Theoretical Results Using Stoichiometry Solution Guide

Before conducting the experiment, the theoretical quantities for the carbon dioxide produced can be determined using stoichiometry, as described below.

From the Introduction/Motivation section of the activity, we know that:

In the presence of water, citric acid [$C_6H_8O_7$] and sodium bicarbonate [$NaHCO_3$] (aka baking soda) react to form sodium citrate [$Na_3C_6H_5O_7$], water, and carbon dioxide [CO_2]

$$C_6H_8O_7 + 3NaHCO_3 \longrightarrow Na_3C_6H_5O_7 + 3H_2O + 3CO_2$$

From this information, we know that 1 molecule of citric acid reacts with 3 molecules of sodium bicarbonate to produce 3 molecules of carbon dioxide.

We can then look up (or calculate) the following molecular weights:
$C_6H_8O_7$ (citric acid; CA): 192.12 g/mol
$NaHCO_3$ (sodium biocarbonate; SB): 84.007 g/mol
CO_2 (carbon dioxide): 44.01 g/mol
$Na_3C_6H_5O_7$ (carbonic acid is 62.03 g/mol

Now, we can calculate the following theoretical results to answer questions 1 and 2 on the Exposed Reaction Worksheet, page 5):

Group A:
1 g CA, 2.6g SB
1 g CA x (1 mol CA/192.12 g CA) = 0.0052 mol CA
2.6 g SB x (1 mol SB/ 84.007g SB) = 0.0309 mol SB

Therefore, CA is the limiting reactant, and the reaction will produce 3 x 0.0052 mol CO_2 = 0.0156 mol CO2 x 44.01 g/mol CO2 = **0.687 grams CO_2**

(Note: since CA is the limiting reactant, ***in theory***, all CA will be used up, but some SB will remain once the reaction has occurred.)

Group B:
4 g CA, 5.2 g SB
4 g CA x (1 mol CA/192.12 g CA) = 0.0208 mol CA
5.2 g SB x (1 mol SB/ 84.007g SB) = 0.0619 mol SB

Therefore, SB is the limiting reactant, and the reaction will produce 0.0619 mol CO_2 x 44.01 g/mol CO_2 = **2.724 grams CO_2**

(Note: in this case, ***in theory***, SB should all be used up, and almost all of the CA will also be used up; theoretically, we expect only about 0.032 g CA left over.)

Group C:
2 g CA, 5.2 g SB
2 g CA x (1 mol CA/192.12 g CA) = 0.0104 mol CA
5.2 g SB x (1 mol SB/ 84.007g SB) = 0.0619 mol SB

Therefore, CA is the limiting reactant, and the reaction will produce 3 x 0.0104 mol CO_2 = 0.0312 mol CO_2 x 44.01 g/mol CO_2 = **1.374 grams CO_2**

(Note: since CA is the limiting reactant, ***in theory***, all CA will be used up, but some SB will remain once the reaction has occurred.)

Group D:
6 g CA, 7.8 g SB
6 g CA x (1 mol CA/192.12 g CA) = 0.0312 mol CA
7.8 g SB x (1 mol SB/ 84.007g SB) = 0.0928 mol SB

Therefore, SB is the limiting reactant, and the reaction will produce 0.0928 mol CO_2 x 44.01 g/mol CO_2 = **4.084 grams CO_2**

(Note: in this case, ***in theory***, SB should all be used up, and almost all of the CA will also be used up; theoretically, we expect only about 0.051 g CA left over.)

How can we explain differences between theoretical results and actual results? We expect that experimental results for grams of CO_2 will be **lower** than these theoretical values, because it is possible that not all the CO_2 produced will be collected and it is possible that not all of the limiting reactant will react to produce the theoretical product quantities.

In Table 3 on page 6, students use the **experimental results** above to calculate costs. Using the **theoretical values**, we expect the results to be:

Group A: $0.09
Group B: $0.12
Group C: $0.08
Group D: $0.23

Thus, we predict that the reaction performed by Group D will be the most profitable.

Bonus question: *Is there any way to calculate how much carbonic acid is in the CO_2 stream?*

The theoretical quantities of carbonic acid produced in each reaction can be determined mathematically, in the same way we've provided theoretical values for carbon dioxide produced in each reaction. For every 3 molecules of carbon dioxide produced, 1 molecule of carbonic acid should be produced. The molecular weight for carbonic acid is 62.03 g/mol. Therefore:

For Group A: In theory, 0.0156 mol CO_2 will be produced.

0.0156 mol CO_2 x (1 mol carbonic acid/3 mol CO_2) = 0.0052 mol carbonic acid x 62.03 g/mol carbonic acid = 0.323 g carbonic acid

For Group B: In theory, 0.0619 mol CO_2 will be produced.

0.0619 mol CO_2 x (1 mol carbonic acid/3 mol CO_2) = 0.0206 mol carbonic acid x 62.03 g/mol carbonic acid = 1.28 g carbonic acid

For Group C: In theory, 0.0312 mol CO_2 will be produced.

0.0312 mol CO_2 x (1 mol carbonic acid/3 mol CO_2) = 0.0104 mol carbonic acid x 62.03 g/mol carbonic acid = 0.645 g carbonic acid

For Group D: In theory, 0.0928 mol CO_2 will be produced.

0.0928 mol CO_2 x (1 mol carbonic acid/3 mol CO_2) = 0.0309 mol carbonic acid x 62.03 g/mol carbonic acid = 1.92 g carbonic acid

Alternatively, students could determine the moles of CO_2 produced by dividing the grams of CO_2 they measure experimentally by the molecule weight of CO_2 (44.01 g/mol) and then use that resulting number of moles of CO_2 produced in the calculations above to determine the grams of carbonic acid that should have been produced in their experiments. This option makes the results based more on experimental results and not just theory and ideal stoichiometry.