Name	Student Number

03-59-250	Midterm 1	16/10/18 (80 min)

Note: Exams written in pencil will NOT be re-marked.

Fill out your name on each page. Make sure all pages are handed in at the end.

The distribution of marks for the questions is approximate, and may change. You may use the back of any page for additional space or rough work.

Group 1	Group 2	Group 3	Group 4	Group 5	Group 6	Group 7	Group 8	Group 9	Group 10	Group 11	Group 12	Group 13	Group 14	Group 15	Group 16	Group 17	Group 18
1 **H** 1.0078																	2 **He** 4.0026
3 **Li** 6.938	4 **Be** 9.012											5 **B** 10.806	6 **C** 12.011	7 **N** 14.007	8 **O** 15.999	9 **F** 18.998	10 **Ne** 20.180
11 **Na** 22.990	12 **Mg** 24.305											13 **Al** 26.982	14 **Si** 28.085	15 **P** 30.974	16 **S** 32.059	17 **Cl** 35.45	18 **Ar** 39.948
19 **K** 39.098	20 **Ca** 40.078	21 **Sc** 44.956	22 **Ti** 47.867	23 **V** 50.942	24 **Cr** 51.996	25 **Mn** 54.938	26 **Fe** 55.845	27 **Co** 58.933	28 **Ni** 58.693	29 **Cu** 63.546	30 **Zn** 65.38	31 **Ga** 69.723	32 **Ge** 72.630	33 **As** 74.922	34 **Se** 78.971	35 **Br** 79.904	36 **Kr** 83.798
37 **Rb** 85.468	38 **Sr** 87.62	39 **Y** 88.906	40 **Zr** 91.224	41 **Nb** 92.906	42 **Mo** 95.95	*43* *Tc* *(98)*	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** 1.008
55 **Cs** 132.91	56 **Ba** 137.33		72 **Hf** 178.49	73 **Ta** 180.95	74 **W** 183.84	75 **Re** 186.21	76 **Os** 190.23	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** –		*104* *Rf* –	*105* *Db* –	*106* *Sg* –	*107* *Bh* –	*108* *Hs* –	*109* *Mt* –	*110* *Ds* –	*111* *Rg* –	*112* *Cn* –	*113* *Nh* –	*114* *Fl* –	*115* *Mc* –	*116* *Lv* –	*117* *Ts* –	*118* *Og* –

57 **La** 138.91	58 **Ce** 140.12	59 **Pr** 140.91	60 **Nd** 144.24	61 **Pm** 144.91	62 **Sm** 150.36	63 **Eu** 151.96	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** 173.05	71 **Lu** 174.97
89 **Ac** –	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* –

Common VSEPR geometries					
# of objects	**2**	**3**	**4**	**5**	**6**
Base geometry	*linear*	*trigonal planar*	*tetrahedral*	*trigonal bipyramidal*	*octahedral*

Some (maybe) useful equations and constants

$$\Delta E = h\nu = \Re\left(\frac{1}{{n_l}^2} - \frac{1}{{n_h}^2}\right) \qquad \Re = \frac{2\pi^2 \mu e^4}{(4\pi\varepsilon_0)^2 h^2} = 13.6\ \text{eV}$$

$$c = \lambda\nu \qquad Z^* = Z - \sigma \qquad E_n = -\Re\left(\frac{Z^{*2}}{n^2}\right)$$

Speed of light: $c = 2.998 \times 10^8$ m/s Planck's constant: $h = 6.6261 \times 10^{-34}$ J·s
Avogadro's constant: $N = 6.022 \times 10^{23}$ mol^{-1}

$D_{(A-B),theory} = \frac{1}{2}(D_{(A-A)} + D_{(B-B)})$ $\Delta'_{(A-B)} = D_{(A-B),experiment} - D_{(A-B),theory}$
$\chi_A - \chi_B = 0.102\ (\Delta'_{(A-B)})^{1/2}$

Born-Mayer equation $$\Delta U_0 = 1390\ \text{Å} \times \left(\frac{q_A q_B}{r_0}\right) \times A \times \left(1 - \frac{0.345\ \text{Å}}{r_0}\right)\ \text{in}\ \frac{\text{kJ}}{\text{mol}}$$

