

# Calculations in IB Chemistry SL and HL

Below is a list of the calculations are expected to be able to do in IB chemistry. This needs committing to memory, and each type of calculation will need practice to master. Good luck!

Calculations shaded in grey are only required at HL.

## Quantitative Chemistry

| Purpose                                                                          | The Calculation                                                                                                                                                                                                                                                                                                                                                                                                       | Notes                                                                                                                                                                                                                                                                |
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| 1. Calculating a quantity in moles from a number of particles                    | $n = \frac{N}{L}$ <p>n = the quantity in moles<br/>N = the number of particles<br/>L = Avogadro's constant, <math>6.02 \times 10^{23}</math></p>                                                                                                                                                                                                                                                                      | <ul style="list-style-type: none"> <li>When calculating numbers of atoms within molecules, multiply the number of particles (N) by the number of atoms in the formula</li> <li>To find out numbers of particles, rearrange to: <math>N = n \cdot L</math></li> </ul> |
| 2. Determine relative molecular or formula mass, $M_r$                           | $M_r = \sum (\text{number of atoms} \cdot \text{atomic mass})$                                                                                                                                                                                                                                                                                                                                                        | <ul style="list-style-type: none"> <li><math>M_r</math> has no unit as it is a relative value</li> <li>To calculate molar mass, <math>M_m</math>, just stick a 'g' for grams on the end</li> </ul>                                                                   |
| 3. Calculate a quantity in moles, from a mass of a substance                     | $n = \frac{m}{M_m}$ <p>n = the quantity in moles<br/>m = the mass of substance you are given in grams<br/><math>M_m</math> = the molar mass of the substance</p>                                                                                                                                                                                                                                                      | <ul style="list-style-type: none"> <li>To determine the mass of a given number of moles of a substance use:<br/><math>m = M_m \cdot n</math></li> <li>To determine the molar mass of a given mass of a substance:<br/><math>M_m = \frac{m}{n}</math></li> </ul>      |
| 4. Determine empirical formula from % composition by mass                        | <ol style="list-style-type: none"> <li>Divide each % by the atomic mass</li> <li>Divide each answer to Step 1 by the smallest answer to Step 1</li> <li>Multiply all answers to Step 1 to remove any obvious fractions                             <ol style="list-style-type: none"> <li>If there is a '.5' multiply everything by 2</li> <li>If there is a '.3' multiply everything by 3 etc</li> </ol> </li> </ol> |                                                                                                                                                                                                                                                                      |
| 5. Determine molecular formula from empirical formula                            | $F_m = \frac{M_r}{m(F_e)} \cdot F_e$ <p><math>F_m</math> = molecular formula<br/><math>M_r</math> = relative molecular mass<br/><math>F_e</math> = empirical formula<br/><math>m(F_e)</math> = empirical formula mass</p>                                                                                                                                                                                             | <ul style="list-style-type: none"> <li>This and the previous calculation are often combined together in exam questions</li> </ul>                                                                                                                                    |
| 6. Use mole ratios to determine the number of moles of B that can be made from A | $n(B) = n(A) \cdot \frac{\text{number of B} \in \text{equation}}{\text{number of A} \in \text{equation}}$                                                                                                                                                                                                                                                                                                             | <ul style="list-style-type: none"> <li>The second term in this equation is the mole ratio</li> <li>You must use a fully balanced equation</li> <li>This is the central step in many stoichiometry calculations</li> </ul>                                            |

