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Topological analysis of five-vertex clusters of group IVA elements

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Summary. Net sign analyses of eigenvectors and eigenvalues of five-vertex chemical graphs were performed. The five-vertex graphs are denoted as G_{5m}, where the first subscript 5 stands for the number of vertices and m for the number of edges. G_{54} is the path with 5 vertices, hence 4 edges, isomorphic with the hydrogen-depleted graph of *n*-pentane. In most cases, the ordering according to the net sign is found to be similar to the ordering according to the energy eigenvalues. Applications of net sign analysis to the investigation of ground-state geometry of five-vertex clusters of carbon, silicon and germanium are also discussed.

Key words: Five-vertex graphs – Group IVA elements

1. Introduction

Recently there has been a growing interest in the chemistry and physics of small atomic clusters partly due to its practical significance in the combustion [1–3], laser evaporation [4–6], catalysis [7], semiconductor industries [8–9], astrochemistry [10–12], and partly because the challenge its intriguing dynamics and structure presents to theoreticians [13–16]. The state of art is reflected in a collection of recent works in this field [17]. Among the various facets of clusters, we attempt to explore the topological feature involved in the stability problem of clusters from the graph-theoretical point of view.

Determination of the ground state geometry of clusters is the central problem in cluster science. Small carbon clusters have been studied using simple molecular orbital scheme [18–19], extended Hückel method [20], MINDO [21–23], and *ab initio* calculations at different levels of sophistication [24–31]. The ground-state geometry is still a problem of controversy [21–23]. Clusters made of silicon [32–37], germanian [32, 38], tin [37], rare gas [39, 40], alkali metal [41], transition metal [42, 43] and etc. [44–46] present the same problem. We report here the results of topological analysis of five-vertex chemical graphs [47] in order to shed some insight into this problem.

Topological aspects of cluster bonding have been studied by several investigators. George et al. [48] calculated the relative stabilities of the alkali-like metal clusters up to $n = 9$ using Hückel-type calculation. They concluded that the agreement between the most stable HMO structures and the equilibrium geometry predicted by *ab initio* calculations [49–52] is excellent. King [53–57] and several others [14, 58, 59] studied the cluster topology using graph theory and developed an electron counting rule for predicting the stabilities of organo-metallic clusters. The introduction of the concept of internal connectivity [60–65] by the author provides a rather simpler way, namely, the net sign analysis, to approach this problem. In this paper, net sign approach was performed to analyze the topological feature of Hückel molecular orbitals of chemical graphs having five vertices.

Chemical compounds with five vertices may have various external structural features ranging from acyclic form, three-membered ring, four-membered ring, and five-membered ring. The number of edges is four for acyclic isomers and five for cyclic isomers containing a three-membered ring. As the intra-ring connections increase, the number of edges varies from five to seven for isomers having a four-membered ring and it varies from five to ten for isomers having a five-membered ring. It is interesting to investigate the internal connections hidden behind the external varieties.

In Sect. 2, the essence of the net sign analysis is introduced using an acyclic 5-vertex-4-edge graph (G_{54}) and one of the cyclic 5-vertex-5-edge graphs (G_{55}) as model graphs. The signed graphs containing the graphical features of the eigenvectors are then built up. The graph of each eigenvector is then found to belong to the class of vertex-signed graphs (VSG's). The graphs characterizing the internal connections are edge-signed graphs (ESG's). In order to study the relative stabilities of various structures, a total energy-like quantity, computed as summation of orbital occupation number times its net sign, is introduced. Results of the net sign analysis of other five-vertex graphs as well as the corresponding total-energy-like quantities are also presented and discussed in Sect. 3. Comparisons were made with the results of other calculations. Conclusions are given in Sect. 4.

2. Method and model

A graph is defined as a mathematical entity containing a set of vertices and a set of edges. Each edge represents the connection between two neighboring vertices. The intuitive connection between a chemical structure and a mathematical graph is rather straightforward. If only the topological features are of main concern, a weighted factor a_{ij} $(i = j)$, is given as follows:

$$\begin{cases} a_{ij} = 1 & \text{for connection between vertices } i \text{ and } j \\ a_{ij} = 0 & \text{for no connection between vertices } i \text{ and } j \end{cases} \tag{1}$$

In this way, we can establish a N by N topological matrix, the adjacency matrix, for each N-vertex graph to characterize the external connectivity of a graph. Taking into account the presence of heteroatoms, weighted loops can be added to the hetero-vertices and the edges connecting hetero-vertices are also given different weights. In such cases, we obtain vertex- and edge-weighted graphs and the corresponding weighted adjacency matrices [66, 67]. Weighted graphs are useful in the investigations of quantitative structure-activity relationship (QSAR) of the heterocyclic compounds [68, 69].

