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Application of Matlab in the thermochemical studies of some organic compounds

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ABSTRACT

Thermochemical studies of some organic compounds have been done in the present communication. The enthalpy of combustion values, ΔH_c, of the compounds have been determined experimentally by measuring temperature rise per gram of the sample and obtaining the time-temperature plot by the application of Matlab. These data have been used in the calculation of standard enthalpies of formation of the compounds, ΔH_f^0.

Key words*:* Enthalpy of combustion, Matlab, Enthalpy of formation.

INTRODUCTION

In continuation with our earlier studies[1, 2], this communication deals with the thermo-chemical studies of some organic compounds, this can also form complexes. From experimentally measured rise in temperature of the sample due to bomb calorimetric combustion, the time-temperature plots have been obtained using Matlab. The temperature rise per gram of the sample thus obtained, Δt, has been used to determine the enthalpy of combustion of the compound, ΔH_c. By substituting the auxiliary thermochemical data, standard enthalpy of formation of the sample, ΔH_f^0, has been determined. These ΔH_f^0 values for the samples compare well with the earlier reported ones[3].

EXPERIMENTAL

Certified grade crystalline compounds were used for calorimetric studies. Before commencement of experiment, the temperature was stabilized for half an hour by running the static oxygen bomb calorimeter. The instrument was then standardized making use of certified grade benzoic acid and the water equivalent of calorimeter, W, was determined.

The temperature rise per gram of the sample, Δt, was measured experimentally in a bomb calorimeter by burning a weighed sample in an excess of oxygen in known quantity of water.

RESULTS AND DISCUSSION

The water equivalent of the calorimeter, W, was determined by burning a weighed sample of certified grade benzoic acid and measuring the temperature rise per gram of the sample, Δt, in known quantity of water. The time-temperature plot (Fig.1) for benzoic acid was obtained in Matlab[4] as follows:

Time in Minutes;
x = [0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0]

Temp. in ^{0}C;
y = [1.000 1.001 1.002 3.496 3.501 3.500 3.499 3.498]
Plot(x, y)
Grid on

The enthalpies of combustion per mole for the organic compounds shown in Table-1 were determined from the relation,
x label ('Time in min.')
y label ('Temperature in Deg C')

The value of Δt was obtained as 2.501 ^{0}C gm^{-1} for benzoic acid.

The heat of combustion per gram of benzoic acid = -26434 joules gm^{-1}.

From the relation $\Delta H_c = W.\Delta t$,

$$W = 10569 \text{ joules } °C^{-1} \quad ...(1)$$

The enthalpies of combustion per mole for the organic compounds shown in Table-1 were determined from the relation,

$$\Delta H_c = W.M.\Delta t \text{ kJ mol}^{-1} \quad ...(2)$$

Where W is the water equivalent of the calorimeter, M is the gram molecular weight of the sample and "t, the temperature rise per gram of the sample measured experimentally with the help of time temperature plot using Matlab as discussed earlier. As the compounds under study were having elemental composition C, H and O, their combustion products were CO_2(gas) and H_2O (liq.) in their standard states as follows:

$$C_xH_yO_z(\text{cryst.}) + O_2(\text{excess}) = xCO_2 + y/2\ H_2O, \quad \Delta H = \Delta H_c \quad ...(3)$$

Where $C_xH_yO_z$ is the general formula of the crystalline organic compounds.

Their standard enthalpies of formation, ΔH_f^0 were determined from the relation ΔH_c=-

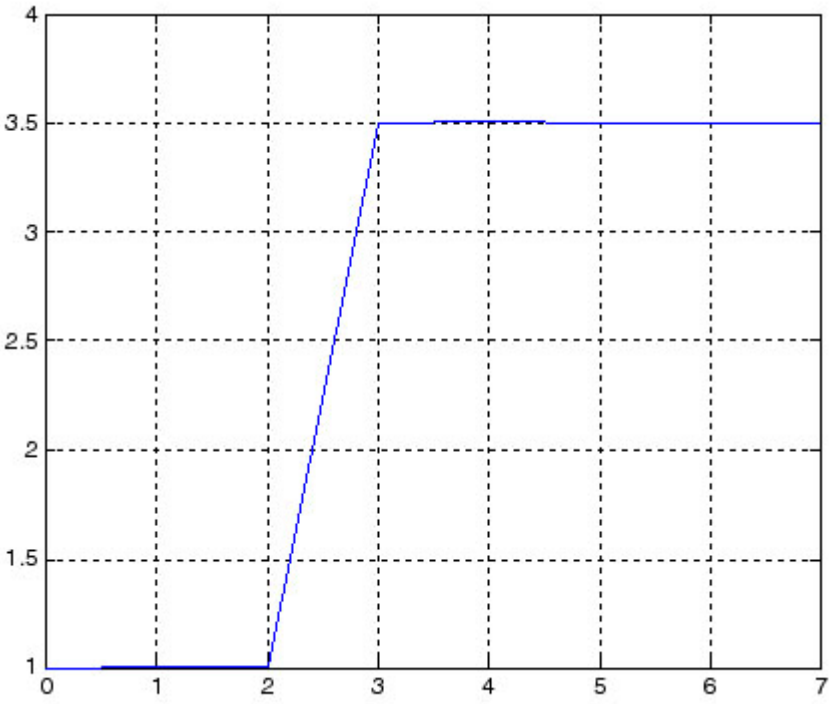

Fig. 1: The time-temperature plot

Table 1: Thermochemical Data of some Organic Compounds

S. No.	Name of the Compound	Formula of Compound	Δt ^0C gram^{-1}	ΔH_c kJ mol^{-1}	ΔH_f^0 kJ mol^{-1}
1.	Benzoic acid	C_6H_5COOH	2.501	-3227	-384
2.	Methyl benzoic acid	$CH_3C_6H_4COOH$	2.683	-3861	-430
3.	Ethyl benzoic acid	$C_6H_4(C_2H_5)COOH$	2.849	-4520	-451
4.	Tetra methyl benzoic acid	$C_6H(CH_3)_4COOH$	3.094	-5824	-505
5.	Succinic acid	$HOOCCH_2CH_2COOH$	1.194	-1490	-941
6.	Methyl succinic acid	$HOOCCH_2CH(CH_3)COOH$	1.542	-2153	-958
7.	Citric acid	$HOOCCH_2C(OH)COOH\text{-}CH_2COOH$	0.965	-1959	-1545

ΔH_f^0(products) - -ΔH_f^0(reactants) as follows:

$$\Delta H_f^0\ C_xH_yO_z\ (cryst.) = x\ \Delta H_f^0\ CO_2\ (g) + y/2\ \Delta H_f^0\ H_2O\ (l) - \Delta H_c \quad ...(4)$$

The enthalpies of formation of the combustion products CO_2(g) and H_2O(l) were obtained from standard source[5]. The enthalpies of formation thus obtained for the compounds have been shown in Table 1.

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