| Purpose                                                                             | The Calculation                                                                                                                                                                                                                                                                 | Notes                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
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| <b>7.</b> Calculate theoretical yield                                               | 1. Use <b>Calculation 6</b> to determine the expected quantity of product in moles<br>2. Use a rearranged <b>Calculation 3</b> to determine the expected mass.                                                                                                                  | <ul style="list-style-type: none"> <li></li> </ul>                                                                                                                                                                                                                                                                                                                                                                                                                       |
| <b>8.</b> Determine limiting and excess reactants                                   | Divide moles of each reactant by their coefficient in the balanced equation<br>a. Smallest value = limiting<br>b. Largest value = excess                                                                                                                                        | <ul style="list-style-type: none"> <li>You would often then need to combine this with Calculation 6 to determine a quantity of product (in moles).</li> </ul>                                                                                                                                                                                                                                                                                                            |
| <b>9.</b> Calculating percentage yield.                                             | $\text{Yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \cdot 100$                                                                                                                                                                                                 | <ul style="list-style-type: none"> <li>Actual and theoretical yield must have the same units.</li> <li>You might sometimes be required to rearrange this equation, or use it to work backwards from this to find the amount of reactant you started with.</li> </ul>                                                                                                                                                                                                     |
| <b>10.</b> Apply Avogadro's Law to calculate reacting volumes of gases              | $\frac{V_1}{n_1} = \frac{V_2}{n_2}$ <p> <math>V_1</math> = the initial volume of gas<br/> <math>n_1</math> = the initial quantity of gas in moles<br/> <math>V_2</math> = the final volume of gas<br/> <math>n_2</math> = the final volume of gas in moles           </p>       | <ul style="list-style-type: none"> <li>Only applies when temperature and pressure remain constant.</li> <li>Units of V do not matter. But must be the same.</li> <li>This is really a special case of the Ideal Gas Law where the pressure, temperature and gas constant terms cancel each other out.</li> </ul>                                                                                                                                                         |
| <b>11.</b> Calculate molar quantities of gases at standard temperature and pressure | $n = \frac{V}{22.4}$ <p> <math>n</math> = quantity in moles<br/> <math>V</math> = the volume of gas in <math>\text{dm}^3</math><br/>           22.4 is the molar volume of an ideal gas at 273K and 101,000 Pa         </p>                                                     | <ul style="list-style-type: none"> <li>Only applies at standard conditions:               <ul style="list-style-type: none"> <li>273 K (0°C)</li> <li>101,000 Pa (1.00 atm)</li> </ul> </li> <li>If volume of gas is given in <math>\text{m}^3</math>, use <math>2.24 \times 10^{-5}</math> as your molar volume.</li> <li>Molar volumes are given in the data booklet and do not need memorising.</li> </ul>                                                            |
| <b>12.</b> The ideal gas equation                                                   | $PV = nRT$ <p> <math>P</math> = pressure in Pa<br/> <math>V</math> = volume of gas in <math>\text{m}^3</math><br/> <math>n</math> = quantity of gas in moles<br/> <math>R</math> = the gas constant, 8.31<br/> <math>T</math> = temperature in Kelvin (°C + 273)           </p> | <ul style="list-style-type: none"> <li>In practice, you can often use:               <ul style="list-style-type: none"> <li><math>V</math> in units of <math>\text{dm}^3</math></li> <li>Pa in units of kPa</li> </ul> </li> <li>You will need to be comfortable rearranging this equation to change the subject.</li> <li>This takes time to use, so only use it in non-standard conditions, or when the laws in <b>Calculation 13</b> would not be quicker.</li> </ul> |

| Purpose                                                          | The Calculation                                                                                                                                                                                                                                                                                                                                                                                                                                                               | Notes                                                                                                                                                                                                                                                                                                    |
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| <b>13.</b> Relationship between temperature, pressure and volume | <p><b>Charles' Law</b>, at fixed pressure:</p> $\frac{V_1}{T_1} = \frac{V_2}{T_2}$ <p><b>Gay-Lussac's Law</b>, at fixed volume:</p> $\frac{P_1}{T_1} = \frac{P_2}{T_2}$ <p><b>Boyle's Law</b>, at fixed temperature:</p> $P_1 V_1 = P_2 V_2$ <p><math>V_1</math> and <math>V_2</math> are initial and final volume<br/> <math>P_1</math> and <math>P_2</math> are initial and final pressure<br/> <math>T_1</math> and <math>T_2</math> are initial and final temperature</p> | <ul style="list-style-type: none"> <li>These only work where the quantity in moles remains fixed.</li> <li>All of these are just special cases of the ideal gas law, where the remaining terms just cancel each other out.</li> </ul>                                                                    |
| <b>14.</b> Molar Concentration                                   | $c = \frac{n}{V}$ <p><math>c</math> = concentration in mol dm<sup>-3</sup><br/> <math>n</math> = the quantity in moles<br/> <math>V</math> = the volume in dm<sup>3</sup> (litres)</p>                                                                                                                                                                                                                                                                                        | <ul style="list-style-type: none"> <li>Units are pronounced 'moles per decimetre cubed'</li> <li>You need to be able to use any rearrangement of this equation</li> </ul>                                                                                                                                |
| <b>15.</b> Concentration by mass                                 | $c = \frac{m}{V}$ <p><math>c</math> = concentration in g dm<sup>-3</sup><br/> <math>m</math> = the quantity in grams<br/> <math>V</math> = the volume in dm<sup>3</sup> (litres)</p>                                                                                                                                                                                                                                                                                          | <ul style="list-style-type: none"> <li>Units are pronounced 'grams per decimetre cubed'</li> <li>You need to be able to use any rearrangement of this equation</li> <li>Generally, if you have a concentration like this, you should convert it into a molar concentration before proceeding.</li> </ul> |

