Name **Student number**

Problem 1 (35 points)

a) For the following elements, (1) give the electron configuration with the correct atomic orbitals, (2) clearly indicate which electrons are the core electrons and which electrons are the valence electrons, and (3) give the charge and electron configuration of the most stable ion formed by these elements. (6pt)

(i) Te

[redacted] 52 e^- $\overbrace{1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,4s^2\,3d^{10}\,4p^6}^{core}\,\underline{\underline{5s^2}}\,\overbrace{4d^{10}}^{core}\,\underline{\underline{5p_x^2\,5p_y^1\,5p_z^1}}$

valence

Te^{2-} $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6$

(ii) Sc

21 e^- $\underbrace{1s^2\,2s^2\,2p^6\,3s^2\,3p^6}_{core}\,|\,\underbrace{4s^2\,3d^1}_{valence}$

Sc^{3+} $1s^2 2s^2 2p^6 3s^2 3p^6$

b) Organize the following atoms and ions in terms of size (small to large), and explain your answer (6pt):

Br^-, Ne, Al^{3+}, S^{2-}

Answer: $Al^{3+} < Ne < S^{2-} < Br^-$

Al and S are on the same row, Al^{3+} is much smaller than S^{2-} because of their charges. Br is one row down and therefore the largest. Ne is one row up and therefore small. However, as Al is in the 3+ state, its size is considerably reduced and it becomes smaller than neutral Ne.

You will still score points if you swap A^{l3+} for Ne or S^{2-} for Br^-.

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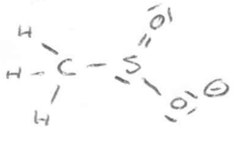
c) Organize the following compounds in terms of their miscibility with water (lower to higher), and explain your answer (6pt).

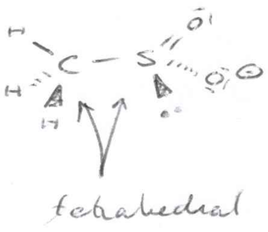
$CH_3CH(OH)CH_2CH_3$ (2-butanol), $CH_3CH_2CH_2CH_3$ (butane), $CH_3C{=}OCH_2CH_3$ (2-butanone)

Miscibility means the ability to mix (i.e. the solubility of one in the other). Typically, polar molecules will mix with other polar molecules, apolar with apolar. Water is very polar, and therefore the most polar molecules will mix the best. 2-butanol can form h-bonds and has a dipole. 2-butanone has a dipole. Butane has only dispersion interactions (they all do). Thus, the order from low to high miscibility is butane < butanone < butanol.

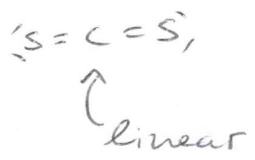
d) What is the 3D structure of (i) $CH_3SO_2^-$, (ii) CS_2 , and (iii) IO_2^- ? Explain your answer using Lewis structure drawings and VSEPR theory (12 points).

i) $CH_3SO_2^{\ominus}$:
C (4)
H (3×1)
S (6)
O (2×6)
$\ominus$ (1)
26 $e^{\ominus}$