Kapustinskii equation $$\Delta U_0 = 1210\ \text{Å} \times n \times \left(\frac{q_A q_B}{r_0}\right) \times \left(1 - \frac{0.345\ \text{Å}}{r_0}\right)\ \text{in}\ \frac{\text{kJ}}{\text{mol}}$$

Relativistic relationships:

$$v = \frac{Ze^2}{2\varepsilon_0 h} \qquad \boldsymbol{m_{rel}} = \frac{\boldsymbol{m_{rest}}}{\sqrt{\mathbf{1} - \left(\frac{\boldsymbol{v}}{\boldsymbol{c}}\right)^{\mathbf{2}}}}$$

$$E_n = -\frac{m_e e^4}{8{\varepsilon_0}^2 h^2}\left(\frac{Z^2}{n^2}\right) \qquad r(n) = n^2 a_0 = n^2 \frac{Ze^2}{m_e 4\pi\varepsilon_0 v^2}$$

$$\boldsymbol{v} \propto \mathbf{Z} \qquad \boldsymbol{E_n} \propto -\boldsymbol{m_e} \qquad \boldsymbol{r(n)} \propto \frac{\mathbf{1}}{\boldsymbol{m_e}}$$

Slater's Rules:

1. Group electron configuration as follows:
$$(1s)(2s, 2p)(3s, 3p)(3d)(4s, 4p)(4d)(4f)(5s, 5p)\ \text{etc}$$
2. Electrons to the right (in higher subshells and shells) of an electron do not shield it.
3. If the electron of interest is an $\boldsymbol{n}s$ or $\boldsymbol{n}p$ electron:
   a) each other electron in the same group contributes 0.35 (0.30 for $1s$)
   b) each electron in an $(\boldsymbol{n} - 1)$ group contributes 0.85
   c) each electron in an $(\boldsymbol{n} - 2)$ or lower group contributes 1.00
4. If the electron of interest is an $\boldsymbol{n}d$ or $\boldsymbol{n}f$ electron:
   a) each other electron in the same group contributes 0.35
   b) each electron in a lower group (to the left) contributes 1.00

Name: ________________________________

1. Quick fire round! Circle or write the correct answer, as appropriate. [1 mark each]
   a) Compounds obeying the octet rule have an octahedral geometry

      True **False**

   b) On the subatomic scale, energy is on a continuum

      True **False**

   c) The earth's crust is mostly made up of elements that are lighter than iron.

      True **False**

   d) The mass of an electron is constant for all elements.

      True **False**

   e) An orbital is described by 3 unique quantum numbers

      True **False**

   f) How many nodes do the orbitals in n = 6 the energy level have?

   g) How many angular nodes does an orbital with ℓ = 3 have?

   h) How many orbitals are there in the n = 5, ℓ = 3 subshell?

   i) Left to right across a period, ionisation energy….

      Increases **Decreases**

   j) Top to bottom down a group, ionisation energy….

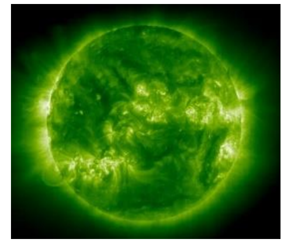
      Increases **Decreases**

   k) After the first ionisation, the radius of an atom…

      Increases **Decreases**

Name: ________________________________

2. This (artificially coloured) image of the sun was recorded by NASA's Atmospheric Imaging Assembly using the light given off by iron atoms that have lost 11 electrons, at a wavelength of 19.3 nm



   a) Calculate the energy (in joules) of one photon of light that is emitted from these iron atoms [2 marks]

   b) What is the energy per mole of photons? [1 mark]