## Atomic Structure

| Purpose                                                         | The Calculation                                                                                                  | Notes                                                                                                                                                                                                                                                                |
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| <b>16.</b> Determine relative atomic mass from % abundance data | $A_r = \sum \left( \frac{\text{abundance}}{100} \times i \right)$ <p><math>A_r</math> = relative atomic mass</p> | <ul style="list-style-type: none"> <li>% abundance may be given in the question, or you may need to read it from a mass spectrum</li> <li>If you convert the percentages to decimals (i.e. 0.8 for 80%, 0.25 for 25%), there is no need to divide by 100.</li> </ul> |

| Purpose                                                    | The Calculation                                                                                                                                                                                                                                                                                                                                                                                                                         | Notes                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
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| <b>17.</b> Determine % abundance from relative atomic mass | <p>If there are two isotopes, label one of them 'a' and one 'b'.</p> <p>Now:</p> $A_r = \frac{xI_a + yI_b}{x + y}$ <p><math>A_r</math> = relative atomic mass<br/> <math>I_a</math> = the mass of isotope a<br/> <math>I_b</math> = the abundance of isotope b<br/> x and y is the abundance of each isotope</p> <p>However, since <math>x + y = 100\%</math>, <math>y = 100 - x</math> so:</p> $A_r = \frac{xI_a + (100 - x)I_b}{100}$ | <ul style="list-style-type: none"> <li><math>A_r</math>, <math>I_a</math> and <math>I_b</math> will be provided in the question, so you can plug the numbers in, and then rearrange to find x.</li> <li>To find y, simply do <math>y = 100 - x</math></li> <li>If you have three isotopes, you must know the abundance of at least one in order to find the other two. You would also need to subtract the abundance of this one from the 100, before doing the rest of the sum.</li> </ul> |

## Periodicity and Bonding

| Purpose                  | The Calculation | Notes |
|--------------------------|-----------------|-------|
| No calculations. Huzzah! |                 |       |

## Energetics

| Purpose                                                          | The Calculation                                                                                                                                                                                                                                                                                              | Notes                                                                                                                                                                                                                                                                                                                                                                                            |
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| <b>18.</b> Calculating the heat change of a pure substance       | $q = mc \Delta T$ <p>q = the heat change in Joules<br/> m = the mass of substance in grams<br/> c = specific heat capacity in <math>\text{J K}^{-1} \text{g}^{-1}</math><br/> <math>\Delta T</math> = temperature rise in K or <math>^{\circ}\text{C}</math></p>                                             | <ul style="list-style-type: none"> <li>Be careful of the units of mass...you may need to convert kg into g</li> <li>Be careful of the units for specific heat capacity, if it is <math>\text{J K}^{-1} \text{kg}^{-1}</math> you will need to convert your mass into kg.</li> </ul>                                                                                                              |
| <b>19.</b> Calculating an enthalpy change from experimental data | $\Delta H = -mc \Delta T$ <p><math>\Delta H</math> = the enthalpy change in Joules<br/> m = the mass of solution in grams<br/> c = specific heat capacity of water: <math>4.18 \text{ J K}^{-1} \text{g}^{-1}</math><br/> <math>\Delta T</math> = temperature rise in K or <math>^{\circ}\text{C}</math></p> | <ul style="list-style-type: none"> <li>The minus sign is needed to ensure that an exothermic reaction has a negative enthalpy change.</li> <li>Units are <math>\text{J}</math> or <math>\text{kJ mol}^{-1}</math></li> <li>The mass of solution is assumed to be the same as its volume in <math>\text{cm}^3</math>.</li> <li>The specific heat capacity of the reactants is ignored.</li> </ul> |