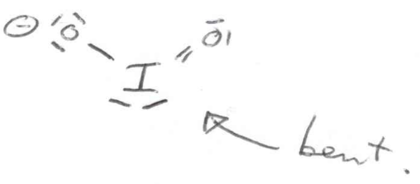




ii) CS_2
C (4)
S (2×6)
16 $e^{\ominus}$

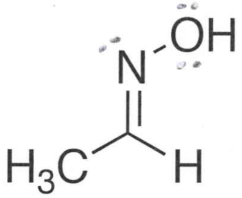


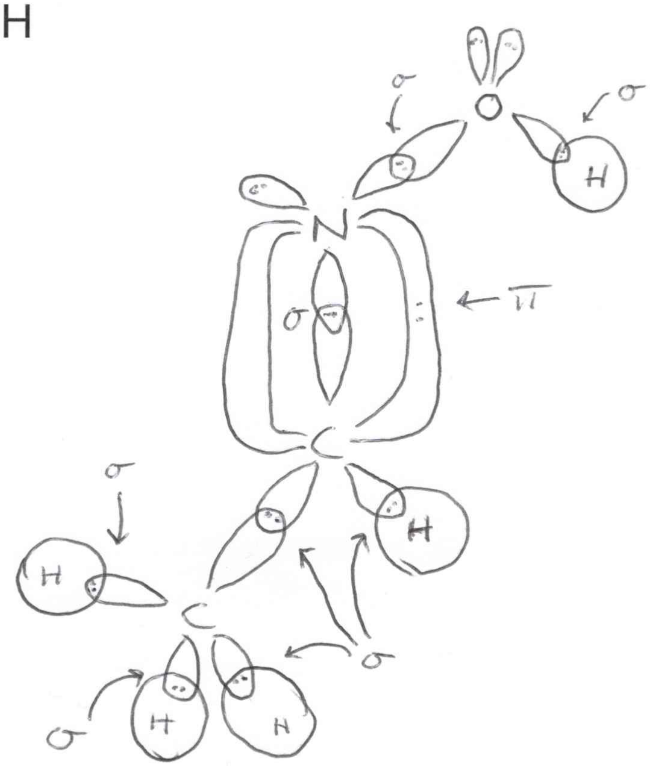
iii) $IO_2^{\ominus}$
I (7)
O (2×6)
$\ominus$ (1)
20 e^-



Name **Student number**

e) Draw all molecular orbitals of $CH_3CH=NOH$. The Lewis structure is shown below. (8pt)





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Problem 2 (18 points)

True or False? Indicate if the statements below are true or false. In each case, explain your answer in 1-2 lines and/or a simple drawing. <u>You will only score points if you provide a valid explanation</u>.

(i) A catalyst increases the rate of a reaction by lowering the energy of the reaction product.

False, a catalyst does nothing to the energies of the starting and product molecules (it does not change equilibrium), but it does change the Activation Energy.

(ii) The osmotic pressure of a 0.07 M ethanol solution is higher than that of a 0.03 M $Mn(SO_4)_3$ solution.

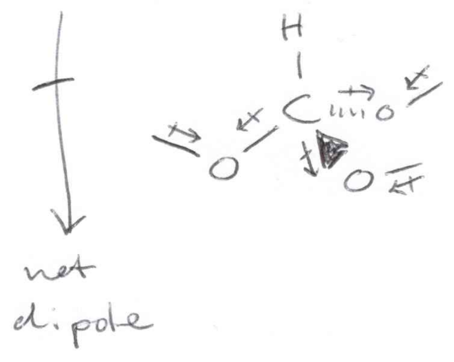
False. Collegiative property, $Mn(SO_4)_3$ gives 4 ions in solution (i=4), ethanol only one molecule. So $Mn(SO_4)_3$ will give 4*0.03*RT, ethanol 0.07RT.

(iii) The N-Cl bond in NCl_3 is an ionic bond.

False, N and Cl are both highly electronegative elements and therefore the difference in electronegativity can never be large enough to get an ionic bond. In fact, the difference is 0, so it is a perfect covalent bond.

(iv) $HC(OCH_3)_3$ is a polar molecule.

True, the CO bonds are polarized and because of the 3D structure of the molecule a net dipole is present, giving a polar molecule.



(v) Dissolving Fe^{3+} ions in water will result in a basic solution because the Fe^{3+} will repel H^+

<u>False</u>, it will result in an acidic solution as Fe^{3+} will bind to water molecules, making H^+ detach more easily from water.

(vi) The triple bond between C and N in the cyanide anion (NC^-) indicates that the orbitals on N are sp^3 hybridized.

False, the triple bond indicates that N must be sp hybridized.

(vii) n-Octane has a higher boiling point than iso-octane (2,2,4-trimethylpentane).