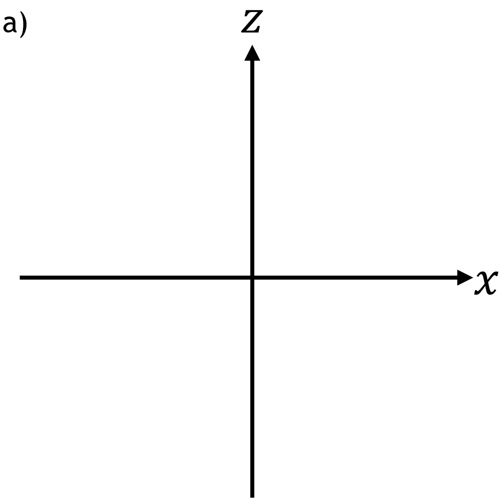
   c) Assuming the atoms are following the Aufbau rules, what is the electronic configuration of these iron atoms? (Do not use noble gas abbreviations, write it all out!) [2 marks]

   d) The ground state electronic configuration of iron metal (on earth!) is $[\mathrm{Ar}]3d^6 4s^2$. What is the effective nuclear charge experienced by these d-electrons in iron? [3 marks]

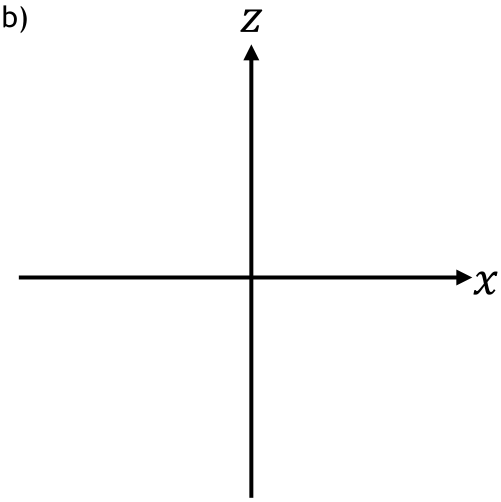
Name: ______________________________

3. Sketch the following orbitals:
   a) $1s$; b) $2p_z$ [1 mark each]; c) $3p_z$; d) $3d_{z^2}$; e) $4d_{xz}$ [2 marks each]

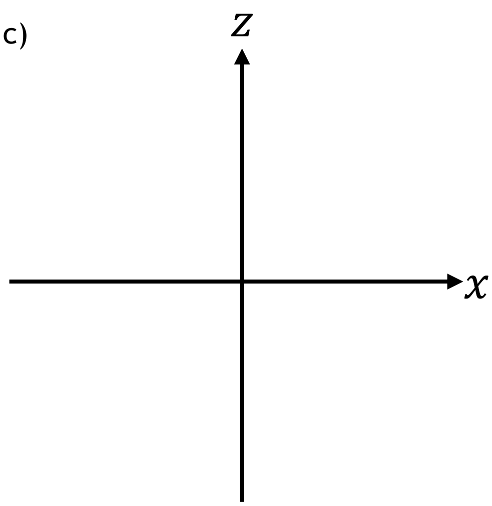
a)



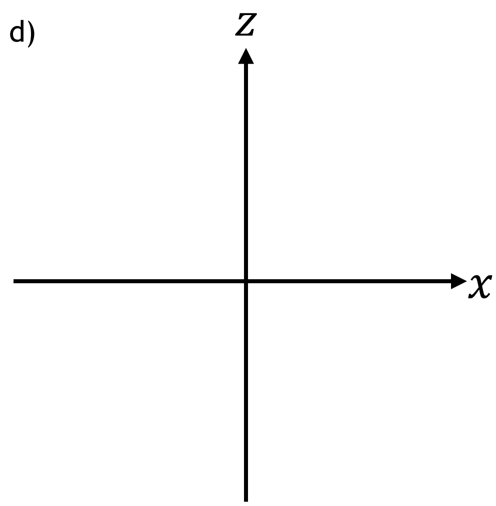
b)