The adjacency matrix is one of the basic topological matrices of a graph. Most of the chemical applications of graph theory are established on the properties derived directly from the adjacency matrices [70–78] combined with the knowledge of combinatorics [79]. Successful applications of graph theory have been found in the applications of the conjugated systems [70–72], in drug design and research [73], in QSAR [74, 75], in isomer enumeration [76, 77], in organometallic chemistry [53–57, 58], in structural chemistry of cluster compounds [48, 58, 59], etc.

The equivalence relation between the adjacency matrix of a chemical graph and the Hückel secular matrix of a molecule has been pointed out by several authors [80–83]. Applications of this equivalence relationship to the alternate π-conjugated systems yield all features at the Hückel level, including the spectra [84], charge densities and bond orders [85]. Graph theory has been successfully applied to a variety of fields of chemistry [70–78] based only on the external topology, i.e., the spectra of a graph and the connections or bonds among vertices. For the complete usage of graph theory to chemistry, the internal topological features embedded in the eigenvectors of the adjacency matrices need to be extracted and put in use. Chemical graphs containing two to four vertices have been analyzed by Lee et al. using net sign approach [60–65]. In this section, net sign analysis is illustrated by examining the topological features of two model five-vertex graphs, G_{54} and G_{55}.

G_{54}. The G_{54} graph is one of the simplest five-vertex connected graphs. It belongs to the class of tree graphs. Organic compounds which are isomorphic to such a graph are n-pentane and 1,3-pentadienyl ion. Acyclic compounds always has $N-1$ edges where N is the number of vertices.

For G_{54}, the adjacency matrix, $A(G_{54})$, according to Eq. (1), is given by:

$$A(G_{54}) = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix} \tag{2}$$

Eigenvalues and eigenvectors are resulted from diagonalization of $A(G_{54})$. The eigenvalues, ζ_i, and the corresponding eigenvectors; χ_i, are:

$$\zeta_1 = -1.73, \quad \chi_1 = (0.29, 0.50, 0.58, 0.50, 0.29) \tag{3a}$$

$$\zeta_2 = -1.00, \quad \chi_2 = (0.50, 0.50, 0.00, -0.50, -0.50) \tag{3b}$$

$$\zeta_3 = 0.00, \quad \chi_3 = (0.58, 0.00, -0.58, 0.00, 0.58) \tag{3c}$$

$$\zeta_4 = -1.00, \quad \chi_4 = (0.50, -0.50, 0.00, 0.50, -0.50) \tag{3d}$$

$$\zeta_5 = -1.73, \quad \chi_5 = (0.29, -0.50, 0.58, -0.50, 0.29) \tag{3e}$$

The eigenvectors of the adjacency matrix are equivalent to the eigenvectors of the Hückel secular matrix. Thus the eigenvectors in Eqs. (3a)–(3e) correspond to Hückel molecular orbitals (HMO) of a pentadienyl-ion-like molecule. Due to the connection factor as given by $+1$, opposite to the negative value of the off-diagonal terms in the Hückel secular matrix, eigenvectors with positive and negative eigenvalues correspond to bonding HMO's and antibonding HMO's, respectively, The net sign of an ESG is obtained by summing the signs of the edges of a given ESG which is built up from eigenvectors. Net signs of the five eigenvectors are 4, 2, 0, −2, −4. The ordering in the net signs is parallel to the ordering in the eigenvalues.

G_{55}. If the number of edges is greater than or equal to the number of vertices in a connected graph, there must be a cyclic or ring structure in the graph. Dimethylene-cyclopropenyl ion, ethyl-cyclopropene, methylene-cyclobutenyl ion, and cyclopentadienyl ion are typical examples which are isomorphic to the G_{55} graph. Here we take ethyl-cyclopropene as an example.

