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A study of matrix energy during peptide formation through chemical graphs

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Abstract

Amino acids, the monomer units of protein, play an important role in all biological species. Two amino acids combine by the elimination of a molecule of water to produce a dipeptide and the linkage is known as peptide link or peptide bond. Chemical graphs serve as a convenient model of any real or abstract chemical system. The energy of a chemical graph is the sum of the absolute eigen values of the adjacency matrix of the graph. The aim of this work is to make a theoretical estimation of the energies of graphs associated with the amino acids constituting the dipeptide and that of the peptide itself. It is found that the energy during the formation of dipeptide is conserved for various di-peptides.

Keywords: Graph spectra, eigen value, topological indices, di peptides.
AMS Subject Classification(2010): 94C15, 05C10.

1 Introduction

Chemical Graph theory is used to mathematically model the molecules in order to gain insight into their physical and chemical properties [1]. It is also an important tool in drug designing. E.Estraade [4] and coworkers made a review on the use of topological indices in drug design and discovery. Natarajan [7] and Nirdosh worked on application of topological indices to QSAR modeling and selection of mineral collectors. Sharma [9] et al calculated the excess isentropic compressibility KsE values using density values of the binary and ternary mixtures and graph theory. Basak [2] employed topostructural (TS) and topochemical (TC) indices in the development of QSAR models of the aryl hydrocarbon (Ah) receptor binding potency of a set of dibenzofurons. The correlation between the eigen values and the atomic mass for twenty amino acids using chemical graphs has been calculated [6]. Amino acids, the monomer units of protein molecule play an important role in all biological species. The combination and proportion of the amino acids in different cells depend on the type of cells and this gives the difference in behavior of cells. Relatively simple monomeric subunits provide the key to the structure of the thousands of different proteins. This group of 20 precursor molecules may be regarded as the alphabet in which the language of protein structure is written.

Two Amino acids, for example, Alanine and Glycine can combine together with the elimination of a molecule of water to produce a dipeptide . It is possible for this to happen in one of two different ways (Figure-1). Three amino acids combine to form tri-peptides. More than three amino acids combine to form poly peptides. The peptide chain is made up of amino acid residues. The end of the peptide

chain with NH_2 group is known as N- terminal and the end with COOH group is known as the C - terminal.The peptide chain is known as the backbone and the R groups are known as the side chains.

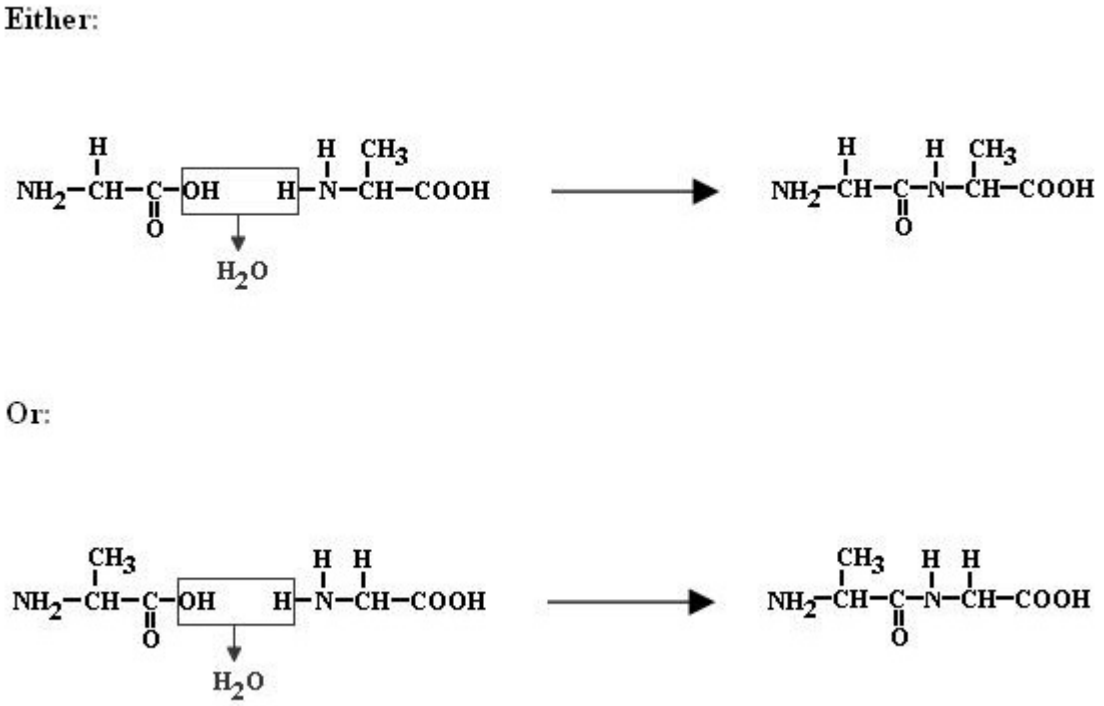

Figure 1: *Formation of di-peptide.*

2 Estimation of energies

The adjacency matrix of the molecule represents the topology of the molecules. The non zero entries appear only alongside the principal diagonal. It is noted that all Eigen values appear in pairs. The energy of a chemical graph is the sum of absolute eigen values of the adjacency matrix of the graph [8].

