

# Strain Energy in Organic Compounds - Bomb Calorimetry

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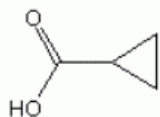
**Goal:** Bomb calorimeter measurements are presented for cyclopropanecarboxylic acid and 1,4-cyclohexane-dicarboxylic acid and the heat of combustion is determined for both compounds. Students are then guided to learn about strain energy by comparing the results obtained for these two compounds.

**Prerequisites:** An introductory knowledge of thermal chemistry and calorimeter measurement and analysis.

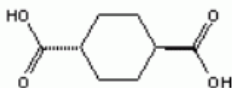
**Resources you will need:** While the calculations associated with this exercise can be carried out by hand, you are encouraged to use a software environment that is capable of data manipulation.

## Background:

Cyclopropanecarboxylic acid and 1,4-cyclohexane-di-carboxylic acid have the same empirical formula ( $C_2H_3O$ ), but different molecular formulas ( $C_4H_6O_2$  for cyclopropanecarboxylic acid;  $C_8H_{12}O_4$  for 1,4-cyclohexane-di-carboxylic acid); the former has a three-ring aliphatic cyclic chain while the later has a six-ring aliphatic cyclic chain. The molar mass of 1,4-cyclohexane-di-carboxylic acid is twice as much as cyclopropanecarboxylic acid. The structures of these two compounds are shown below:



(Cyclopropanecarboxylic acid)



(1,4, Cyclohexane-di-carboxylic Acid, Trans-)

If the heat of formation and combustion of 1,4, cyclohexane-di-carboxylic acid differ from twice as those of cyclopropanecarboxylic acid, the difference provides information regarding the structural stabilities of these two compounds.

## Experimental Data:

Heats of combustion of cyclopropanecarboxylic acid and 1,4 cyclohexane-di-carboxylic acid were obtained using an adiabatic bomb calorimeter. The calorimeter is initially calibrated with a known amount of benzoic acid having a known amount of heat of combustion,  $Q_m = 26414 \pm 3$  J/g. The temperature rise is measured, and the calorimeter heat capacity,  $C$ , is obtained from:

$$C = Q_{tot} / \Delta T. \quad (1)$$

Both the heat of combustion of benzoic acid and the heat released by the combustion of the nichrome wire contribute to  $Q_{tot}$ , and therefore the heat due to combustion of the wire must be subtracted from  $Q_{tot}$  to obtain accurate results for the compound under investigation. Thus, we have:

$$Q_{tot} = Q_m m + q_1. \quad (2)$$

$q_1$  is obtained by measuring the change in length of the nichrome fuse after ignition and multiplying this value by the conversion factor. For the No.34 - gauge nichrome wire used in this experiment, this value is 9.6 J/cm; hence

where  $L_0$  and  $L$  are the initial and final lengths of the nichrome fuse, respectively, in centimeters,

$$q_1 = 9.6(L_0 - L) \quad (3)$$

Once the calibration was carried out, two trials were conducted for each compound in question. In the case of the 1,4-cyclohexane-dicarboxylic acid, a pellet of approximately 1 gram mass was created and the same procedure used to calibrate the bomb was followed again to measure the temperature change associated with the combustion of the compound. For the cyclopropanecarboxylic acid trials a benzoic acid pellet of .7 -.8 gram mass was made, and liquid cyclopropanecarboxylic acid was pipette onto it until the mass of the pellet and solution was approximately 1 gram. The following data were obtained in the physical chemistry laboratory of UW-Green Bay.

Sample	$\Delta T$ (K)	$(L_0 - L)$ - (cm)	Mass- (gm)
Benzoic Acid (trial #1)	2.50	3.5	0.9938
Benzoic Acid (trial #2)	2.50	3.8	0.9940
1,4-cyclohexane-dicarboxylic acid (trial #1)	2.10	5.8	0.9950
1,4-cyclohexane-dicarboxylic acid (trial #2)	2.05	5.7	0.9980
cyclopropanecarboxylic acid (dropped on benzoic acid pellet), (trial #1)	2.40	5.3	0.3046 gm (on 0.6892 gm benzoic acid pellet)
cyclopropanecarboxylic acid (dropped on benzoic acid pellet), (trial #2)	2.41	6.6	0.2082 gm (on 0.7751 gm benzoic acid pellet)

### Exercise:

- Using the benzoic acid data, calculate the heat capacity of the calorimeter using Equations (1-3).
- Is the heat of combustion of benzoic acid,  $Q_m = 26414 \pm 3$  J/g, shown in the Experimental Data Section above, a  $\Delta E$  (an internal energy change of combustion), or a  $\Delta H$  (enthalpy change of combustion)? Give your reason. You can check your answers from the following website: [webbok.nist.gov](http://webbok.nist.gov).
- What is the relationship between  $\Delta H$  and  $\Delta E$  for benzoic acid, for 1,4-cyclohexane-di-carboxylic acid, and for cyclopropanecarboxylic acid?
- Calculate the heat of combustion ( $\Delta H$ ) for 1,4-cyclohexane-di-carboxylic acid based on the calibration data of benzoic acid.
- Since liquid specimens of cyclopropanecarboxylic acid were pipeted into a known amount of benzoic acid and both benzoic acid and the liquid sample were combusted together in the calorimeter, the resulting temperature rise of the calorimeter came from both sources. Based on this information, calculate the heat of combustion ( $\Delta H$ ) of cyclopropanecarboxylic acid.

6. Write a three paragraph essay to discussing the heats of combustion data of both cyclopropanecarboxylic acid and 1,4-cyclohexane-di-carboxylic acid and what your results imply about the relative structural stabilities of these two compounds.

Suggestions for improving this web site are welcome. You are also encouraged to submit your own data-driven exercise to this web archive. All inquiries should be directed to the curator: Tandy Grubbs, Department of Chemistry, Unit 8271, Stetson University, DeLand, FL 32720.

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