The adjacency matrix of G_{55} graph is built in the same way as in the case of G_{54} generating:

$$A(G_{55}) = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 & 0 \end{bmatrix} \tag{4}$$

The resulting eigenvalues and eigenvectors are:

$$\zeta_1 = 2.21, \qquad \chi_1 = (0.15, 0.34, 0.60, 0.50, 0.50) \tag{5a}$$

$$\zeta_2 = 1.00, \qquad \chi_2 = (0.63, 0.63, 0.00, -0.32, -0.32) \tag{5b}$$

$$\zeta_3 = -0.540, \qquad \chi_3 = (0.67, -0.36, -0.48, 0.31, 0.31) \tag{5c}$$

$$\zeta_4 = -0.100, \qquad \chi_4 = (0.00, 0.00, 0.00, 0.71, -0.71) \tag{5d}$$

$$\zeta_5 = -1.67, \qquad \chi_5 = (-0.35, 0.59, -0.64, 0.24, 0.24) \tag{5e}$$

The positive and negative eigenvalues also correspond to the bonding HMO's and antibonding HMO's. Note that the numbering of the vertices is 12345 starting from the ethyl group outside the 3-membered ring. Net signs of the five eigenvectors are 5, 2, −1, −1, −3.

Signed graphs. Very few chemical applications of signed graphs have been found in the literature. Only in the description of the Möbius structures [86, 87], the ESG's with one minus-signed edge have been used. Similar notions were used by Heilbronner and Straub [88], by Heilbronner and Bock [89], and by Herndon and Silber [90] in simplifying the energy calculation in Hückel MO theory. For complete descriptions of the topological features of internal connectivities, both ESG's and VSG's are used.

The VSG's representing the eigenvectors of both G_{54} and G_{55} graphs are shown in Fig. 1. Each eigenvector is represented by one VSG in which '+' stands for positive coefficient, '−' for negative one, and no sign for zero one. From the VSG's, we can build up their corresponding ESG's. The constructions of these VSG's and ESG's are described elsewhere [60–65].

In Fig. 2, the ESG's recording the internal connections of acyclic 5-vertex graphs are presented. ESG's of cyclic 5-vertex graphs having three-, four-, and five-membered ring are also shown in Figs. 3, 4, and 5, respectively.

One should note that the nodal properties of Hückel MO's are not fully understood. For instance, it is difficult to predict the ordering of HMO's having the same number of nodal planes [91]. Lee et al. had proposed a net sign approach [60–65] to tackle the puzzling nodal properties of HMO's. In the net sign approach, the net sign of an ESG is simply obtained by summing the signs

