

**Chemistry of Industry Solutions****1. Atwater System of Caloric Measurement**

The food industry uses the Atwater system to estimate the caloric content of food by adding up the calories in macronutrients such as proteins, carbohydrates, and fats. The system assumes that a gram of carbohydrates and a gram of protein both yield 4 kcals, and one gram of fat yields 9 kcals. You are working for IGotTheCheese Inc., and have been asked to report caloric information using the Atwater system on a new chicken sandwich.

The gram amounts of macronutrients in each of the ingredients for the sandwich are given below.

	<b>Sandwich bun</b>	<b>Chicken breast</b>	<b>1 tablespoon Vegetable Oil</b>
<b>Total Fat (g)</b>	2	4	14
<b>Total Carbohydrates (g)</b>	29	0	0
<b>Total Protein (g)</b>	7	31	0

a) Calculate the number of kcals in one sandwich bun.

$$(2 \text{ g fat})(9 \text{ kcal/g}) + (29 \text{ g carbs})(4 \text{ kcal/g}) + (7 \text{ g protein})(4 \text{ kcal/g}) = 18 + 116 + 28 = 162 \text{ kcal}$$

b) Each ingredient is placed in its own bomb calorimeter, where the ingredient is combusted entirely, and heat energy from the food is perfectly transferred to a surrounding 5000 mL water bath. How much does the water's temperature increase for each food item? (Note: 1 kcal = 1 Calorie. Specific heat of water (C) is  $1 \frac{\text{kcal}}{\text{kg}\cdot^{\circ}\text{C}}$ , and density of water is 1 g/mL. Show all work.

$$\text{Sandwich bun: } 162 \text{ kcal. } \Delta T = \frac{Q}{mC_s} = \left( \frac{162 \text{ kcal}}{5 \text{ kg} \cdot 1 \frac{\text{kcal}}{\text{kg}\cdot^{\circ}\text{C}}} \right) = 32.4 \text{ }^{\circ}\text{C}$$

$$\text{Chicken breast: } 160 \text{ kcal. } \Delta T = 32 \text{ }^{\circ}\text{C}$$

$$\text{Vegetable oil (1 tbsp): } 126 \text{ kcal. } \Delta T = 25.2 \text{ }^{\circ}\text{C}$$

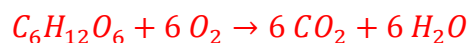
**(This question continues on the next page.)**

- c) The following day, your supervisor, Mike Romahnejer tells you to measure the temperature change in the water of the calorimeter for 1.50 grams of glucose ( $C_6H_{12}O_6$ ; MW = 180 g/mol). To your dismay, the machine breaks, and you are unable to use it anymore to determine energy.
- i. Perform the necessary calculations to show your boss the theoretical change in temperature of the 5000 mL of water in the calorimeter if you had burned the glucose. The heat of combustion of glucose is -2800 kJ/mol. The specific heat of water is  $4.184 \frac{J}{g \cdot ^\circ C}$ , and density is 1 g/mL. Assume that your reaction goes to completion.

$$(1.5 \text{ g glucose}) \left( \frac{1 \text{ mol glucose}}{180 \text{ g glucose}} \right) \left( \frac{2800 \text{ kJ}}{1 \text{ mol glucose}} \right) = 23.33 \text{ kJ released}$$

$$\Delta T = \frac{Q}{mC_s} = \frac{23.33 \times 10^3}{5000 \text{ g} \cdot 4.184 \frac{J}{g \cdot ^\circ C}} = 1.115 \text{ }^\circ C$$

- ii. How many grams of  $CO_2$  will this combustion reaction produce?



$$(1.5 \text{ g glucose}) \left( \frac{1 \text{ mol glucose}}{180 \text{ g glucose}} \right) \left( \frac{6 \text{ mol } CO_2}{1 \text{ mol glucose}} \right) \left( \frac{44 \text{ g } CO_2}{1 \text{ mol } CO_2} \right) = 2.2 \text{ g}$$

**2. Greenhouse Gases**

Global warming has been connected to the presence of greenhouse gases in the atmosphere. Greenhouse gases are molecules that can absorb and re-emit infrared radiation. One way for a molecule to be able to do this is by having a non-zero dipole moment. Many academic and industrial efforts have been focused on taking these gases out of the atmosphere.

