

## **Bomb Calorimetry: Heat of Combustion of Naphthalene and Sucrose**

Mary Grace Sanders

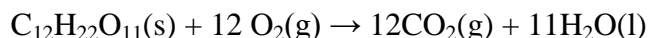
Lab Partners: Alex Schoening-Hudson,  
Brittney Westermeyer, Jessica Withey

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## **Introduction**

The purpose of this lab was to determine the standard heat of combustion of the common hydrocarbon sucrose ( $C_{12}H_{22}O_{11}$ ). Since sucrose produces known products under specific conditions we can measure heat flow associated with a controlled and stoichiometrically known reaction. The important reaction for the experiment is:



A bomb calorimeter was the apparatus used to run the experiment. When the sample is a solid, which was used in this experiment, it is put into the bomb in the form of a compressed pellet. The combustion is triggered by sending an electric current through a thin-gauge nickel-chromium wire that touches the top of the pellet. This becomes very hot when current (voltage source ~20VAC) passes through it. The hot wire causes the sample to ignite in the presence of the high  $O_2$  pressure.

## **Experimental Method**

The experimental method began with calibration of the bomb calorimeter. The combustion is carried out inside the bomb and the container in which the bomb is inside is called the bucket. Thick-walled stainless steel that is capable of withstanding a lot of stress makes up the bomb. The bucket does not allow heat exchange and contains a known quantity of water. The temperature of the calorimeter bucket is determined by using a calibrated mercury thermometer, which is highly precise. When used with a magnifying glass, this thermometer can be read to  $\pm 0.01^\circ C$ . The heat released by the reaction is absorbed by the calorimeter. For any substance:

$$q = C\Delta T \quad (1)$$

With this equation, we can know the heat capacity of the calorimeter and the total temperature change it undergoes in order to determine the amount of heat released from the previous stated chemical reaction. We also need to use the chemical standard, a known amount of pure substance having a known heat of combustion, which is ignited in the calorimeter. The calorimeter heat capacity is measured,  $C_{cal}$ , and can be obtained from:

$$C_{cal} = q_{tot}/\Delta T \quad (2)$$

$q_{tot}$  is the total amount of heat liberated in the calorimeter from combustion. This provides the conversion between the measured temperature change and the absolute heat from that caused that temperature rise in the calorimeter. The mass of the bomb (~8 kg) and the mass of the water surrounding the bomb in the bucket (~2 kg) prove to be the most significant component of the calorimeter.

The heat released by the combustion from the nichrome wire and the heat associated with the formation of the product must be considered experimental correction terms. The amount of product (acid) produced can be found by titrating.

Calculation of heat flow is also important, in carrying out a combustion reaction, heat flow is expressed as:

$$q_{\text{total}} = q_{\text{m}}m + q_1 + q_2 \quad (3)$$

$q_{\text{m}}m$  is the heat liberated by the combustion of the sample and  $q_1 + q_2$  are the correctional terms mentioned earlier.  $q_1$  is obtained by measuring the change in the length of the nichrome wire before and after ignition and multiplying this value by the conversion factor, which is provided by the manufacturer  $9.6 \text{ J cm}^{-1}$ ; therefore:

$$q_1 = 9.6 \text{ J/cm} (L_o - L) \quad (4)$$

The bomb was purged with  $\text{O}_2$  before combustion, eliminating a lot of air. This eliminates the second correctional term. The equation becomes:

$$C_{\text{cal}} = q_{\text{total}}/\Delta T = q_{\text{m}}m + [9.6 \text{ J/cm} (L_o - L)] + \sim 0/\Delta T \quad (5)$$

Solving for the  $q_{\text{m}}m$  term we can get the total amount of heat liberated by the combustion reaction and gives us:

$$q_{\text{m}}m = C_{\text{cal}} \Delta T - [9.6 \text{ J/cm} (L_o - L)] \quad (6)$$

Earlier, the stoichiometry of the reaction was considered and displayed. If that is known we can use the definition of  $\Delta H$

$$\Delta H = \Delta E + \Delta(PV) \rightarrow \Delta H = \Delta E + V\Delta P \text{ (at constant volume)} \quad (7)$$

There is a change in pressure so we can see:

$$\Delta H = \Delta E + V (\Delta nRT/V) = \Delta E + \Delta nRT \quad (8)$$

Calculation of the change in T is also important, it is also the least precise quantity that is directly measured in the experiment. When the temperature is taken, it is taken every 1 minute for 5 minutes and then every 30 seconds until it levels off.  $\Delta T$  is determined from:

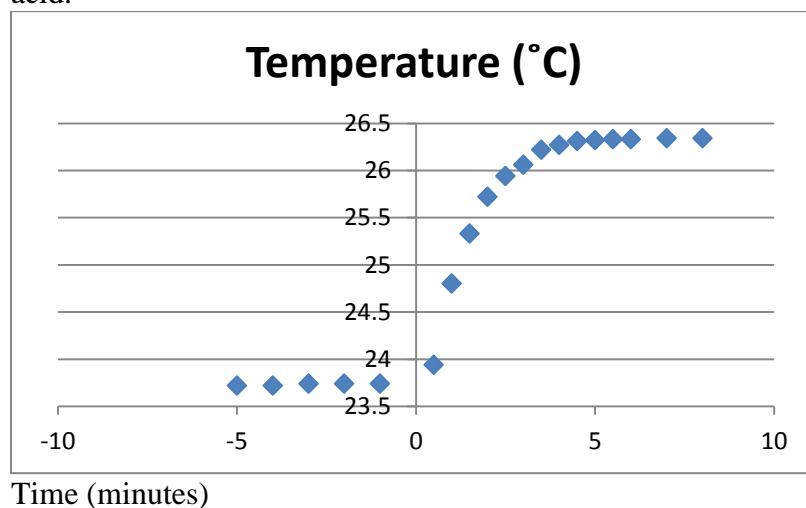
$$\Delta T = T_c - T_a - r_1 (b-a) - r_2 (c-b)$$

In the procedure the bomb calorimeter is first calibrated using 0.1 mg of 1-g benzoic acid pellet. Then the 10-cm length of nichrome ignition wire is connected to the bomb electrodes (not touching the fuel capsule in any way, only touching the top of the pellet. Water will be placed inside the bomb for condensation and the professor will purge the bomb with  $\text{O}_2$  before combustion (as stated earlier). Voltage will be applied creating the combustion to begin and the temperature will be measured in the way discussed previously. Two standardization runs will be run to insure internal consistency, using the benzoic acid. Next, sucrose will be run twice and the results will be checked for consistency.

The other group will run naphthalene twice, but since only one bomb calorimeter worked for our lab group we will just focus on sucrose. Also, the lab was very warm, with the heater near the lab table the experiment was performed on.

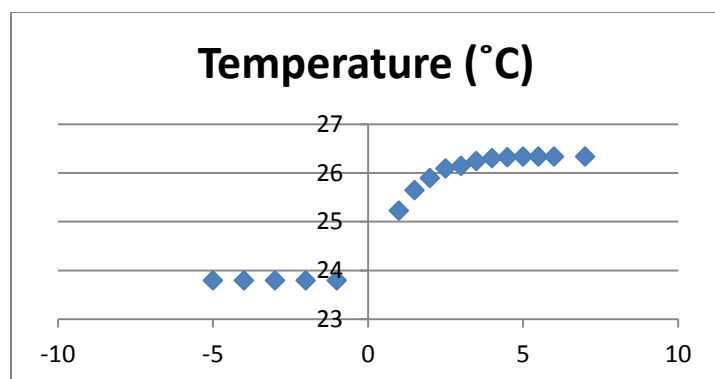
### Results and Calculations

Figure 1: Temperature change over time (thermogram) of the first combustion run of benzoic acid.



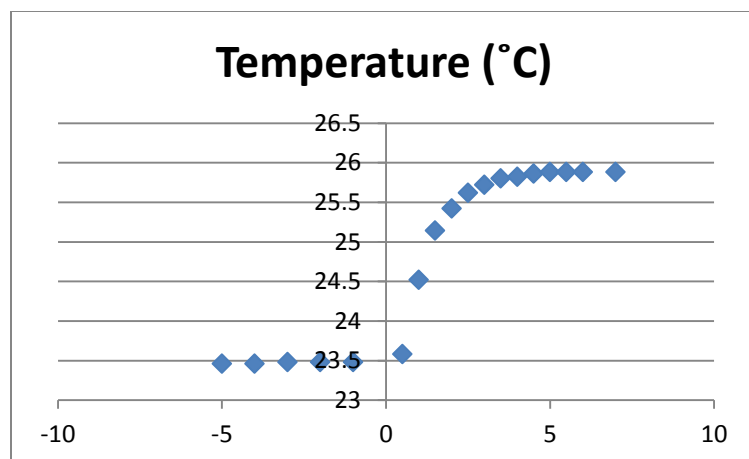
The wire length was 3.1 after the combustion reaction.

Figure 2: Temperature change over time of the second combustion run of benzoic acid.