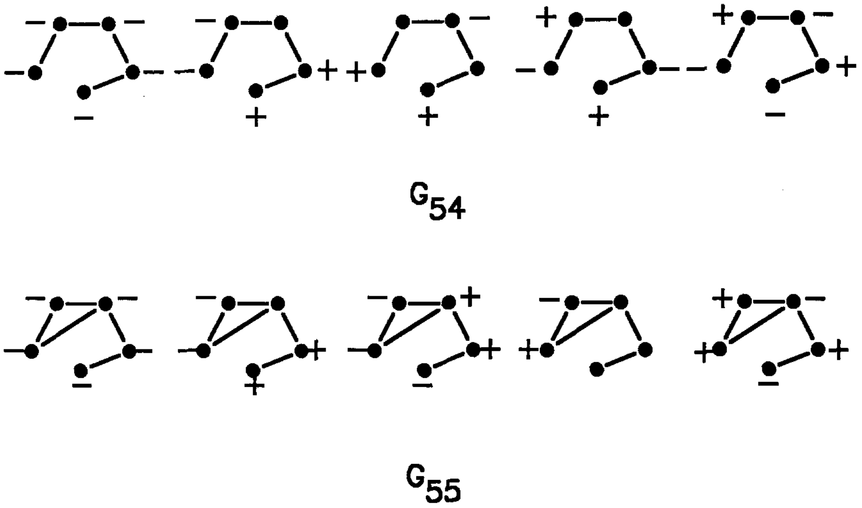

Fig. 1. Vertex-signed graphs of G_{54} and G_{55}

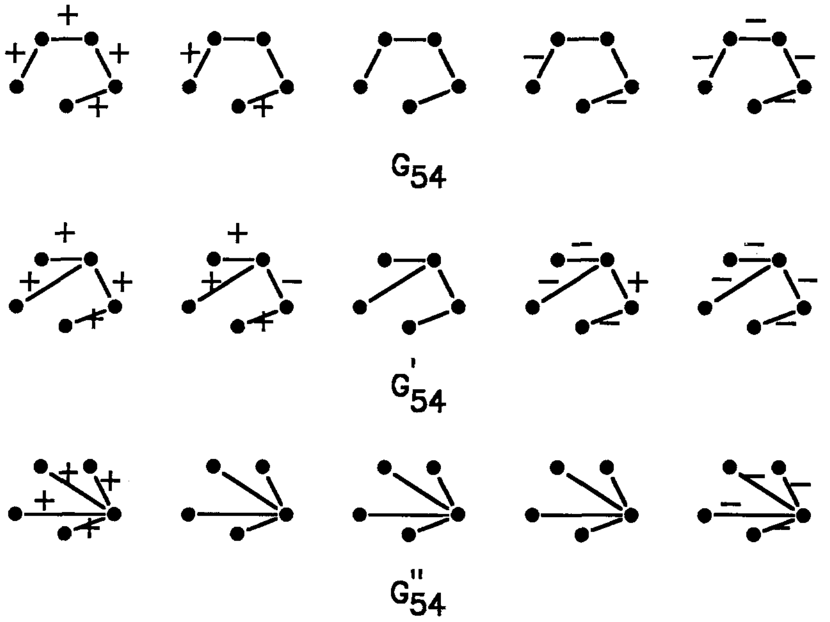

Fig. 2. Edge-signed graphs of acyclic 5-vertex graphs. Some of the ESG's have no signed edges due to the nodal plane passes through at least one of the vertices

of the edges of a given ESG. The net signs of the ESG's of acyclic 5-vertex graphs are given in Table 1. We can see that the net signs of ESG's in Table 1 have the same ordering as the corresponding eigenvalues of the adjacency matrix. Real examples such as pentadienyl-radical and cyclopentadienyl-anion [92] can be found to be exactly similar to the G_{54} and G_{55}^{iv}. The net signs of the ESG's of

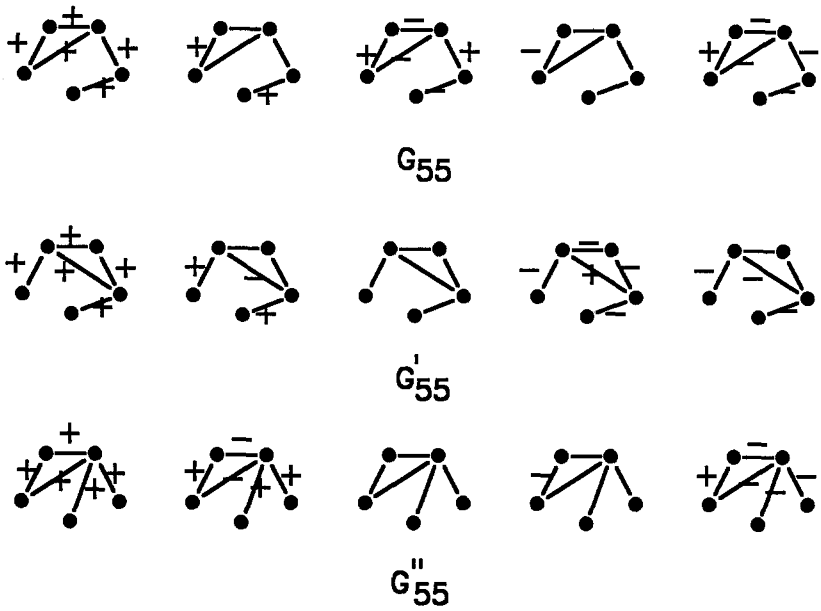

Fig. 3. Edge-signed graphs of 5-vertex graphs having three-membered ring

cyclic 5-vertex graphs having three-, four-, and five-membered rings are given individually in Tables 2–4.

In most cases the ordering according to net signs is similar to the ordering according to the energies. Inconsistent ordering in the net signs can be found compared to the ordering in the energies in certain cases. However, for orbitals

Table 1. Net signs of ESG's and energy levels of Hückel MO's for acyclic 5-vertex graphs

Graph	Energy	Net sign
G_{54}	1.73	4
	1.00	2
	0.00	0
	−1.00	−2
	−1.73	−4
G'_{54}	1.85	4
	0.77	2
	0.00	0
	−0.77	−2
	−1.85	−4
G''_{54}	2.00	4
	0.00	0
	0.00	0
	0.00	0
	−2.00	−4