In the case of Alanine - Glysine dipeptide, we get the following results.
The eigen values of the adjacency matrix of Alanine are:
-2.7163, -2.0000, -1.5474, - 0.8976, -0.6493, , 0.0000, 0.0000, 0.0000, 2.7163, 2.0000 , 1.5474, 0.8976, 0.6493.
Energy of Alanine E_A = 15.62.

The eigen values of the adjacency matrix of Glysine are:
-2.662, -1.7925, -1, -0.8384,0.0000, 0.0000, 2.662, 1.7925, 1, 0.8384
Energy of Glysine E_G = 12.59 .

The eigen values of the Alanine - Glysine dipeptide are:
-2.8055, -2.5779, -2.0279, -1.5704, -1.4851, -0.8758, - 0.7243, - 0.6386, 0.0000, 0.0000, 0.0000, 0.0000, 0.6386, 0.7243, 0.8758, 1.4851, 1.5704, 2.0279, 2.5779, 2.8055.
Energy of Alanine - Glysine dipeptide E_{AG} = 25.41.

The energy of the water molecule E_w is 2.83.

It is interesting to note that the sum of the energies of the individual amino acids constituting the dipeptide is equal to the sum of the the energies of the dipeptide and water molecule, that is, $E_A + E_B = E_{AB} + E_w$ and so the energy is conserved during the formation of dipeptides.

The energies of all the 20 amino acids and that of the peptides formed by Alanine with itself and other 19 amino acids have been calculated from their adjacency matrices.

For want of space the adjacency matrix AG of Alanine - Glysine dipeptide alone is given.

$$AG = \begin{pmatrix}
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0
\end{pmatrix}$$

The eigen values of the matrices were evaluated using **SCILAB** and energy is obtained as the sum of the absolute eigen values.

The estimated energies of the other di peptides are given in Table.1.
From the table one can conclude that during the formation of dipeptide,
$E_A + E_B = E_{AB} + E_w$, and hence the energy is conserved during this reaction.

Table 1: *Energies of some di peptides.*

Amino acid	Energy E_A	Energy E_B	Peptide Energy E_{AB}	E_A + E_B	E_{AB} + E_w
Glycine	12.59	15.62	25.41	28.21	28.24
Alanine	15.62	15.62	28.46	31.24	31.29
Serine	17.4	15.62	30.23	33.02	33.06
Proline	20.91	15.62	33.75	36.53	36.58
Valine	21.83	15.62	34.66	37.45	37.49
Theonine	20.46	15.62	33.30	36.08	36.13
Cystine	17.4	15.62	30.23	33.02	33.06
Isoleusine	24.99	15.62	37.82	40.61	40.65
Aspargine	22.41	15.62	35.24	38.03	38.07
Asparticacid	21.61	15.62	34.44	37.23	37.27
Leucine	24.97	15.62	37.81	40.59	40.64
Glutamine	25.55	15.62	38.39	41.17	41.22
Lysine	27.64	15.62	40.47	43.26	43.30
Glutamicacid	24.76	15.62	37.60	40.38	40.43
Methionine	22.7	15.62	35.54	38.32	38.37
Histidine	27.3	15.62	40.13	42.72	42.96
Phynilealnine	32.00	15.62	44.84	47.62	47.67
Arginine	31.74	15.62	44.57	47.36	47.40
Tyrosine	33.28	15.62	46.12	48.90	48.95
Tryptophan	38.91	15.62	51.75	54.53	54.58

Conclusion: Many topological indices like Hosoya index, Wiener index, etc have been used for analyzing physicochemical properties of molecules. We have used chemical graph theory to calculate the energies during the formation of di-peptides from amino acids and found that the energy is conserved during this reaction. Further study is being made on the other properties of amino acids and peptides using chemical graph theory.

References

[1] A.T. Balaban, *Chemical applications of Graph Theory*, Acadamic Press, 1976.

[2] S.S. Basak, D. Mills, M. Murnataz and K. Balasubramanian, *Ind. J. Chem..*, Vol.42A, 2003,pp.1385.

[3] Donald T. Haynie, *Biological Thermodynamics*, 2nd Edition, Cambridge University Press,2002.

[4] E. Estraade, G. Patlewicz and E. Uriarte, *Ind.J.Chem.*, Vol. 42A, 2003,pp.1315.

[5] S. Lalitha, Ph.D Thesis, *S*olvation study of aqueous solutions of Amino acids, Alagappa University, 2003.

[6] S. Lalitha , Mathavi Manisekar, *Mathematical and Experimental Physics*, Narosa Publishing House Pvt.Ltd.,2010,India.

[7] Natarajan, P. Kamalakannan and I. Nirdosh, *Ind. J. Chem.*., Vol.42A, 2003.

[8] Nenad Trinajstic, *Chemical Graph Theory*, Vol.1, CRC Press Inc., 1983.

[9] V.K. Sharma, Romi and S. Kumar, I*nd. J. Chem.*, Vol.42A, 2003,pp.1379.