 = 2.85$$

$$S_{4p} = 1 \times 0.35 + 7 \times 0.35 + 10 \times 0.85 + 8 \times 0.85 + 8 \times 1.00 + 2 \times 1.00 = 27.75$$

$$Z_{eff_{4p}} = 38 - 27.75 = 10.25$$

$$Z_{eff_{3s}} \text{ for Cd} = 36.75$$

$$Z_{eff_{3s}} \text{ for Sr} = 26.75$$

Problem 6

For the series (I looked them up!) of ruthenium, rhodium, and palladium, calculate the Z_{eff} for the outer most orbital. Rationalize the ionization energies for the atoms based on your calculations; Do the same for Fe, Co, Ni.

element	Ionization energy	e-configuration	Z_{eff} outer e
Ru	710.2	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^1 4d^7$	$Z_{eff_{5s}} = 44 - 40.75 = 3.25$
Rh	719.7	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^1 4d^8$	$Z_{eff_{5s}} = 45 - 41.60 = 3.40$
Pd	804.4	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^0 4d^{10}$	$Z_{eff} = 46 - 39.15 = 6.85$
Fe	762.5	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$	$Z_{eff} = 26 - 22.25 = 3.75$
Co	760.4	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^7$	$Z_{eff} = 27 - 23.1 = 3.9$

element	Ionization energy	e-configuration	Z_{eff} outer e
Ni	737.1	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^8$	$Z_{\text{eff}} = 28 - 23.95 = 4.05$

Before we do the math, consider our electron of interest; for Ru and Rh, the electron is in 5s, while Pd has its electron in 4d. Palladium has a full 4d shell and an empty 5s shell; this is very stable and will be difficult to ionize.

$$\text{Ru: } (1s)^2(2s2p)^8(3s3p)^8(3d)^{10}(4s4p)^8(4d)^7(4f)^0(5s5p)^{1-1}$$

$$S = 0 \times 0.35 + 7 \times 0.85 + 8 \times 0.85 + 10 \times 1.00 + 8 \times 1.00 + 8 \times 1.00 + 2 \times 1.00 = 40.75$$

$$Z_{\text{eff } 5s} = 44 - 40.75 = 3.25$$

$$\text{Rh: } (1s)^2(2s2p)^8(3s3p)^8(3d)^{10}(4s4p)^8(4d)^8(4f)^0(5s5p)^{1-1}$$

$$S = 0 \times 0.35 + 8 \times 0.85 + 8 \times 0.85 + 10 \times 1.00 + 8 \times 1.00 + 8 \times 1.00 + 2 \times 1.00 = 41.60$$

$$Z_{\text{eff } 5s} = 45 - 41.60 = 3.40$$

$$\text{Pd: } (1s)^2(2s2p)^8(3s3p)^8(3d)^{10}(4s4p)^8(4d)^{10-1}(4f)^0(5s5p)^0$$

$$S = 9 \times 0.35 + 8 \times 1.00 \text{ [see the copper example]} + 10 \times 1.00 + 8 \times 1.00 + 8 \times 1.00 + 2 \times 1.00 = 39.15$$

$$Z_{\text{eff}} = 46 - 39.15 = 6.85$$

While for Fe, Co, Ni

$$(1s)^2(2s,2p)^8(3s,3p)^8(3d)^6(4s,4p)^{2-1}$$

$$S_{\text{Fe}} = 2 \times 1.00 + 8 \times 1.00 + 8 \times 0.85 + 6 \times 0.85 + 1 \times 0.35 = 22.25$$

$$Z_{\text{eff}} = 26 - 22.25 = 3.75$$

$$(1s)^2(2s,2p)^8(3s,3p)^8(3d)^7(4s,4p)^{2-1}$$

$$S_{\text{Co}} = 2 \times 1.00 + 8 \times 1.00 + 8 \times 0.85 + 7 \times 0.85 + 1 \times 0.35 = 23.1$$

$$Z_{\text{eff}} = 27 - 23.1 = 3.9$$

$$(1s)^2(2s,2p)^8(3s,3p)^8(3d)^8(4s,4p)^{2-1}$$

$$S_{\text{Ni}} = 2 \times 1.00 + 8 \times 1.00 + 8 \times 0.85 + 8 \times 0.85 + 1 \times 0.35 = 23.95$$

$$Z_{\text{eff}} = 28 - 23.95 = 4.05$$

At first glance, it seems as if both series should show an increase in the ionization energies, since all of the Z_{eff} are increasing. So maybe the answer is more complex. We can easily explain the rise in Palladium's ionization energy is also probably due to the stability of filled shells. The 4d sub shell is lower in energy than an 5s sub shell, so the electrons are closer to the nucleus and with the added effect of the nuclear charge, we expect a large ionization energy.

We predict that it will be easier to ionize the 3d metals because the electrons are in lower energy shells. When we compare Fe and Ru (762 vs 710) and Co and Rh (760 vs 719) we see an expected trend.