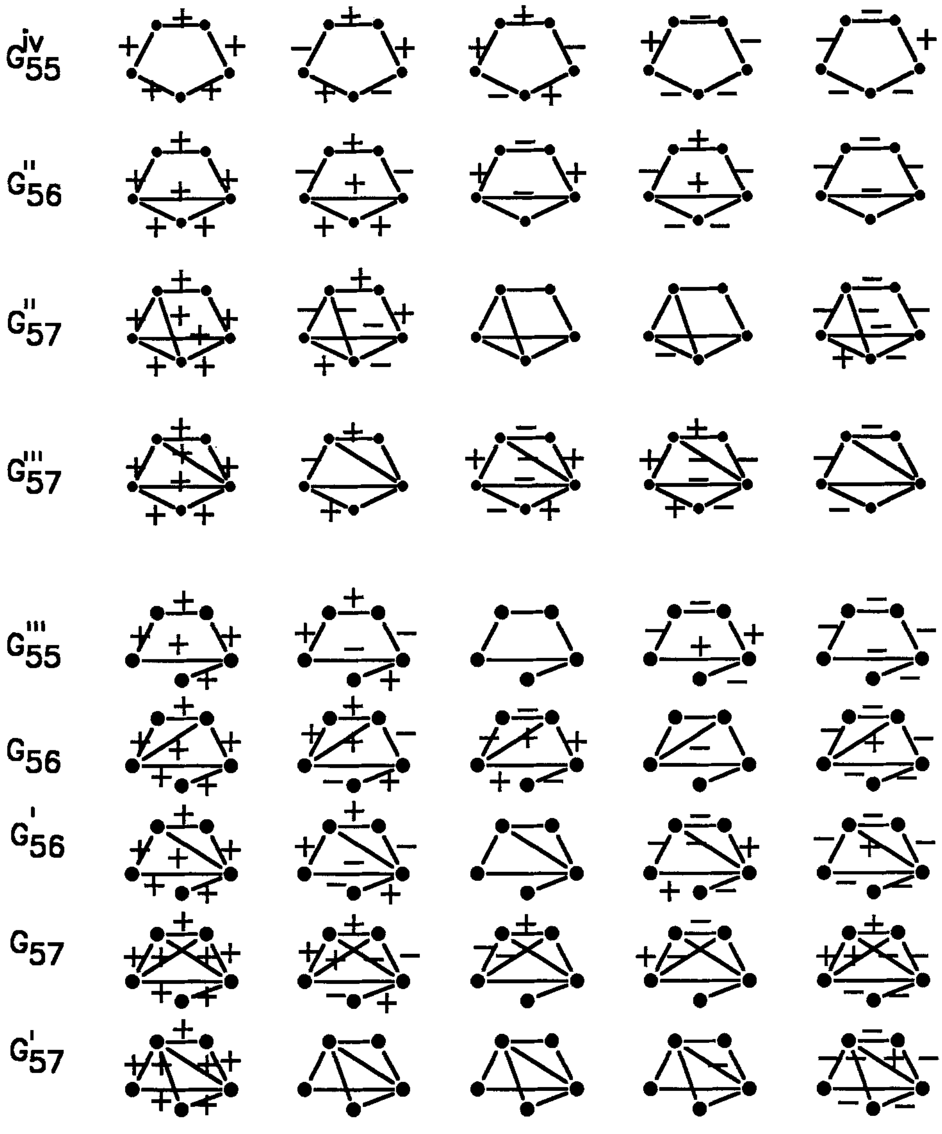

Fig. 4. Edge-signed graphs of 5-vertex graphs having four-membered ring

having one nodal place in all 5-vertex graphs, the net sign approach yielded the correct ordering. Same conclusions have been addressed for more complicated systems such as naphthalene, anthracene, pyrene, etc. by Lee et al. [60–65].

The partially inconsistent ordering found in the 5-vertex graphs and pyrene is certainly not a special case in view of the simplicity of the net sign approach. Further investigations on the relationship among the energy ordering, number of nodal planes, and the net sign from a more fundamental point of view pointed out that the oscillating theorem of one-dimensional quantal system could not be straightforwardly extended to two-dimensional quantal systems [93].