True, the bruto formula is the same but the surface area of n-octane is much larger, giving rise to larger dispersion interactions and thus a higher boilingpoint.

n-octane ⇒ more area for dispersion interactions

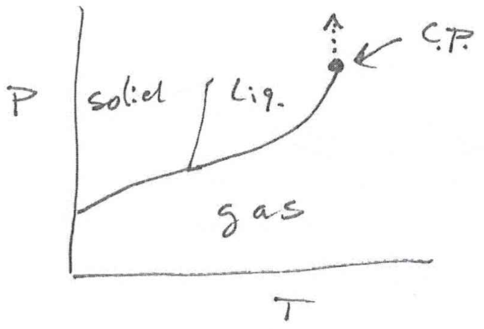
⇓

iso-octane

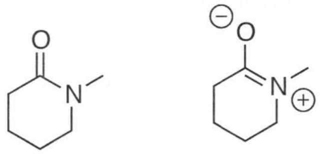
higher b.p. ⇒ <u>True</u>

(viii) When you increase the pressure at the critical point in a typical phase diagram, you immediately get a solid.

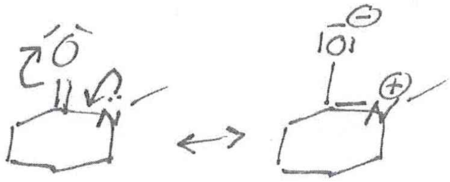
False, the critical point is at the end of the vaporization curve, separating liquid from gas. This, when you increase the pressure you will either get a liquid or a supercritical fluid, but never a solid.



(ix) The following structures are two resonance forms of the same molecule.



True.



Problem 3 (20 points)

Consider the following exothermic reaction:

$NCl_3 + H_2O \rightleftarrows NCl_2H + HOCl$

In the reaction, compound NCl_3 first reacts to give first intermediate X, which then reacts with H_2O to finally give products NCl_2H and HOCl. Analysis of the initial rates (at 298K) at which NH_3 is formed at various initial concentrations of NCl_3 and H_2O shows the following:

Experiment	initial rate of formation of NCl_2H (M/s)	$[NCl_3]$ (M)	$[H_2O]$ (M)
1	1.25 ×1	0.3 ×2	0.125 ×1
2	1.25	0.6	0.125
3	×4 5.00	×1 0.6	×2 0.25
4	5.00	0.3	0.25

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a) Write down the reaction rate equation for the formation of product NCl_2H as a function of the concentrations of NCl_3 and H_2O. Explain your answer. (6 points)

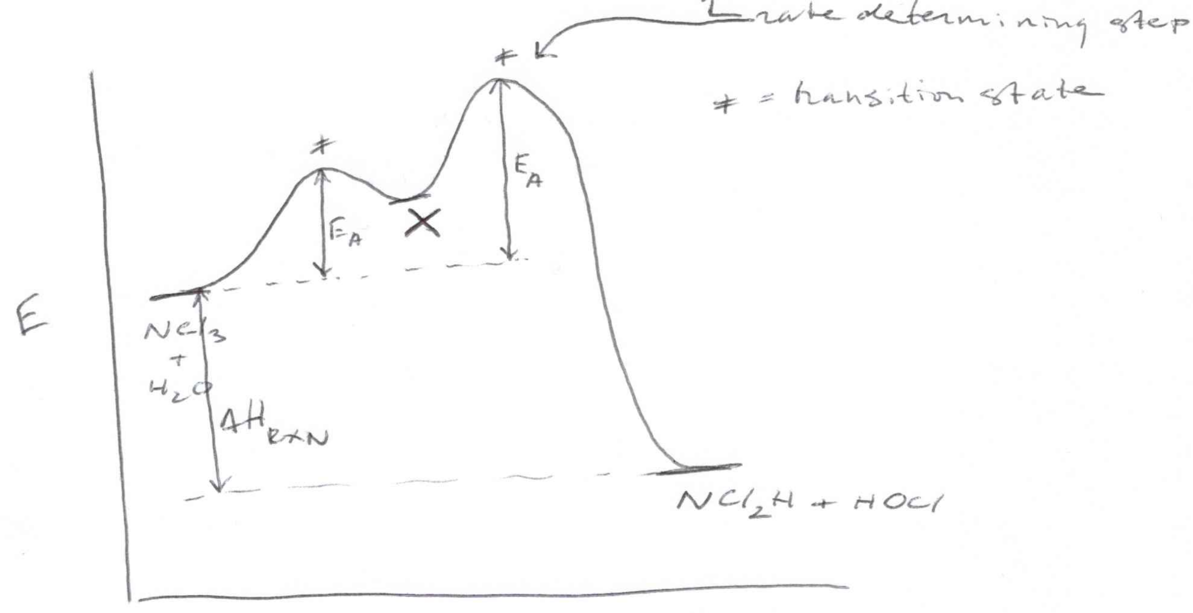
In the table: - when $[NCl_3]$ is doubled, nothing happens ⇒ 0th order.