[illegible]

First, find the electron configuration to calculate Z_{eff} :

Element	Melting Point (°C)	Electron Configuration	Z_{eff}
Na	98	$(1s)^2(2s2p)^8(3s3p)^1$	$Z_{\text{eff}} = 11 - [2(1.00) + 8(0.85)] = 2.20$
Mg	650	$(1s)^2(2s2p)^8(3s3p)^2$	$Z_{\text{eff}} = 12 - [2(1.00) + 8(0.85) + 1(0.35)] = 2.85$
Al	660	$(1s)^2(2s2p)^8(3s3p)^3$	$Z_{\text{eff}} = 13 - [2(1.00) + 8(0.85) + 2(0.35)] = 3.50$
Si	1414	$(1s)^2(2s2p)^8(3s3p)^4$	$Z_{\text{eff}} = 14 - [2(1.00) + 8(0.85) + 3(0.35)] = 4.15$
P	44	$(1s)^2(2s2p)^8(3s3p)^5$	$Z_{\text{eff}} = 15 - [2(1.00) + 8(0.85) + 4(0.35)] = 4.80$
S	115	$(1s)^2(2s2p)^8(3s3p)^6$	$Z_{\text{eff}} = 16 - [2(1.00) + 8(0.85) + 5(0.35)] = 5.45$
Cl	-101.5	$(1s)^2(2s2p)^8(3s3p)^7$	$Z_{\text{eff}} = 17 - [2(1.00) + 8(0.85) + 6(0.35)] = 6.10$
Ar	-189	$(1s)^2(2s2p)^8(3s3p)^8$	$Z_{\text{eff}} = 18 - [2(1.00) + 8(0.85) + 7(0.35)] = 6.75$

¹ Order of filling is always a sticky subject because we (meaning me too!) don't have the total background needed to fully understand the subject. I liked the way this website explains filling, which is similar to how I think about degenerate orbitals and filling orders: <http://www.chemguide.co.uk/atoms/properties/3d4sproblem.html>

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condensed phases. Thus, melting point might be considered a periodic property, but requires an understanding of all the bonding attractions in place for each substance.

Problem 8

Atom	neutral configuration	cation configuration	Slater Z_{eff}	Second Ionization Potential
K	$[\text{Ar}]4s^1$	$[\text{Ar}] = (1s)^2(2s2p)^8(3s3p)^8$	$Z_{\text{eff}} = 19 - [7(0.35) + 8(0.85) + 2(1.00)] = 7.75$	31.625 eV
Ca	$[\text{Ar}]4s^2$	$[\text{Ar}]3d^1 = (1s)^2(2s2p)^8(3s3p)^8(3d)^1$	$Z_{\text{eff}} = 20 - [18(1.00)] = 2.0$	11.871 eV
Sc	$[\text{Ar}]4s^23d^1$	$[\text{Ar}]3d^2 = (1s)^2(2s2p)^8(3s3p)^8(3d)^2$	$Z_{\text{eff}} = 21 - [1(0.35) + 18(1.00)] = 2.65$	12.80 eV
Ti	$[\text{Ar}]4s^23d^2$	$[\text{Ar}]3d^3 = (1s)^2(2s2p)^8(3s3p)^8(3d)^3$	$Z_{\text{eff}} = 22 - [2(0.35) + 18(1.00)] = 3.30$	13.58 eV
V	$[\text{Ar}]4s^23d^3$	$[\text{Ar}]3d^4 = (1s)^2(2s2p)^8(3s3p)^8(3d)^4$	$Z_{\text{eff}} = 23 - [3(0.35) + 18(1.00)] = 3.95$	14.65 eV

Z_{eff} nicely parallels the second ionization potential. It is hard to ionize K^+ and the large Z_{eff} indicates this. All the other elements ionize more readily and the second ionization potentials steadily increase along with Z_{eff} .

The electron configuration for Ca^+ is d^1 , the same as any transition metal element. If the ion were $4s^1$, then the Slater Z_{eff} would be $= 20 - [8(0.85) + 10(1.00)] = 3.20$, which is out line with the observations. $Z_{\text{eff}} = 3.2$ suggests an ionization potential closer to Ti^+ .

Problem 9

Element	Electron Configuration	Z_{eff} (Calculated)	EA, kJ/mol
Li	$(1s^2)(2s^1)$	$3 - [2(0.85)] = 1.30$	-60
Be	$(1s^2)(2s^2)$	$4 - [2(0.85) + 1(0.35)] = 1.95$	0
B	$(1s^2)(2s^22p^1)$	$5 - [(2(0.85) + 2(0.35))] = 2.60$	-27
C	$(1s^2)(2s^22p^2)$	$6 - [2(0.85) + 3(0.35)] = 3.25$	-122
N	$(1s^2)(2s^22p^3)$	$7 - [2(0.85) + 4(0.35)] = 3.90$	7
O	$(1s^2)(2s^22p^4)$	$8 - [2(0.85) + 5(0.35)] = 4.55$	-141
F	$(1s^2)(2s^22p^5)$	$9 - [2(0.85) + 6(0.35)] = 5.20$	-328
Ne	$(1s^2)(2s^22p^6)$	$10 - [2(0.85) + 7(0.35)] = 5.85$	$\approx +29$

Generally, Z_{eff} and EA give the same trend. However, N and Ne are very low: N is half-filled and Ne is filled, neither want to remove this stability and add an electron. Li is a bit high perhaps, maybe because the product anion is a filled shell. Be is a mystery. Possibly the electron affinity has not been measured. The search for possible answers and values continues. It helps to draw the box diagram for these atoms and the formed anion.