| Purpose                                                   | The Calculation                                                                                                                                                                                                                                                                                                                                                                                            | Notes                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
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| 20. Calculating $\Delta H_r$ using a Hess cycle           | Once you have produced your Hess cycle:<br>1. Write the relevant $\Delta H$ onto each arrow<br>2. Multiply each $\Delta H$ in accordance with the stoichiometry<br>3. To do your sum, add when you go with an arrow, and subtract when you go against one.                                                                                                                                                 | <ul style="list-style-type: none"> <li>See the 'Energetics' PowerPoint for advice on constructing Hess cycles.</li> </ul>                                                                                                                                                                                                                                                                                                                                                                     |
| 21. Calculating $\Delta H_r$ from average bond enthalpies | <b>Method 1:</b> Make a Hess cycle, then do as in Calculation 20.<br><br><b>Method 2:</b><br>$\Delta H_r = \sum (\text{reactant bonds}) - \sum (\text{product bonds})$                                                                                                                                                                                                                                     | <ul style="list-style-type: none"> <li>It is more reliable to use Hess cycles and you can easily forget whether it is reactants - products or vice versa.</li> <li>Average bond enthalpies can be found in Table 10 of the data booklet.</li> <li>You only need to worry about the bonds that broken and made. If a bond, for example a C-H is present at the start and finish, you can ignore it....this can save time in exams.</li> </ul>                                                  |
| 22. Calculating $\Delta H_r$ from enthalpies of formation | <b>Method 1:</b> Make a Hess cycle, then do as in Calculation 20.<br><br><b>Method 2:</b><br>$\Delta H_r = \sum \Delta H_f^\circ(\text{products}) - \sum \Delta H_f^\circ(\text{reactants})$<br><br>$\Delta H_r = \sum \Delta H_f^\circ(\text{products}) - \sum \Delta H_f^\circ(\text{reactants})$<br><br>$\Delta H_r$ = enthalpy change of reaction<br>$\Delta H_f^\circ$ = enthalpy change of formation | <ul style="list-style-type: none"> <li>It is more reliable to use Hess cycles and you can easily forget whether it is products - reactants or vice versa.</li> <li><math>\Delta H_f^\circ</math> for elements in their standard states is zero.</li> <li><math>\Delta H_f^\circ</math> values for many compounds can be found in Table 11 of the data booklet.</li> <li>In some questions, you may also need to take a state change into account, if standard states are not used.</li> </ul> |

| Purpose                                                                             | The Calculation                                                                                                                                                                                                                                                                                                                            | Notes                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
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| <b>23.</b> Calculating $\Delta H_r$ from enthalpies of combustion                   | <p><b>Method 1:</b> Make a Hess cycle, then do as in Calculation 20.</p> <p><b>Method 2:</b></p> $\Delta H_r = \sum \Delta H_c^\circ(\text{products}) - \sum \Delta H_c^\circ(\text{reactants})$ <p><math>\Delta H_r</math> = enthalpy change of reaction<br/> <math>\Delta H_c^\circ</math> = enthalpy change of combustion</p>           | <ul style="list-style-type: none"> <li>It is more reliable to use Hess cycles and you can easily forget whether it is reactants - products or vice versa.</li> <li><math>\Delta H_c^\circ</math> for <math>\text{CO}_2</math> and <math>\text{H}_2\text{O}</math> is zero.</li> <li><math>\Delta H_c^\circ</math> values for many compounds can be found in Table 12 of the data booklet.</li> </ul>                                                  |
| <b>24.</b> Calculating lattice enthalpy                                             | You need to build a Born-Haber cycle....see the Energetics PowerPoint for help.                                                                                                                                                                                                                                                            |                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| <b>25.</b> Calculating $\Delta S$ from standard entropy values                      | $\Delta S^\circ = \sum S^\circ(\text{products}) - \sum S^\circ(\text{reactants})$ <p><math>\Delta S^\circ</math> = standard entropy change of reaction<br/> <math>S^\circ</math> = standard entropy of each substance</p>                                                                                                                  | <ul style="list-style-type: none"> <li>Units are <math>\text{J K}^{-1} \text{mol}^{-1}</math></li> <li><math>S^\circ</math> values can be found in Table 11 of the data booklet</li> <li>You cannot assume that <math>S^\circ</math> of an element is zero. It is not.</li> </ul>                                                                                                                                                                     |
| <b>26.</b> Calculating $\Delta G_r$ standard Gibb's Free Energy of Formation values | <p><b>Method 1:</b> Make a Hess cycle, then do similar to Calculation 20.</p> <p><b>Method 2:</b></p> $\Delta G_r = \sum \Delta G_f^\circ(\text{products}) - \sum \Delta G_f^\circ(\text{reactants})$ <p><math>\Delta G_r</math> = Gibb's free energy of reaction<br/> <math>\Delta G_f^\circ</math> = Gibb's free energy of formation</p> | <ul style="list-style-type: none"> <li>Units are <math>\text{J}</math> or <math>\text{kJ mol}^{-1}</math></li> <li>It is more reliable to use Hess cycles and you can easily forget whether it is products - reactants or vice versa.</li> <li><math>\Delta G_f^\circ</math> for elements in their standard states is zero.</li> <li><math>\Delta G_f^\circ</math> values for many compounds can be found in Table 11 of the data booklet.</li> </ul> |
| <b>27.</b> Calculating $\Delta G_r$ from experimental data                          | $\Delta G = \Delta H - T \Delta S$ <p><math>\Delta G</math> = Gibb's free energy<br/> <math>\Delta H</math> = Enthalpy change<br/> <math>T</math> = Temperature in Kelvin<br/> <math>\Delta S</math> = Entropy change</p>                                                                                                                  | <ul style="list-style-type: none"> <li>If <math>\Delta H</math> is in <math>\text{kJ mol}^{-1}</math>, you will need to divide <math>\Delta S</math> by 1000 to convert it to units of <math>\text{kJ K}^{-1} \text{mol}^{-1}</math></li> <li>You may first need to calculate <math>\Delta H</math> and <math>\Delta S</math> using <b>Calculations 23 and 24.</b></li> </ul>                                                                         |