- a) Draw the Lewis dot structures for water, nitrogen, and carbon monoxide (CO) and identify which are greenhouse gases and which are not. Explain your reasoning.

Draw the correct the atoms for each of the molecules, lone pairs, assign formal charges, and recognize that water and CO have dipole moments, while nitrogen doesn't (arrow optional). The bent angle in water is very necessary for recognizing its dipole moment! Thus water and CO are greenhouse gases while nitrogen is not.

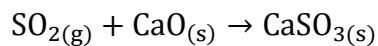


- b) If we took the water molecule and replaced oxygen with sulfur, how would this affect the dipole moment, and why? Support your answer with a discussion of the appropriate periodic trend and the reasoning behind it.

Replacing the oxygen with sulfur would make the dipole moment smaller since sulfur is less electronegative than oxygen. Periodic trend: electronegativity decreases down a row. This is because the valence electrons are an entire subshell further out, meaning they experience a smaller effective nuclear charge due to increased shielding from inner electrons as well as increased distance from the nucleus. This means they are less tightly held, meaning lower electronegativity.

Name (Last, First): \_\_\_\_\_ ID Number: \_\_\_\_\_

- c) Processes that generate major greenhouse gases ( $\text{CO}_2$ ,  $\text{CH}_4$ , etc) also create compounds like sulfur dioxide that contribute to acid rain. One way that companies limit their emissions of sulfur dioxide is by the following reaction:



If an industrial plant produced 100 moles of calcium sulfite last, what is the volume, in liters, of sulfur dioxide (at 1 atm, 298 K) that is kept out of the atmosphere? Assume ideal gas behavior.

100 mol  $\text{SO}_2$  kept out of atmosphere, because 1: 1 ratio

$$V = \frac{nRT}{P} = \frac{(100 \text{ mol}) \left(0.0821 \frac{\text{L} \cdot \text{atm}}{\text{K} \cdot \text{mol}}\right) (298 \text{ K})}{1 \text{ atm}} = 2446.6 \text{ L}$$

**3. Pharma Company**

You're a pharmacist on a product development team at Happy Medicine pharmaceutical company. Your team is working on developing a new line of antacid tablets.

- a) Your team is considering 3 different compounds (shown in the table below) to be used for the product. Considering the cost and the balanced equation for the neutralization reaction for each compound, which compounds would be most cost-effective in neutralizing gastric acid (HCl)? Please show all your work including balanced chemical equations for each neutralization. Assume all reactions go to completion, and there is no need to consider equilibrium.

Compound	Molecular Weight (g/mol)	Cost
Magnesium carbonate	84.313	\$ 0.28 / g
Sodium bicarbonate	84.006	\$ 0.13 / g
Magnesium hydroxide	58.319	\$ 0.12 / g