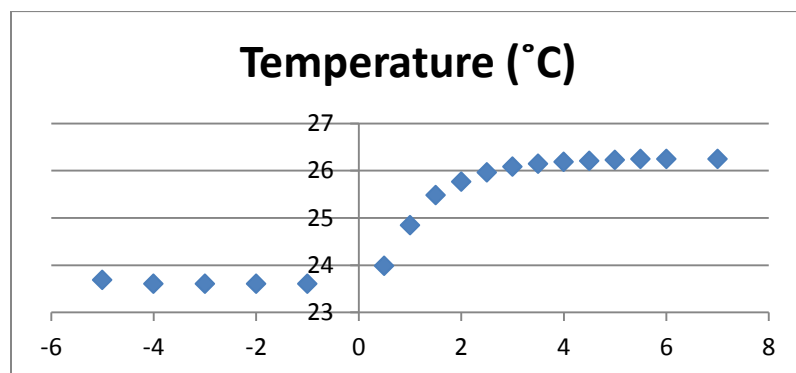
The wire length was 4.4 cm after the combustion. The two runs were very similar.

Figure 3: The temperature over time of the first sucrose combustion run.



The wire length was 5.3 cm after combustion and the beginning weight of sucrose was 1.5 g.

Figure 4: The temperature over time of the second sucrose combustion run.



The wire length was 3.3 cm after combustions and the beginning weight of the sucrose was 1.6 g.

The total amount of heat liberated for each benzoic acid tablet was 26,434 J. This was attained from  $q_{mM} = (1 \text{ g})(26.434 \text{ kJ/g}) = 26.434 \text{ kJ}$  or 26,434 J.

From this calculation, the heat capacity of the bomb calorimeter can be found.

$$C_{\text{cal}} = q_{\text{total}}/\Delta T = q_{mM} + [9.6 \text{ J/cm} (L_o - L)] + \sim 0/\Delta T \text{ so,}$$

$$C_{\text{cal}} = (26,434\text{J} + [9.6 \text{ J/cm}(10-3.1 \text{ cm})])/2.62^\circ\text{C}$$

$$C_{\text{cal}} = 10,112.60 \text{ J/C}^\circ$$

$$C_{\text{cal}} = (26,434\text{J} + [9.6 \text{ J/cm}(10-4.4\text{cm})])/2.54^\circ\text{C}$$

$$C_{\text{cal}} = 10,428.25 \text{ J/C}^\circ$$

The heat of combustion for the sucrose can be found by using the equation:

$$q_{mM} = C_{\text{cal}} \Delta T - [9.6 \text{ J/cm} (L_o - L)].$$

$$q_{mM} = 10,114.60 (2.62) - [9.6\text{J/cm}(10-3.1)]$$

$$q_{mm} = 26,434.012 \text{ J}$$

$$q_{mm} = 10,428.25 (2.54) - [9.6 \text{ J/cm} (10-4.4)]$$

$$q_{mm} = 26,433.995 \text{ J}$$

Next, the  $\Delta E_{\text{combustion}}$  and the  $\Delta H_{\text{combustion}}$  can be determined. By using the stoichiometric equation and  $\Delta H = \Delta E + \Delta nRT$  we can do this.

$$\text{CO}_2 = 393.5, \text{H}_2\text{O} = -285.8 \text{ and } \text{C}_{12}\text{H}_{22}\text{O}_{11} = -5,652 \text{ kJ/mol}$$

$$\Delta H = 26,434.012 \text{ J} + ((-2213.8)(8.314)(276.54)) ???$$

$$\Delta H = 5, 116,300.163 \text{ J}$$

$$\Delta H = 26,433.995 \text{ J} + ((-2213.8)(8.314)(276.62))$$

$$\Delta H = 5, 064,904.599 \text{ J}$$

CRC handbook standard combustion enthalpy for sucrose was -2,226,100 J/mol.

$$((\text{my result} - \text{accepted}) / \text{Accepted})(100) = \% \text{ error}$$

$$((-5,078,121.596 - 2,226,100) / 2,226,100) \times 100 = 128 \% \text{ error}$$

$$\Delta H = 43,260 \text{ J} + ((8.459 \text{ mol})(8.314)(298 \text{ K}))$$

$$\Delta H = 64,217.78$$

### Discussion

The percent error was 128%. This means my calculations went wrong somewhere, but there was error in the problem. There were two potential sources of error in this experiment. The first was in the approximation for calculating the change in temperature. If we calculated the temperature to be high that would lower the heat capacity in the calculation and therefore in the heat liberated equation that would be off, decreasing that too. This would cause a higher percent error in the end calculations. If the temperature were approximated too low, the opposite would occur. If the nitrogen was not removed from the bomb when it was purged with oxygen the calculations would also be off. This error would have to be considered in the heat capacity equation as  $q_2$ . Without this number included the calculations would have further errors. During the lab itself, the room became very hot. The heater was right next to the equipment being used in the lab. This could cause the approximated temperature change be measured incorrectly causing the percent error to increase.