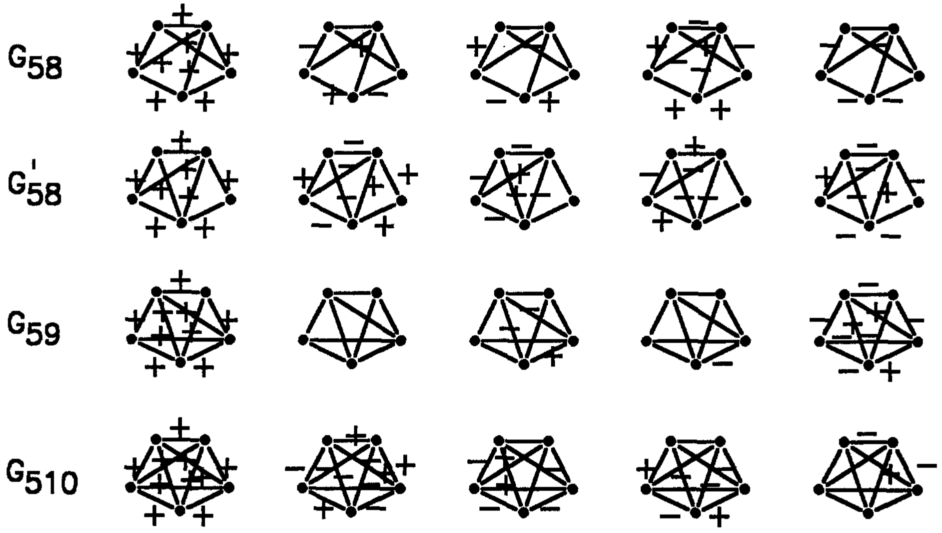

Fig. 5. Edge-signed graphs of 5-vertex graphs having five-membered ring

Total-energy-like quantities. In order to study the relative stabilities of different structures of five-vertex clusters, a total-energy-like quantity, $E(G)$, is defined as the total net sign, $S(G)$, of the structure times the interaction between two vertices, β. The total net sign of a graph is computed as:

$$S(G) = \sum_i n_i S_i \tag{6}$$

where n_i is the occupation number of the ith orbital, S_i is the net sign of the corresponding signed graph. The summation is taken over all occupied orbitals. Thus, the relative stabilities of the two graphs G and G' can be qualitatively obtained by investigating the difference of $E(G)$ and $E(G')$.

$$E(G) - E(G') = \sum_i (n_i(G)S_i(G)\beta(G) - n_i(G')S_i(G')\beta(G')) \tag{7}$$

where $\beta(G)$ and $\beta(G')$ are inter-vertex interactions of graphs G and G', respectively. Provided that inter-vertex interactions are same in different graphs, the total net sign would be a good index for the stability problem of clusters. In real molecular systems, the inter-vertex interactions are different in different graphs and are found to be approximately proportional to overlap integrals as used in the Wolfsberg–Helmholtz formula [94]. By adopting the formula of overlap integrals from Roothaan's [95] and Ruedenberg's [96] paper, we use the average inter-vertex distance of the optimized geometry from other calculations, and excellent agreement with the results of the *ab initio*-type calculations for the stability problem among different graphs of carbon clusters can be reached. It should be noted that we do not attempt to solve this arduous problem in our crude treatment, we would rather point out the topological essence among five-vertex clusters of different elements.

3. Results and discussions

Net sign analysis. Net signs of ESG's for acyclic 5-vertex graphs are given in Table 1 along with the energies of HMO's. As can be seen in Table 1, the ordering according to the net sign is similar to the ordering according to the energy. For G_{54} and G'_{54}, the systems are basically one-dimensional graphs. One-dimensional quantal particles should obey the oscillating theorem [97], and their eigenvalues can be predicted by the net sign approach [93]. Graph G''_{54}, which belongs to the class of star graphs and have a vertex with four edges, could not have a corresponding counterpart in real π systems. This graph may be of importance in the topological study of cluster compounds and chemical graphs containing a central atom. The ordering according to the net sign for this star graph is also in perfect agreement with the ordering according to the energy.

Net signs of ESG's of 5-vertex graphs having three-membered rings are given in Table 2 along with the corresponding eigenvalues. Agreements between the ordering according to the net signs and the eigenvalues are quite satisfactory. Two exceptions exist when the difference between two energy levels is less than 0.46β, where β is the interaction between two neighboring vertices. Graphs G_{55} and G'_{55} have partners in the real systems, namely, ethylene-cyclopropenyl-anion and dimethylene-cyclopropenyl-anion. Graph G''_{55} could find its usage in the cluster compounds due to the existence of a 4-edged vertex.