**Answer A:**

Compound	Chemical Formula	Chemical Reaction
Magnesium Carbonate	$\text{MgCO}_3$	$\text{MgCO}_3(\text{s}) + 2 \text{HCl}(\text{aq}) \rightarrow \text{MgCl}_2(\text{aq}) + \text{H}_2\text{O}(\text{l}) + \text{CO}_2(\text{g})$ <p>Also accept:</p> $\text{MgCO}_3(\text{s}) + 2 \text{H}^+(\text{aq}) + 2 \text{Cl}^-(\text{aq}) \rightarrow \text{Mg}^{2+}(\text{aq}) + 2 \text{Cl}^-(\text{aq}) + \text{H}_2\text{O}(\text{l}) + \text{CO}_2(\text{g})$
Magnesium Hydroxide	$\text{Mg}(\text{OH})_2$	$\text{Mg}(\text{OH})_2(\text{s}) + 2 \text{HCl}(\text{aq}) \rightarrow \text{MgCl}_2(\text{aq}) + 2 \text{H}_2\text{O}(\text{l})$ <p>Also accept:</p> $\text{Mg}(\text{OH})_2(\text{s}) + 2 \text{H}^+(\text{aq}) + 2 \text{Cl}^-(\text{aq}) \rightarrow \text{Mg}^{2+}(\text{aq}) + 2 \text{Cl}^-(\text{aq}) + 2 \text{H}_2\text{O}(\text{l})$
Sodium Bicarbonate	$\text{NaHCO}_3$	$\text{NaHCO}_3(\text{aq}) + \text{HCl}(\text{aq}) \rightarrow \text{NaCl}(\text{aq}) + \text{H}_2\text{O}(\text{l}) + \text{CO}_2(\text{g})$ <p>Also accept:</p> $\text{Na}^+ + \text{HCO}_3^-(\text{aq}) + \text{H}^+(\text{aq}) + \text{Cl}^-(\text{aq}) \rightarrow \text{NaCl}(\text{aq}) + \text{H}_2\text{O}(\text{l}) + \text{CO}_2(\text{g})$

Name (Last, First): \_\_\_\_\_ ID Number: \_\_\_\_\_

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**NOTE:**

- State of matter [(s), (aq), (l), and (g)] aren't necessary as long as right compounds are included in the balanced equation.

Compounds	Molecular Weight	How much compound need for neutralizing one mole of HCl	Cost Effectiveness
Magnesium Carbonate	84.313g/mol	(1 mol MgCO <sub>3</sub> / 2 mol HCl)*(84.313g MgCO <sub>3</sub> / 1 mol MgCO <sub>3</sub> ) = 42.1565g MgCO <sub>3</sub> /1 mol HCl	42.1565g*(\$0.28/g)=\$11.80
Magnesium Hydroxide	58.3188g/mol	(1 mol Mg(OH) <sub>2</sub> / 2 mol HCl)*(58.3188g Mg(OH) <sub>2</sub> / 1 mol Mg(OH) <sub>2</sub> )= 29.1594g Mg(OH) <sub>2</sub> /1 mol HCl	29.1594g*(\$0.12/g)=\$3.50
Sodium Bicarbonate	84.0059g/mol	(1 mol NaHCO <sub>3</sub> /1 mol HCl)*(84.0059g NaHCO <sub>3</sub> / 1 mol NaHCO <sub>3</sub> )= 84.0059g NaHCO <sub>3</sub>	84.0059g*(\$0.13/g)=\$10.92

**Final Answer: Magnesium Hydroxide most cost effective.**

Name (Last, First): \_\_\_\_\_ ID Number: \_\_\_\_\_

- b) If you want one antacid tablet to increase the pH of the stomach contents from 0.9 to 1.5, how many grams of the compound chosen in part (a) should be in each tablet? Model the stomach as a 75 mL solution of HCl. Assume neutralization goes to completion, addition of the pill doesn't cause a significant change in volume, and that after neutralization, further reactions have negligible effect on pH. If you did not obtain an answer for part A, use sodium carbonate ( $\text{Na}_2\text{CO}_3$ ; MW = 105.99 g/mol) as your compound.

