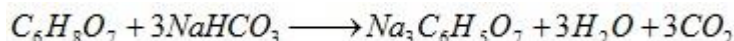


Theoretical Results Using Stoichiometry **Solution Guide**

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 [C₆H₈O₇] and sodium bicarbonate [NaHCO₃] (aka baking soda) react to form sodium citrate [Na₃C₆H₅O₇], water, and carbon dioxide [CO₂]



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:

C₆H₈O₇ (citric acid; CA): 192.12 g/mol

NaHCO₃ (sodium bicarbonate; SB): 84.007 g/mol

CO₂ (carbon dioxide): 44.01 g/mol

Na₃C₆H₅O₇ (sodium citrate): 238.07 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 CO₂ = 0.0156 mol CO₂ x 44.01 g/mol CO₂ = **0.687 grams CO₂**

(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 CO₂ x 44.01 g/mol CO₂ = **2.724 grams CO₂**

(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 CO₂ = 0.0312 mol CO₂ x 44.01 g/mol CO₂ = **1.374 grams CO₂**

(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

$6 \text{ g CA} \times (1 \text{ mol CA}/192.12 \text{ g CA}) = 0.0312 \text{ mol CA}$

$7.8 \text{ g SB} \times (1 \text{ mol SB}/84.007 \text{ g SB}) = 0.0928 \text{ mol SB}$

Therefore, SB is the limiting reactant, and the reaction will produce $0.0928 \text{ mol CO}_2 \times 44.01 \text{ g/mol CO}_2 = \mathbf{4.084 \text{ grams CO}_2}$

(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 CO₂ will be **lower** than these theoretical values, because it is possible that not all the CO₂ 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 CO₂ 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 CO₂ will be produced.

$0.0156 \text{ mol CO}_2 \times (1 \text{ mol carbonic acid}/3 \text{ mol CO}_2) = 0.0052 \text{ mol carbonic acid} \times 62.03 \text{ g/mol carbonic acid} = 0.323 \text{ g carbonic acid}$

For Group B: In theory, 0.0619 mol CO₂ will be produced.

$0.0619 \text{ mol CO}_2 \times (1 \text{ mol carbonic acid}/3 \text{ mol CO}_2) = 0.0206 \text{ mol carbonic acid} \times 62.03 \text{ g/mol carbonic acid} = 1.28 \text{ g carbonic acid}$

For Group C: In theory, 0.0312 mol CO₂ will be produced.

$0.0312 \text{ mol CO}_2 \times (1 \text{ mol carbonic acid}/3 \text{ mol CO}_2) = 0.0104 \text{ mol carbonic acid} \times 62.03 \text{ g/mol carbonic acid} = 0.645 \text{ g carbonic acid}$

For Group D: In theory, 0.0928 mol CO₂ will be produced.

$0.0928 \text{ mol CO}_2 \times (1 \text{ mol carbonic acid}/3 \text{ mol CO}_2) = 0.0309 \text{ mol carbonic acid} \times 62.03 \text{ g/mol carbonic acid} = 1.92 \text{ g carbonic acid}$

Alternatively, students could determine the moles of CO₂ produced by dividing the grams of CO₂ they measure experimentally by the molecule weight of CO₂ (44.01 g/mol) and then use that resulting number of moles of CO₂ 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.