# Kinetics

| Purpose                                                            | The Calculation                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | Notes                                                                                                                                                                                                                                                                                                                              |
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| 28. Calculate the rate of a reaction                               | $Rate = \frac{-\Delta[R]}{\Delta t} = \frac{\Delta[P]}{\Delta t}$ <p> <math>\Delta[R]</math> = change in reactant concentration<br/> <math>\Delta[P]</math> = change in product concentration<br/> <math>\Delta t</math> = change in time                 </p>                                                                                                                                                                                                                                               | <ul style="list-style-type: none"> <li>Units are <math>\text{mol dm}^{-3} \text{ s}^{-1}</math></li> <li>The minus sign in front of <math>\Delta[R]</math> is because the concentration of reactants decreases</li> </ul>                                                                                                          |
| 29. Calculate the gradient of a slope                              | $Gradient = \frac{\text{change in } y}{\text{change in } x}$                                                                                                                                                                                                                                                                                                                                                                                                                                                 | <ul style="list-style-type: none"> <li>Used for calculating rate from graph of concentration (y-axis) over time (x-axis)</li> </ul>                                                                                                                                                                                                |
| 30. Determine the order of reaction with respect to a reactant, x. | <ol style="list-style-type: none"> <li>Identify two experiments, where the concentration of 'x' has changed, but all others have remained the same.</li> <li>Compare the change in [x] to the change in rate:                         <ol style="list-style-type: none"> <li>If doubling [x] has no effect on rate, then 0<sup>th</sup> order.</li> <li>If doubling [x] doubles rate, then 1<sup>st</sup> order.</li> <li>If doubling [x] quadruples rate, then 2<sup>nd</sup> order.</li> </ol> </li> </ol> | <ul style="list-style-type: none"> <li>Sometimes, you can't find two cases where only [x] has changed, in which case you may need to take into account the order of reaction with respect to other reactants.</li> </ul>                                                                                                           |
| 31. Deduce a rate expression                                       | $Rate = k[A]^x[B]^y[C]^z$ <p> <math>k</math> = rate constant (see below)<br/> <math>[A/B/C]</math> = concentration of each reactant<br/> <math>x/y/z</math> = order of reaction with respect to each reactant                 </p>                                                                                                                                                                                                                                                                           | <ul style="list-style-type: none"> <li>Reactants with a reaction order of zero can be omitted from the rate equation</li> <li>Given suitable information, you may need to calculate the value of the rate constant if given rates, concentrations and reaction order, or the expected rate given the other information.</li> </ul> |

| Purpose                                                | The Calculation                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | Notes                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
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| <b>32.</b> Determining the units for the rate constant | $\text{Units} = \frac{\text{mol dm}^{-3} \text{ s}^{-1}}{\text{mol}^x (\text{dm}^{-3})^x}$ <ul style="list-style-type: none"> <li>Mol and <math>\text{dm}^{-3}</math> terms on the top and the bottom should be cancelled out</li> <li>Remaining mol and <math>\text{dm}^{-3}</math> terms on the bottom should then be brought to the top by inverting their indices.</li> </ul> <p><math>x</math> = the overall order of the reaction</p>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | <ul style="list-style-type: none"> <li>If you can't understand this, try to memorise: <ul style="list-style-type: none"> <li>0<sup>th</sup> order: <math>\text{mol dm}^{-3} \text{ s}^{-1}</math></li> <li>1<sup>st</sup> order: <math>\text{s}^{-1}</math></li> <li>2<sup>nd</sup> order: <math>\text{mol}^{-1} \text{ dm}^3 \text{ s}^{-1}</math></li> <li>3<sup>rd</sup> order: <math>\text{mol}^{-2} \text{ dm}^6 \text{ s}^{-1}</math></li> </ul> </li> </ul> |
| <b>33.</b> Determining activation energy               | <p>The Arrhenius equation:</p> $k = A e^{\frac{-E_a}{RT}}$ <p>Where:</p> <ul style="list-style-type: none"> <li><math>k</math> = rate constant</li> <li><math>A</math> = Arrhenius constant</li> <li><math>e</math> = exponential constant</li> <li><math>E_a</math> = activation energy</li> <li><math>R</math> = gas constant, 8.31</li> <li><math>T</math> = temperature in Kelvin</li> </ul> <p>This rearranges to:</p> $\ln k = \frac{-E_a}{R} \cdot \frac{1}{T} + \ln A$ <p>Which is basically the equation for a straight line in the form '<math>y=mx+c</math>' where:</p> <ul style="list-style-type: none"> <li>'<math>y</math>' is <math>\ln k</math></li> <li>'<math>x</math>' is <math>1/T</math></li> <li>'<math>m</math>' is <math>-E_a/R</math></li> <li>'<math>c</math>' is <math>\ln A</math></li> </ul> <p>So, if we do a reaction at a range of temperatures and calculate <math>\ln k</math>, then:</p> <ul style="list-style-type: none"> <li>Draw a graph with <math>1/T</math> along the x-axis, and <math>\ln k</math> on the y-axis</li> <li>Draw a straight line of best fit.</li> <li>Determine the gradient of the line</li> <li>Then:</li> </ul> $E_a = -\text{Gradient} \times R$ | <ul style="list-style-type: none"> <li>Units of <math>E_a</math> are <math>\text{kJ mol}^{-1}</math></li> <li>From the graph, you might also be asked to calculate <math>A</math>: <ul style="list-style-type: none"> <li>'<math>\ln A</math>', is the y-intercept of the graph, so simply raise 'e' to the power of this intercept.</li> </ul> </li> </ul>                                                                                                        |