If using  $\text{Mg}(\text{OH})_2$  which is the right answer from part A:

Initial condition pH=0.9

$$\text{pH} = -\log[\text{H}^+]$$

$$0.9 = -\log[\text{H}^+]$$

$$[\text{H}^+] = 0.12589\text{M}$$

$$\text{H}^+ \text{ mol} = (0.12589\text{M}) \cdot (0.075\text{L}) = 0.00944\text{mol}$$

Final condition pH=1.5

$$\text{pH} = -\log[\text{H}^+]$$

$$1.5 = -\log[\text{H}^+]$$

$$[\text{H}^+] = 0.0316\text{M}$$

$$\text{H}^+ \text{ mol} = (0.0316\text{M}) \cdot (0.075\text{L}) = 0.00237\text{mol}$$

Change in moles of  $\text{H}^+$  = moles of HCl neutralized

$$\text{Change in mol of H}^+ = 0.00944\text{mol} - 0.00237\text{mol} = 0.00707\text{mol}$$

$$(0.00707 \text{ mol H}^+) \cdot (1 \text{ mol HCl} / 1 \text{ mol H}^+) \cdot (1 \text{ mol Mg}(\text{OH})_2 / 2 \text{ mol HCl}) \cdot (58.3188\text{g Mg}(\text{OH})_2 / 1 \text{ mol Mg}(\text{OH})_2) = \mathbf{0.206\text{g Mg}(\text{OH})_2}$$

If using sodium carbonate:

Initial pH and final pH still same thus mole of HCl neutralized still same as above.

Change in mol of  $\text{H}^+$  = 0.00944mol - 0.00237mol = 0.00707mol = mole of HCl neutralized.

$$(0.00707 \text{ mol H}^+) \cdot (1 \text{ mol HCl} / 1 \text{ mol H}^+) \cdot (1 \text{ mol Na}_2\text{CO}_3 / 2 \text{ mol HCl}) \cdot (105.988\text{g Na}_2\text{CO}_3 / 1 \text{ mol Na}_2\text{CO}_3) = \mathbf{0.375\text{g Na}_2\text{CO}_3}$$

Name (Last, First): \_\_\_\_\_ ID Number: \_\_\_\_\_

- c) If another company has an antacid tablet with 500 mg of calcium carbonate in each tablet, what would be the appropriate amount of active ingredient (basic compound from part b) to have in your tablet to neutralize twice as much HCl as your competitor's tablet?

If using  $\text{Mg}(\text{OH})_2$ :



Chemical equation for  $\text{CaCO}_3$  tablet's neutralization.

Amount of HCl that  $\text{CaCO}_3$  tablet of competitor company =  $(0.500\text{g CaCO}_3) * (1 \text{ mol CaCO}_3 / 100.086\text{g CaCO}_3) (2 \text{ mol HCl} / 1 \text{ mol CaCO}_3) = 0.00999 \text{ mol HCl}$

Since we want to neutralized twice the amount of HCl competitor's tablet can neutralize.  
 $\text{HCl neutralized} = 2 * 0.00999 \text{ mol} = 0.0200 \text{ mol}$

Amount of  $\text{Mg}(\text{OH})_2$  needed to neutralize 0.0200 mol of HCl =  $(0.0200 \text{ mol HCl}) * (1 \text{ mol Mg}(\text{OH})_2 / 2 \text{ mol HCl}) (58\text{g Mg}(\text{OH})_2 / 1 \text{ mol Mg}(\text{OH})_2) = \mathbf{0.583\text{g Mg}(\text{OH})_2}$

If using  $\text{Na}_2\text{CO}_3$ :

Same amount of HCl that needs to be neutralized = 0.0200 mol HCl. (See work above)

Amount of  $\text{CaCO}_3$  needed to neutralize 0.02 mol HCl =  $(0.0200 \text{ mol HCl}) * (1 \text{ mol Na}_2\text{CO}_3 / 2 \text{ mol HCl}) (105.988\text{g Na}_2\text{CO}_3 / 1 \text{ mol Na}_2\text{CO}_3) = \mathbf{1.06\text{g Na}_2\text{CO}_3}$



d) You have decided to titrate the active ingredient (Calcium hydroxide) in the competitor's antacid tablet with 0.1M HCl. The pH of the analyte was taken throughout. The initial pH reading showed that the analyte was indeed basic prior to the titration, but the pH reading at equilibrium point tells you that the solution is slightly basic at the equivalence point. You realize that you have made a mistake and that the solution that was supposed to be HCl is actually not HCl.