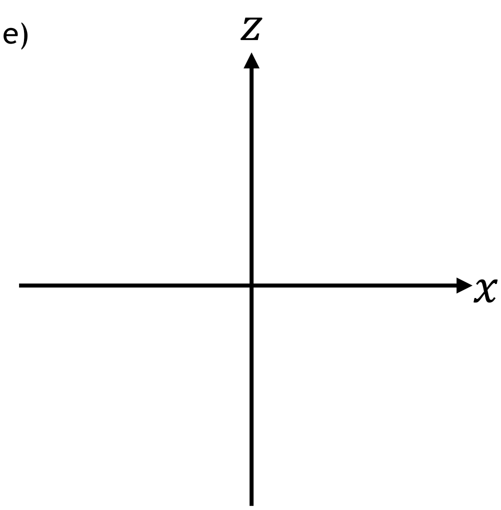
c)



d)



e)



Bonus: Sketch and label any f orbital. Draw your own axes ☺ [2 bonus marks]

Name: ________________________________

4.

a) Sketch two diagrams for possible configurations of the p electrons in nitrogen. [2 marks]

b) Based on your diagrams above, write expressions for the energy of both of your arrangements in terms of Π_c (coulombic) and Π_e (exchange). [4 marks]

c) Which of the two arrangements would you expect to be the lowest energy? [1 mark]

d) Estimate the ionisation energy of oxygen (in eV), given that the effective nuclear charges experienced by the valence electrons in O and O+ are 4.55 and 4.90, respectively. [3 marks]

e) The experimental first ionisation energy for oxygen is 13.6 eV. Is this value higher or lower than your calculated value? Suggest a reason for this discrepancy [2 marks]

Name: ________________________________

5. This question is about the group 6 metals.
   a) The ground state electronic configuration of chromium is $[\mathrm{Ar}]3d^5 4s^1$ rather than $[\mathrm{Ar}]3d^4 4s^2$. Why? [1 mark]

   b) What is the spin multiplicity of Cr? [1 mark]

   c) The ground state of molybdenum is $[\mathrm{Kr}]4d^5 5s^1$; however, the ground state of tungsten is $[\mathrm{Xe}]5d^4 6s^2$. Suggest why tungsten breaks the trend, with a BRIEF explanation. (Think: what might be affecting the energy difference between the $5d$ and $6s$ orbitals?) [2 marks]

   d) The only compound of chromium that is +5 is CrF_5. However, molybdenum forms MoF_5 and $MoCl_5$; and tungsten forms WF_5, WCl_5 and WBr_5. Why do you think this might be?
   [2 marks]

Name: ________________________________

6.

a) Using the following data, estimate the value of $\Delta U_0(\mathrm{KBr})$. [3 marks]

$r^+(\mathrm{K}^+)$ = 1.33 Å $r^-(\mathrm{Br}^-)$ = 1.82 Å

b) Using the following thermochemical data, construct a Born-Haber cycle for KBr(s) [3 marks] and hence determine the experimental value of $\Delta U_0(\mathrm{KBr})$ [3 marks].

Note: Bromine is a liquid in its standard state. Dealing with this properly is worth 1 of the 6 marks in this question, so if you're not sure don't worry too much!

$\Delta H^\circ_{sublimation}$($K_{(s)}$) = +89 kJ/mol $\Delta H^\circ_{vapourisation}$($Br_{2(l)}$) = +29.8 kJ/mol $\Delta H^\circ_{dissociation}$($Br_{2(g)}$) = +193 kJ/mol

ΔH°_{ie}($K_{(g)}$) = +418.8 kJ/mol ΔH°_{ea}($Br_{(g)}$) = −324.6 kJ/mol ΔH°_{f}($KBr_{(s)}$) = −393.8 kJ/mol

Name: ________________________________

c) The Kapustinskii equation is remarkably accurate for most compounds, usually giving a value within approx. 50 kJ/mol of the actual value (hint!). However, when $\Delta U_0(\mathrm{AgBr})$ is predicted using the equation, the magnitude of the lattice enthalpy is 220 kJ/mol *smaller* than the real value.

Suggest why the Kapustinskii equation not give a good value for AgBr. What assumptions are made when using the Kapustinskii equation? [2 marks]

7.

a) What is a molecular ion? (Briefly!) [1 mark]

b) Predict the structure of the PF_6^- ion [2 marks]

c) Predict the structure of the PF_4^- ion [3 marks]