# Equilibrium

| Purpose                                             | The Calculation                                                                                                                                      | Notes                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
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| 34. Determining the equilibrium constant expression | <p>For the reaction:</p> $wA + zB \rightleftharpoons yC + zD$ $K_c = \frac{[C]^y [D]^z}{[A]^w [B]^z}$ <p><math>K_c</math> = equilibrium constant</p> | <ul style="list-style-type: none"> <li>Only applies to reactants for which there is a concentration: <ul style="list-style-type: none"> <li>Aqueous substances are included</li> <li>Solids and pure liquids are omitted as they do not have a concentration per se</li> </ul> </li> <li>For reactions involving gases, use partial pressures instead of concentrations.</li> <li>At SL, you only need be able to construct the expression.</li> <li>At HL, you may need to calculate <math>K_c</math> from the expression and suitable data, or to determine reactant equilibrium concentrations of reactants, given <math>K_c</math> and suitable information.</li> </ul> |

# Acids and Bases

| Purpose                                                | The Calculation                                                                                                                                                                                                   | Notes                                                                                                                                         |
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| 35. Determining changes in $[H^+]$ given changes in pH | <ul style="list-style-type: none"> <li>For each increase of '1' on the pH scale, divide <math>[H^+]</math> by 10.</li> <li>For each decrease of '1' on the pH scale, multiply <math>[H^+]</math> by 10</li> </ul> | <ul style="list-style-type: none"> <li>At SL, you do not need to be able to calculate pH, just to understand it in relative terms.</li> </ul> |

| Purpose                                                                        | The Calculation                                                                                                                                                                                                                                                                                                                                                    | Notes                                                                                                                                                                                                                                                                                                       |
|--------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 36. Deduce $[H^+]$ and $[OH^-]$ given $K_w$                                    | $+ \overset{\cdot}{\underset{\cdot}{H}}$ $- \overset{\cdot}{\underset{\cdot}{OH}}$ $K_w = \overset{\cdot}{\underset{\cdot}{H}} \overset{\cdot}{\underset{\cdot}{OH}}$ <p>So:</p> $+ \overset{\cdot}{\underset{\cdot}{H}}$ $- \overset{\cdot}{\underset{\cdot}{OH}}$ <p>And:</p> $- \overset{\cdot}{\underset{\cdot}{OH}}$ $+ \overset{\cdot}{\underset{\cdot}{H}}$ | <ul style="list-style-type: none"> <li>At standard conditions, <math>K_w = 1.00 \times 10^{-14}</math></li> <li><math>K_w</math> varies with temperature, so it is important to know how to do this calculation.</li> </ul>                                                                                 |
| 37. Calculating pH from $[H^+]$ and vice versa                                 | $+ \overset{\cdot}{\underset{\cdot}{H}}$ $pH = -\log_{10} \overset{\cdot}{\underset{\cdot}{H}}$ $\overset{\cdot}{\underset{\cdot}{H}} = 10^{-pH}$                                                                                                                                                                                                                  | <ul style="list-style-type: none"> <li>With strong acids, you can assume <math>[H^+]</math> is the same as the concentration of the acid (adjusted for the stoichiometry)</li> <li>With weak acids, you will need to calculate <math>[H^+]</math> using <math>K_a</math> or <math>pK_a</math>.</li> </ul>   |
| 38. Calculating pH from $[OH^-]$ and vice versa                                | $- \overset{\cdot}{\underset{\cdot}{OH}}$ $pOH = -\log_{10} \overset{\cdot}{\underset{\cdot}{OH}}$ $\overset{\cdot}{\underset{\cdot}{OH}} = 10^{-pOH}$                                                                                                                                                                                                             | <ul style="list-style-type: none"> <li>With strong bases, you can assume <math>[OH^-]</math> is the same as the concentration of the acid (adjusted for the stoichiometry)</li> <li>With weak acids, you will need to calculate <math>[OH^-]</math> using <math>K_b</math> or <math>pK_b</math>.</li> </ul> |
| 39. Determining $K_a$ and $K_b$ of acids/bases and their conjugate bases/acids | $K_w = K_a \cdot K_b$ <p>So:</p> $K_a = \frac{K_w}{K_b}$ <p>And:</p> $K_b = \frac{K_w}{K_a}$                                                                                                                                                                                                                                                                       | <ul style="list-style-type: none"> <li>This is useful when trying to determine the strength the conjugate base of a weak acid, and the conjugate acid of a weak base.</li> </ul>                                                                                                                            |