1. Explain how you realized that your titrant was not HCl.
2. If there were only 5 other solutions in your cabinet beside HCl, which of the following solutions do you suspect was used as the analyte? Explain your choice.

0.1M HNO<sub>3</sub>   0.1M KBr   0.1M CaO   0.1M HCN   0.1M NaNO<sub>3</sub>

Since HCl and Ca(OH)<sub>2</sub> are a strong acid and strong base. The pH at equilibrium point should be pH=7. The fact that solution was basic at the equilibrium point suggest that the acid used for the titration must have been a weak acid. Out of the 5 solutions that are given, only HCN is a weak acid. Thus, the acid that was used for the titration must have been 0.1M HCN solution.

e) From a foreign country with lax food and drug safety laws, you have obtained a pure sample of an effective but mysterious antacid active ingredient. You dissolve 31.02 g of the compound into 500 g water ( $K_f = 1.86 \text{ }^\circ\text{C/molal}$ ), and the freezing point drops to  $-1.37 \text{ }^\circ\text{C}$ . Assuming the compound is non-volatile and essentially insoluble, suggest how these results lead you to believe that the foreign antacid is using one of the three compounds you were originally considering.

$\Delta t = K_f m$  where  $K_f$  is a freezing point depression constant,  $m$  is molality of the solution, and  $\Delta t$  is change in temperature in Celcius.

$$\Delta t = K_f m$$

$t_{\text{initial}}$  = normal freezing point of water =  $0^\circ\text{C}$

$t_{\text{final}}$  = final freezing point of solution =  $-1.37^\circ\text{C}$

$$\Delta t = 1.37^\circ\text{C}$$

$$K_f = 1.86 \text{ }^\circ\text{C/molal}$$

Thus,  $1.37 \text{ }^\circ\text{C} = (1.86 \text{ }^\circ\text{C/molal}) \cdot (\text{molality of solution})$

Molality of solution = mole of solute / kg of solvent =  $0.73656 \text{ m}$

$0.73656 \text{ m} = x \text{ mole of solute} / 0.500 \text{ kg of water}$

$$x = 0.368 \text{ mol}$$

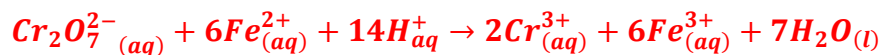
Molar mass =  $31.02 \text{ g} / 0.368 \text{ mol} = 84.29 \text{ g/mol}$

Molar mass closest to Magnesium carbonate. Thus, conclude that the mysterious substance must be Magnesium carbonate.

**4. Chromium Water Toxicity**

In a study of major city drinking water quality, St. Louis' water treatment plants have been found to have the second highest chromium (VI) levels at an average of 1.21 ppb.<sup>1</sup> Chromium (VI) in large amounts is considered dangerous (levels in St. Louis water fall well within safe levels) while chromium (III) is an essential nutrient.<sup>2</sup> You have been hired as a water treatment specialist to remove the chromium (VI) through a process called electrocoagulation. This requires a redox reaction with iron cathodes and anodes. (Note: this problem has been simplified from the actual electrocoagulation reactions, but the fundamental principles are the same).

- a) Suppose the reaction is to be run at a low pH. Write the balanced redox reaction that will be employed to convert chromium (VI) to chromium (III). The reactants are  $Cr_2O_7^{2-}(aq)$  and  $Fe^{2+}(aq)$  and the products are  $Cr^{3+}(aq)$  and  $Fe^{3+}(aq)$ . Also identify which species is the oxidizing agent and which species is the reducing agent.



