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Application of Linear Fitting on Predicting Homologues Combustion Heat and the Determination of Structure of Organic Matter

[1]Hao Li, [2]Shuangjun Yang, [3]Yiwei Wang, [4]Zheze Zhao and [1]Yizhou Li
[1]College of Chemistry,
[2]College of Light Industry,
[3]West China School of Pharmacy,
[4]College of Life Sciences, Sichuan University, Chengdu, Sichuan 610064, China

Abstract: Predicting the combustion heat of hydrocarbon and its homologues is significant in fire protection. Moreover it is also difficult to determine the structures of unknown organic compounds by using limited instruments. In this study, in order to solve the problems, we made a new application of linear fitting. Firstly, according to the research on the thermal variation on combustion of the homologues of alkanes, alkenes and alkynes, a mathematical linear fitting method was proposed to predict the combustion heat of hydrocarbon and its homologues. Then, a model of determining the structures of organic compounds is designed. The structure of an unknown substance could be predicted through the transformation of the determination formula of combustion heat. On the basis of the high linear correlation coefficient, the method is proved to be effective and applicable. Our study suggests that linear fitting should be promising in prediction of combustion heat and the determination of unknown organic compounds and even in the further exploration.

Key words: Prediction of combustion heat, hydrocarbon homologues, Q/M value, determination of unknown structure

INTRODUCTION

The heat of combustion is the energy released as heat when a compound undergoes complete combustion with oxygen under standard conditions. It is generally measured in unit of energy released during the combustion of the amount of substance, unit mass or unit volume of fuel. The combustion reaction is the combustion of hydrocarbons in oxygen which generates carbon dioxide, water and releases heat. The heat of combustion can be measured with a oxygen bomb calorimeter, or be calculated by referring to the heat of combustion tables.

"Material structure determines properties and the properties of matter can reflect the structure" is one of the axioms in the academic field. Heat of combustion, as one of the important properties of organic compounds, also has inevitable relevance to the corresponding structure. In recent years, there have been some similar domestic studies on heat of combustion property of organic compounds. In Security Engineering Research Institute of Nanjing University of Technology, Jiang (1996) a researcher of Security Engineering Research Institute of Nanjing University of Technology, cooperating with other people, has made a more in-depth study on Electrotopological state index in prediction of liquid hydrocarbon combustion heat. In addition, Wang (2000), together with his colleagues, has made a response study on the group contribution method calculating combustion heat of liquid alkanes. Besides, Peng (1999), Taskinen and Yliruusi (2003), Albahri (2003), Turker (2004) and Hall and Kier (1995), have also done the relative researches of calculation methods of the components' characterization. The results of the studies above are advanced to some degree but there are still some limitations in them. First of all, the research object is confined to the liquid organic matter while solid, gaseous organic compounds are not discussed. Secondly, the methods they employed are based on a summative law which makes it difficult for analogy expanding and thus those results have some limitations in application.

In this article, linear regression was applied to predict the heat of combustion on organic homologues. Through conditional experiments, an optimal set of organic homologs were selected for linear fitting between the combustion heats and their carbon numbers. The obtained square of the correlation coefficient value is higher than 0.9 and the homogeneous homologues with unknown heat of combustion could also be predicted. In addition, in this study combination of oxygen bomb

Corresponding Author: Yizhou Li, College of Chemistry, Sichuan University, Chengdu, China

calorimeter of solid organic matter combustion heat determination, method of mathematic linear regression and linear fitting provides a new strategy to obtain the structure of organic matter through the method for the determination of organic combustion heat.

FUNDAMENTAL

According to the calculation it was discovered that in hydrocarbon homologues, the amount of combustion heat has to follow certain rules. Here, three kinds of organics: Alkanes, alkenes and alkynes, were taken for instance. (In the following charts, the abscissa is the carbon atom number of the organic compounds; the ordinate is the corresponding standard heat of combustion).

From the charts above, for all three kinds of organics, alkanes, alkenes or alkynes, the amount of homologue combustion follows certain rules. The square of the correlation coefficient values could reach > 0.9 and then regression equation could be worked out based on the data. According to this phenomenon it can be observed that this rule could be applied to predict the heat of combustion of organic homologs.