| Purpose                                                                                 | The Calculation                                                                                                                                                                                                   | Notes                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|-----------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>40.</b> Determining $pK_a$ and $pK_b$ of acids/bases and their conjugate bases/acids | $pK_w = pK_a + pK_b$ <p>So:</p> $pK_a = pK_w - pK_b$ <p>And:</p> $pK_b = pK_w - pK_a$                                                                                                                             | <ul style="list-style-type: none"> <li>This is useful when trying of determine the strength the conjugate base of a weak acid, and the conjugate acid of a weak base.</li> </ul>                                                                                                                                                                                                                                                                                      |
| <b>41.</b> Determining pH from pOH and vice versa                                       | $pK_w = pK_a + pK_b$ <p>So:</p> $pH = 14 - pOH$ <p>And:</p> $pOH = 14 - pH$                                                                                                                                       | <ul style="list-style-type: none"> <li>This is useful to quickly and easily calculate one of pH/pOH from the other (or <math>[H^+]/[OH^-]</math>).</li> </ul>                                                                                                                                                                                                                                                                                                         |
| <b>42.</b> Calculating pH of a solution of a weak acid                                  | $H^+ + A^- \rightleftharpoons HA$ $K_a = \frac{[H^+][A^-]}{[HA]}$ <p>Since <math>[H^+] = [A^-]</math>:</p> $K_a = \frac{[H^+]^2}{[HA]}$ <p>So:</p> $[H^+] = \sqrt{K_a [HA]}$ <p>Then:</p> $pH = -\log_{10} [H^+]$ | <ul style="list-style-type: none"> <li>We assume that <math>[HA]</math> is equal to the concentration stated in the question, as only a very small amount has dissociated.</li> <li>You may need to work backwards from pH to work out <math>K_a</math>:</li> </ul> $[H^+] = 10^{-pH}$ <p>Then:</p> $K_a = [H^+]^2$ <ul style="list-style-type: none"> <li>You will not need to work out problems for polyprotic weak acids that would require quadratics.</li> </ul> |

| Purpose                                          | The Calculation                                                                                                                                                                                                             | Notes                                                                                                                                                                                                                                                                                                                                |
|--------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 43. Calculating pOH of a solution of a weak base | $B + OH^- \rightleftharpoons BOH + OH^-$ $K_b = \frac{[BOH][OH^-]}{[B]}$ <p>Since <math>[B^+] = [OH^-]</math>:</p> $K_b = \frac{[OH^-]^2}{[B]}$ <p>So:</p> $[OH^-] = \sqrt{K_b [B]}$ <p>Then:</p> $pOH = -\log_{10} [OH^-]$ | <ul style="list-style-type: none"> <li>We assume that <math>[BOH]</math> is equal to the concentration stated in the question, as only a very small amount has dissociated.</li> <li>You may need to work backwards from pOH to work out <math>K_b</math>:</li> </ul> $[OH^-] = 10^{-pOH}$ <p>Then:</p> $K_b = \frac{[OH^-]^2}{[B]}$ |

| Purpose                                                            | The Calculation                                                                                                                                                         | Notes                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
|--------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 44. Determining pH of acidic buffer solutions (and alkali buffers) | $\frac{[H^+]}{[A^-]} = K_a$ <p>Now <math>[H^+]</math> is not equal to <math>[A^-]</math>:</p> <p>So:</p> $[H^+] = K_a \cdot [A^-]$ <p>Then:</p> $pH = -\log_{10} [H^+]$ | <ul style="list-style-type: none"> <li>You may need to use your stoichiometry to calculate the <math>[HA]</math> and <math>[A^-]</math> in the buffer solution first.</li> <li>Since additional <math>A^-</math> is added, we now need to use the concentration of <math>A^-</math> from the buffer as our <math>[A^-]</math>.</li> <li><math>[HA]</math> should either be that stated in the question, or that calculated via stoichiometry, depending on the context.</li> <li>For alkali buffers, do the same process but with <math>OH^-</math>, <math>K_b</math> etc.</li> </ul> |