- when $[H_2O]$ is doubled, rate goes up 4x ⇒ 2nd order

$$\Rightarrow \quad \frac{d[NCl_2H]}{dt} = k[H_2O]^2$$

b) Sketch a Reaction Coordinate / Energy diagram for the reaction of NCl_3 to product NCl_2H.
In these diagrams clearly indicate the following elements: reactants, products, transition state, activation energies, reaction enthalpy, rate determining step, intermediate X. (6pt)

the reaction goes $NCl_3 \rightarrow X \xrightarrow{H_2O} NCl_2H + HOCl$



c) The data is given for 298K. Assuming an activation energy of $1.7*10^2$ kJ/mol (independent of temperature), use a calculation to show what happens to the rate constant when the reaction is carried out at 498K instead of 298K. (8pt)

two methods: ① $k = A\,e^{\left(-\frac{E_a}{RT}\right)}$ $T = 298\,K$; $E_a = 1.7 \cdot 10^5$ g/mol

$k = 80\ M^{-1}s^{-1}$ (from data in table)

↓

$A = \sim 5 \cdot 10^{31}\ M^{-1}s^{-1}$

$T = 498\,K$: $k = 5 \cdot 10^{31} \cdot e^{\frac{-1.7\,10^5}{R \cdot 498}} = \sim 7.4 \cdot 10^{13}\ M^{-1}s^{-1}$

② same via

$$\ln \frac{k_2}{k_1} = \frac{E_a}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)$$

$k_1\ \cancel{k} = 80\ M^{-1}s^{-1}$

$T_1 = 298\,K$

$T_2 = 498\,K$

$k_2 \sim 7.4 \cdot 10^{13}\ M^{-1}s^{-1}$

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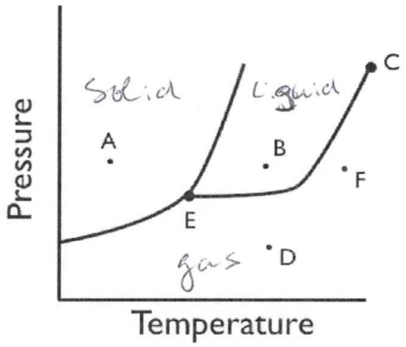
Problem 4 (14 points)

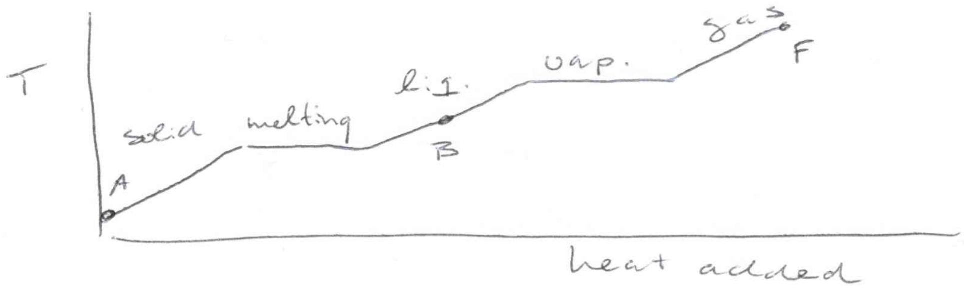


The Figure shows a typical phase diagram for compound Y.

a) What are points E and C? (2p)

E = triple point
C = critical point

b) Sketch a (heat added vs. temperature) diagram for the process going from A to B to F. Indicate in each part of the diagram the phase of compound Y. (6p)



c) What happens to the vaporization curve when a certain amount of sugar is dissolved in compound Y? Explain your answer. (6p)

dissolving sugar leads to a reduction in vapor pressure, and hence a boiling point elevation.