PREDICTION OF COMBUSTION HEAT ON ORGANIC COMPOUNDS

On basis of the principles above it is possible to establish different linear regression equations between heat value of various organic homologs and the carbon atom numbers of homologues organic compounds. The combustion heat of an unknown compounds could therefore be determined. This part will take alkanes, alkenes and alkynes for case studies.

Normal paraffin hydrocarbon homologues: According to the standard alkane combustion heat value, a linear regression equation can be obtained: y = 651.8x+252.1. In order to verify the accuracy of this equation, we substitute x = 12 and then obtain y = 8073.7 . Apparently the predictive value roughly coincides with the actual data.

Normal olefin homologues: According to the standard combustion heat value of olefin, a linear regression equation can be obtained: y = 6846x+15.65 in order to verify the accuracy of this equation, we substitute x = 6 and then obtain y = 6865.65. The predictive value roughly coincides with the actual data.

Normal alkynes homologues: According to the standard combustion heat value of alkyne, a linear regression equation can be obtained: y = 652.0x-11.88. In order to verify the accuracy of this equation, we substitute x = 6 and then obtain y = 3900.12. The predictive value roughly coincides with the actual data.

In summary, the method based on linear fitting can effectively predict the combustion heat of organic homologs which has great application value in the field of fire protection. At the same time, the method can also be applied to other hydrocarbon homologues.

DETERMINATION OF STRUCTURE IN ACCORDANCE WITH THE VALUE OF Q/M

The most common and effective way of determining the combustion heat is utilizing the oxygen bomb calorimeter. The main mathematical formula is showed as follows:

Table 1: Relationship between the value of alkane, alkene and alkyne and the carbon numbers

Carbon No.	Q/M value of alkyne	Q/M value of alkyne	Q/M value of alkyne
1	55.59		2
	51.96	50.34	49.94
3	50.41	48.96	48.4
4	49.58	48.5	48.06
5	48.7	48.18	47.83
6	48.36	47.48	7
	48.12	47.56	8
	47.94	47.45	9
	47.8	47.37	10
	47.68	47.31	