## Oxidation and Reduction

| Purpose                               | The Calculation                                                                                                                                                                               | Notes                                                                                                                                                                                                                                                                                                                                                                          |
|---------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 45. Calculate $E^\circ_{\text{cell}}$ | $E^\circ_{\text{cell}} = E^\circ(\text{cathode}) - E^\circ(\text{anode})$ <p><math>E^\circ_{\text{cell}}</math> = cell potential<br/> <math>E^\circ</math> = standard electrode potential</p> | <ul style="list-style-type: none"> <li>The value should always be positive, so if you get it the wrong way round, just take off the minus sign.</li> <li><math>E^\circ</math> can be found in the data booklet.</li> <li>You do not need to take the stoichiometry of the reaction into account, just use the <math>E^\circ</math> as they are in the data booklet.</li> </ul> |

## Organic Chemistry

| Purpose                  | The Calculation | Notes |
|--------------------------|-----------------|-------|
| No calculations. Huzzah! |                 |       |

## Measurement and Processing

| Purpose                                                                              | The Calculation                                                                             | Notes                                                                                                                    |
|--------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------|
| <b>46.</b> Calculating relative uncertainties (in %)                                 | $\text{Relative uncertainty} = \frac{\text{absolute uncertainty}}{\text{value}} \times 100$ | <ul style="list-style-type: none"> <li>Large measurements have lower relative uncertainties</li> </ul>                   |
| <b>47.</b> Calculating absolute uncertainty when addition/subtraction is involved    | $\text{Total uncertainty} = \sum (\text{absolute uncertainty})$                             | <ul style="list-style-type: none"> <li>This only works when adding and subtracting values with the same units</li> </ul> |
| <b>48.</b> Calculating relative uncertainty when multiplication/division is involved | $\text{Total uncertainty} = \sum (\text{relative uncertainty})$                             | <ul style="list-style-type: none"> <li>For use when you are multiplying/dividing values with different units</li> </ul>  |

## Human Biochemistry

| Purpose                                                              | The Calculation                                                                                                                                                                                                                                                                                                       | Notes                                                                                                                                                                                            |
|----------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>47.</b> Calculating the energy value of food from combustion data | <p>Use:</p> $q = mc \Delta T$ <p> <math>q</math> = the heat change in Joules<br/> <math>m</math> = the mass of substance in grams<br/> <math>c</math> = specific heat capacity in <math>\text{J K}^{-1} \text{g}^{-1}</math><br/> <math>\Delta T</math> = temperature rise in K or <math>^{\circ}\text{C}</math> </p> | <ul style="list-style-type: none"> <li>You may need to convert the energy value into a value per mole by dividing <math>q</math> by the number of moles of substance burnt.</li> </ul>           |
| <b>48.</b> Calculating iodine numbers                                | $N(I_2) = m(I_2) \cdot \frac{100}{m(\text{lipid})}$ <p> <math>N(I_2)</math> = the iodine number<br/> <math>m(I_2)</math> = the mass of iodine reacting in g<br/> <math>m(\text{lipid})</math> = the mass of lipid involved in g         </p>                                                                          | <ul style="list-style-type: none"> <li>All units should be grams</li> <li>You may need to convert from data involving bromine to an 'iodine equivalent'...just use your stoichiometry</li> </ul> |

| Purpose                                                                  | The Calculation                                                                                                                                                                                                                                                                                                                                                                                                                                                               | Notes                                                                                                                          |
|--------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------|
| 49. Calculate the number of double bonds in a lipid using iodine number. | <p>Calculate the quantity in moles of <math>I_2</math> corresponding to the iodine number:</p> $\frac{I}{\frac{N(I_2)}{M_r(I_2)}} = n(I_2)$ <p>Calculate the quantity in moles of lipid in 100g:</p> $n(lipid) = \frac{100}{M_r(lipid)}$ <p>Then the number of double bonds is:</p> $\frac{n(I_2)}{n(lipid)} = \text{Double bonds}$ <p>Where:<br/> <math>N(I_2)</math> = the iodine number<br/> <math>n</math> = quantities in moles<br/> <math>M_m</math> = molar masses</p> | <ul style="list-style-type: none"> <li>This works because each mole of double bonds reacts with one mole of iodine.</li> </ul> |

## Medicines and Drugs

| Purpose                  | The Calculation | Notes |
|--------------------------|-----------------|-------|
| No calculations. Huzzah! |                 |       |