Net signs of ESG's of 5-vertex graphs having four-membered rings are given in Table 3 along with the corresponding eigenvalues. Good agreements between the ordering according to the net signs and the eigenvalues are also obtained. Two exceptions exist when the difference between two energy levels is less than 0.51β, where β is the interaction between two neighboring vertices. Graphs G''_{55} have counterparts in the real systems, namely, methylene-cyclobutadienyl-cation.

Table 2. Net signs of ESG's and energy levels of Hückel MO's for 5-vertex graphs having three-membered ring

Graph	Energy	Net sign
G_{55}	2.21	5
	1.00	2
	−0.54	−1
	−1.00	−1
	−1.68	−3
G'_{55}	2.30	5
	0.62	1
	0.00	0
	−1.30	−3
	−1.62	−3
G''_{55}	2.34	5
	0.47	1
	0.00	0
	−1.00	−1
	−1.81	−3

Table 3. Net signs of ESG's and energy levels of Hückel MO's for 5-vertex graphs having four-membered ring

Graph	Energy	Net sign
G'''_{55}	2.14	5
	0.66	1
	0.00	0
	−0.66	−1
	−2.14	−5
G_{56}	2.64	6
	0.72	2
	−0.59	0
	−1.00	−1
	−1.78	−4
G'_{56}	2.69	6
	0.34	0
	0.00	0
	−1.27	−2
	−1.75	−4
G_{57}	3.09	7
	0.43	1
	−1.00	−1
	−1.00	−1
	−1.51	−1
G'_{57}	3.00	7
	0.00	0
	0.00	0
	−1.00	−1
	−2.00	−5

Graphs G_{56}, G'_{56}, and G_{57} are of use in the study of cluster compounds. Graph G'_{57} is a very interesting graph of propellane-like structure.

Net signs of ESG's of 5-vertex graphs having five-membered rings are given in Table 4 along with the corresponding eigenvalues. Agreements between the ordering according to the net signs and the eigenvalues also hold. One exception exists in the net signs of G''_{57} when the difference between two energy levels is 0.32β, where β is the interaction between two neighboring vertices. Two other exceptions appear in the net signs of G'''_{57} and G_{58}. The energy differences between the reversed ordering levels are 1.01β and 1.47β, respectively and cannot be rationalized. Close examinations of the eigenvectors reveal a common feature in the fourth level of G'''_{57} and G_{58}. This common feature is that a nodal plane intersects all four edges connecting the central vertex and its surrounding four vertices. Only the graphs G^{iv}_{55} have a counterpart in real systems, namely, cyclopentadienyl-anion. All other graphs in this Table might be of usage in the study of cluster compounds.

Ground state geometry. In Table 5, we present the total net signs of some five-vertex clusters which have the same geometry as those used in the semi-

Table 4. Net signs of ESG's and energy levels of Hückel MO's for 5-vertex graphs having five-membered ring

Graph	Energy	Net sign	Graph	Energy	Net sign
G_{55}^{iv}	2.00	5	G_{58}	3.23	8
	0.62	1		0.00	0
	0.62	1		0.00	0
	−1.62	−3		−1.24	0
	−1.62	−3		−2.00	−4
G''_{56}	2.48	6	G'_{58}	3.32	8
	0.69	2		0.36	0
	0.00	0		−1.00	−2
	−1.17	−2		−1.00	−2
	−2.00	−4		−1.68	−4
G''_{57}	2.86	7	G_{59}	3.65	9
	0.32	−1		0.00	0
	0.00	0		−1.00	−1
	−1.00	−1		−1.00	−1
	−2.18	−5		−1.65	−3
G'''_{57}	2.94	7	G_{510}	4.00	10
	0.62	1		−1.00	−2
	−0.46	−1		−1.00	−2
	−1.47	−1		−1.00	−2
	−1.62	−3		−1.00	−2

Table 5. Total net signs $S(G)$, the ordering of total-energy-like quantities $E(G)$ of various five-vertex graphs and the ordering of the relative stabilities of the neutral five-vertex clusters of C, Si and Ge according to other calculations [23, 32, 36, 98]

Graph	$S(G)$	$E(G)$	$C_5{}^a$	$C_5{}^b$	$C_5{}^c$	$Si_5{}^d$	$Si_5{}^e$	$Si_5{}^f$	$Ge_5{}^g$	$Ge_5{}^h$	Symmetry
G_{55}^{iv}	13	3	4	2	4	4	4	–	–	–	D_{5h}
G''_{54}	8	6	5	6	–	–	–	5	4	5	T_d
G_{54}	12	1	3	1	1	–	–	4	5	4	$D_{\infty h}$
G'_{55}	12	4	–	3	2	–	–	–	–	–	C_{2v}
G'''_{57}	15	–	–	–	–	–	–	1	2	3	C_{2v}
G_{58}	16	2	2	5	–	2	3	3	3	1	C_{4v}
G_{59}	17	5	1	4	3	1	1	2	1	2	D_{3h}
G_{510}	14	–	–	–	–	3	2	–	–	–	D_{3h}