**Oxidizing agent is dichromate (1/2 point) and reducing agent is iron (II) (1/2 point).**

**1 point for overall reaction with correct stoichiometry.**

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<sup>1</sup>[http://www.stltoday.com/news/local/metro/tests-show-presence-of-potential-carcinogen-in-st-louis-area/article\\_8ce95670-7dda-551c-a389-71881703e8f0.html](http://www.stltoday.com/news/local/metro/tests-show-presence-of-potential-carcinogen-in-st-louis-area/article_8ce95670-7dda-551c-a389-71881703e8f0.html)

<sup>2</sup><http://pubs.acs.org/doi/abs/10.1021/es050486p>

Name (Last, First): \_\_\_\_\_ ID Number: \_\_\_\_\_

- b) Use the following standard redox potential values to determine if the standard reaction is favorable. Note: the full reactions have been removed to not spoil problem 1. Show your work.

Reaction	E (Volts)
$Cr_2O_7^{2-} \rightarrow Cr^{3+}$	1.33
$Fe^{3+} \rightarrow Fe^{2+}$	0.771

Use  $\Delta G = -nF(E_{oxidant} - E_{reductant})$  (1 point), or see that  $E_{oxidant} - E_{reductant}$  is negative (-0.771-1.33) (1 point), delta G will be positive thus reaction will **not be favorable** (1 point). No credit for multiplying potential with stoichiometric coefficients.

- c) Calculate the average concentration of chromium (VI) in St. Louis' water in units of molality. Assume all of the chromium (VI) is in the form of dichromate and the density of water is 1 kg/L. Molar mass of Cr is 52 g/mol, and for oxygen it is 16 g/mol. (2 points )

$$\frac{1.21 \text{ g}}{10^9 \text{ g of water}} * \frac{1 \text{ mol dichromate}}{216 \text{ grams dichromate}} * \frac{1000 \text{ g}}{1 \text{ kg}} * \frac{1 \text{ kg}}{1 \text{ L}} = 5.6 * 10^{-9} \text{ molal}$$

(partial credit for one arithmetic error)

- d) Suppose we want to calculate the electrical potential of the dichromate reaction to chromium (III) using the concentration calculated in part 3. Assume a pH of 6 and a chromium (III) concentration of  $9 \times 10^{-20}$  molality. What is the new electric potential? Is the overall reaction the same favorability as before? (assume the iron reaction is still under standard conditions and concentrations).

Use Nernst equation (2 points), 1 point for correct potential

$$E_H = 1.33 - 0.059 \log \left( \frac{(5.6 * 10^{-9})^2}{(10^{-6})^{14} (9 * 10^{-20})} \right) = -1.865$$

Now the delta G will be negative (1 point), meaning the reaction is favorable (1 point)

Name (Last, First): \_\_\_\_\_ ID Number: \_\_\_\_\_

- e) Suppose you have run the electrocoagulation process at 3 milliamps for 8 minutes and have converted 0.00010 grams of the  $\text{Fe}_{(\text{aq})}^{2+}$  to  $\text{Fe}_{(\text{aq})}^{3+}$ . What is the efficiency of running this electrocoagulation time? HINT: calculating efficiency is identical to calculating % yield, as in from a lab experiment producing a certain compound.

Need to use the following equation (2 points), (1 point for correct theoretical mass)

$$m_{\text{theoretical}} = \frac{ItM}{zF} = \frac{(3 \text{ milliamps})(480 \text{ seconds}) \left(55.845 \frac{\text{g}}{\text{mol}}\right)}{(6 e^-) \left(98485 \frac{\text{C}}{\text{mol}}\right)} = 0.000136 \text{ g}$$

Where  $m$  is the mass of metal removed,  $I$  is the current,  $M$  is the molecular weight of the metal,  $z$  is the number of electrons transferred, and  $F$  is the Faraday constant (96485 C/mol).

$$\eta = \frac{\text{actual}}{\text{theoretical}} = \frac{0.10 \text{ g}}{0.136 \text{ g}} = 73.5 \%$$

1 point for coming up with efficiency equation, 1 point for correct efficiency value