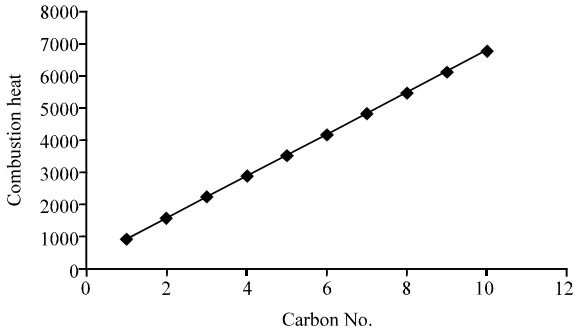

Fig. 1: Law of the alkane's combustion heat

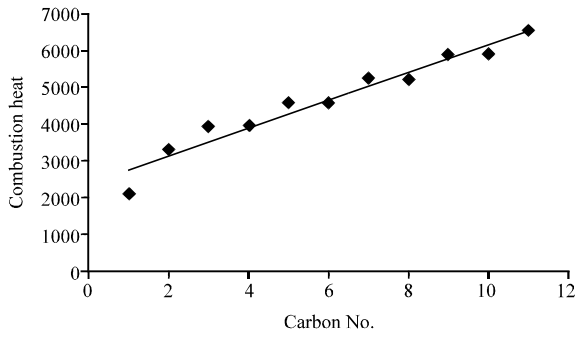

Fig. 2: Lw of the alkene's combustion heat

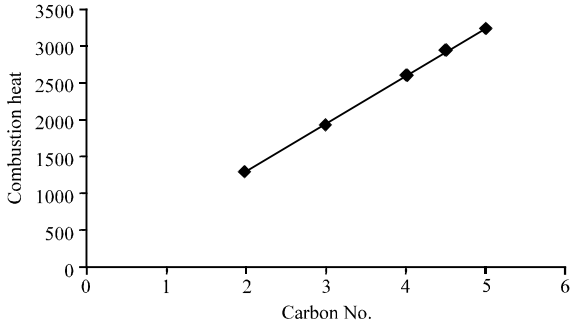

Fig. 3: Law of the alkyne's combustion heat

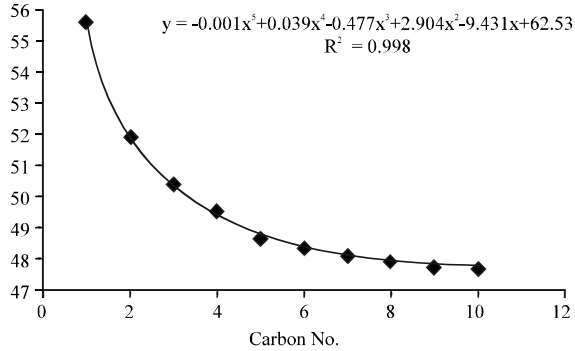

Fig. 4: Q/M curve of alkane

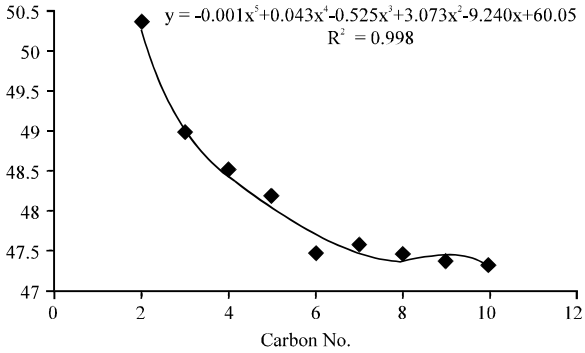

Fig. 5: Q/M curve of alkene

$$mQ/M+\varepsilon b+qc = K\Delta T \quad (1)$$

where, Q represents the Molar constant-volume combustion heat of the determinand; m represents the mass of the determinand; M represents the molar mass of the determinand ε represents the heat value of the Ignition wire b represents the consumption quality of the Ignition wire q represents the heat value of the combustion of cotton c represents the consumption quality of the cotton K represents the constant of the oxygen bomb calorimeter ΔT represents the change value of the system temperature.

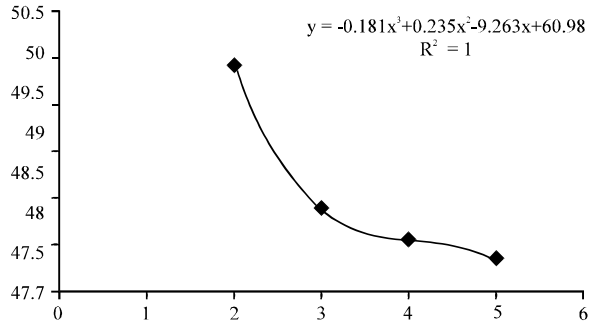

Fig. 6: Q/M curve of alkyne

Transposing the equation (1), we can obtain:

$$QM/ = (K\Delta T-\varepsilon b-qc)/m \quad (2)$$

According to the Eq. 2 it is obvious that the right of the equation has nothing to do with the determinand. Therefore, we only need to take the left of the equation into consideration. According to the equation, the Q/M values could be calculated for the alkane, alkene and alkyne as follows.

According to the Q/M value above, we can obtain the fitting equations as follows.

Now we could draw a conclusion: For alkane, alkene and alkyne, each of their homologues has an independent value of Q/M and it corresponds with the law of polynomial equation (the square of the degree of association is greater than 0.9). Based on this reason, we created a new concept: In the field of the hydrocarbon homologues, hydrocarbon compounds of different carbon number have a different Q/M value. We can determine the Q/M value by determining the combustion heat which acquires the right term of the Eq. 2. Thus the unknown type and structure of the determinand can be determined. Due to the limitation of the data provided by the previous studies, we cannot extend such method to other hydrocarbons with a large number of data. We will do deeper research in the future studies to improve this concept.

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