[a] Data from Ref. [23]. [b] Data from Ref. [98] at HF/D95 or HF/D95* level. [c] Data from Ref. [98] at MP2/D95* level. [d] Data from Ref. [36] at HF, MP2, MP3, and MP4(SDQ) levels. [e] Data from Ref. [36] at MP4 level. [f] Data from Ref. [32] at SCF, SRCI, and full CI levels. [g] Data from Ref. [32] at SCF and SRCI levels. [h] Data from Ref. [32] at full CI level

empirical [23] or *ab initio* calculations [32, 36, 98]. If only the connection pattern among vertices is of main concern, five-vertex clusters would favor a more compact form, G_{58} or G_{59}, than the linear form. Graph G_{59} is isomorphic to a trigonal bipyramidal structure with T_{3d} point group symmetry and G_{58} isomorphic to a square pyramidal structure with C_{4v} point group symmetry. Same conclusions have been pointed out by Sharma [99] in the study of geometrical structures of Hubbard clusters. For comparison, we also present in Table 5 the ordering of relative stabilities of C_5, Si_5 and Ge_5 resulting from calculations at different levels of sophistication. As expected from net sign analysis, Si_5 and Ge_5 clusters favor the compact structures rather than the linear structures. Different levels of *ab initio* calculations gave different ordering as shown in Table 5. However, the preference of the compact form seems to confirm that the topological factor is important in determining the ground-state geometry of Si_5 and Ge_5 clusters. The reason for this can be rationalized by the relatively diffuse basis set provided by each atom in the bounding in clusters.

The situation in C_5 is quite different. Our results agree with those obtained from MINDO calculations [23] and the earlier thermal data. Recent *ab initio* calculations [32, 36, 98] and spectroscopic evidence, on the contrary, favor a linear ground-state geometry. By adopting the formula of overlap integral for $(2p\pi \mid 2p\pi)$ from Refs. [95 and 96], the total-energy-like quantity $E(G)$ of a graph can then be computed. As we compare the ordering of $E(G)$ to the ordering of relative stabilities of different geometries according to a specific level of calculation, the inter-vertex distance is taken as an average value over all bond lengths of the optimized geometry at that level. Variations of the orbital exponents lead to different extents of overlap. As we took 1.625, which is usually used in the extended Hückel calculation, for the orbital exponent, the ordering is found to fit into the ordering of relative stabilities obtained from MINDO calculation [23]. As the orbital exponent is larger than 2, the linear form would be the choice. Excellent agreement with the ordering in the relative stabilities of various geometries of C_5 from the *ab initio* calculations [32, 36, 98] can be reached at a value of 3.375 for the orbital exponent. The reason for this is not clear. However, beyond the topological consideration, the overlapping factor plays a key role in determining the ground-state geometry of the C_5 cluster.

4. Conclusions

Topological analyses of 5-vertex graphs were performed using net sign approach. An adjacency matrix is first established for each graph. Eigenvectors of the adjacency matrix are then described by VSG's, and the internal connectivities in eigenvectors are described by ESG's. The bonding capacity in each ESG is quantified by computing the net sign of the ESG. The ordering of the eigenvectors according to the net sign is found to be parallel to the ordering according to the eigenvalues in most 5-vertex graphs with few exceptions. Most exceptions can be rationalized by the recognition of the small energy difference between the two energy levels with reversed net sign ordering. The other rationale resides on the existence of a nodal plane crossing the four edges surrounding a central vertex. Further investigations of graphs having more than five vertices are currently underway.

For the ground-state geometry of five-vertex clusters composed by carbon, silicon, or germanium, it is found that the prediction of the simple net sign analysis agree quite well with those of *ab initio* calculations of Si_5 and Ge_5 clusters. For the carbon clusters, the prediction of net sign anaysis is found to be of excellent fit with that of the MINDO calculation. Modifications were made by including the overlapping factor in order to fit the results of *ab initio* calculation which predicted a linear geometry for the ground state of the C_5 cluster.

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