

# Molecular Topological Index and Its Application. 4. Relationships with the Diamagnetic Susceptibilities of Alkyl-IVA Group Organometallic Halides

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On the basis of four-energy-level model proposed previously, a new topological index  $H_1$  was introduced in the paper to investigate the diamagnetic susceptibility of the organometallics for the first time, which is essentially a kind of edge-weighted one in terms of the graph theory. The indices  $H_1$ 's of the alkyl-IVA group organometallic halides, including halogen-substituted methanes and ethanes along with those represented by  $(\text{CH}_3)_{4-n}\text{MX}_n$  ( $n = 0-4$ ;  $\text{M} = \text{Si}, \text{Ge}, \text{Sn}$ ), were calculated accordingly. Good linear relations were found between the  $H_1$ 's and the corresponding diamagnetic susceptibilities  $\chi_M$ 's for each series of compounds with similar graphic representations. Moreover, estimation of  $\chi_M$ 's was made as to the compounds whose values are not experimentally measured yet.

## INTRODUCTION

Magnetic susceptibilities  $\chi_M$ 's of stable organic species have long been observed to be approximately fit by a sum of atomic contribution, which was so-called Pascal's constants.<sup>1</sup> A subsequent expansion, motivated by the simple quantum chemical treatment, was developed by Hameka<sup>2,3</sup> and later by Flygare and co-workers,<sup>4</sup> which considers, besides atomic contributions, also bond contributions and bond-bond interactions. But a large number of experimental values of  $\chi_M$  are needed in order to obtain that large families of parameters. In some simple cases the theoretical calculation of  $\chi_M$  seems to be attractive, but most of the results thus obtained are quantitatively incomparable with the experimental values.<sup>5</sup> And for the methyl-IVA group organometallic halides, none of the above approaches proved to yield consistent results.<sup>6</sup>

The diamagnetic property of a compound is determined mainly by its molecular structure other than the bulk as a whole.<sup>7</sup> Hence, the application of graph theory in this connection may be of some merits, though the structures here are approximately represented by the graphs without taking into account of the geometrical details. In fact, many attempts have been made in this direction, from the Wiener<sup>8</sup> or Randić index<sup>9</sup> for alkanes, through the more sophisticated connectivity indices by Kier and Hall,<sup>10,11</sup> for both alkanes and aliphatic alcohols, to the cluster expansion method,<sup>12,13</sup> proposed more recently. As can be seen, a tendency in the construction of new topological indices (TI's) is followed<sup>14</sup> as the incorporation of more electronic structure information into a graph to get so-called chromograph; therefore the elements other than C, N, O, F, Cl, etc. can be fully described,<sup>15-17</sup> and the method can be largely extended to fit the use for the inorganic or organometallic compounds. Practically, there are two strategies to fulfill the aim, which are based on the two kinds of local graph invariants, viz., local vertex invariants associated with vertexes symbolizing atoms and local edge invariants corresponding to edges symbolizing covalent bonds. As we shall see, topological index  $H_1$  falls into the later catalog, and has been proven to

be quite effective in the correlation with the chemical shifts of NMR<sup>16</sup> in  $\text{MoO}_n\text{X}_{4-n}^{2-}$  ( $\text{X} = \text{S}, \text{Se}$ ), Mossbauer isomer shifts<sup>15</sup> in  $\text{SnX}_n\text{Y}_{4-n}$  ( $\text{X}, \text{Y} = \text{halogens}$ ) and the enthalpies of formation for series of compounds.<sup>17</sup> In the present contribution, we will continue to explore its applications to the study of the diamagnetic susceptibilities of group IVA organometallic halides.

## TOPOLOGICAL INDEX $H_1$

The procedure, which was once taken by Lall<sup>18</sup> and Xin,<sup>19</sup> is adopted here, viz., more information is taken into account as to the edges symbolizing the bonds in a molecule. Following Randić,<sup>9</sup> a new topological index  $H_1$  (eq 1) as proposed previously<sup>15</sup> was introduced as

$$H_1 = \left( \sum_i h_i \right)^2 = \left( \sum_i \frac{1}{(1 + \Delta_i)\sqrt{p_i q_i}} \right)^2 \quad (1)$$

where  $p_i$  and  $q_i$  are the degrees of the vertexes bridging the  $i$ th edge,  $h_i$  is the contribution from  $i$ th edge.  $\Delta_i$  is a parameter to describe the interaction in an edge (i.e., a bond), the summation goes over all edges in a molecular graph. It's worthwhile to note that the hydrogens in our graph are not suppressed while unusually done. Based on the four-energy-level assumption,<sup>15-17</sup>  $\Delta_i$  can be expressed as follows:

$$\Delta_i = \alpha[I_i(1) - A_i(2)] + (1 - \alpha)[I_i(2) - A_i(1)] \quad (2)$$


where  $I_i(n)$  and  $A_i(n)$  ( $n = 1, 2$ ) are the first ionization potentials and electron affinities of atoms 1 and 2 connected by the  $i$ th edge (Table 1). As illustrated previously,<sup>15</sup> the first term shows the electron transfer interaction from HAO of atom 1 to LUAO of atom 2, while the last term represents the feed back interaction from HAO of atom 2 to LUAO of atom 1, which may be very important in some cases, e.g., the back-donation of the lone pair of fluorine to the vacant p-orbital of boron greatly increases the stability of  $\text{BF}_3$ . In order to reflect the difference between the two kinds of interactions, the parameter  $\alpha$  can be adjusted. For simplicity, however,  $\alpha$  is empirically taken to be 0.5 in the following calculation, which means that two kinds of interactions are

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**Table 1.** First Ionization Potentials and Electron Affinities of the Atoms Adopted in the Calculations<sup>20</sup> (KJ mol<sup>-1</sup>)

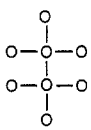
	F	Cl	Br	I	H	C	Si	Ge	Sn
I	1681.0	1251.1	1139.9	1008.4	1312.0	1086.4	786.5	762.2	708.6
A	322.0	348.7	324.5	295.0	72.9	122.0	120.0	116.0	121.0

**Table 2.**  $H_1$ 's and  $\chi_M$ 's (Unit: 10<sup>6</sup> cgs) of Halogen Substituted Methanes

molecular graph	no.	compd	$H_1 (\times 10^{-6})$	$-\chi_M^{\text{exp},21}$	$-\chi_M^{\text{calcd}}$
	1	CH <sub>3</sub> Cl	3.592	32.0	38.9
	2	CH <sub>2</sub> Cl <sub>2</sub>	3.909	46.6	50.5
	3	CHCl <sub>3</sub>	4.238	59.3	62.5
	4	CCl <sub>4</sub>	4.581	66.6	75.1
	5	CCl <sub>3</sub> Br	4.694	73.1	79.2
	6	CCl <sub>2</sub> Br <sub>2</sub>	4.808	81.1	83.4
	7	CBr <sub>4</sub>	5.040	93.7	91.9
	8	CBr <sub>3</sub> H	4.567	82.6	74.6
	9	CBr <sub>2</sub> H <sub>2</sub>	4.118	65.1	58.2
	10	CBrH <sub>3</sub>	3.692	42.8	42.6
	11	CBr <sub>2</sub> ClH	4.456	75.1	70.5
	12	CBrCl <sub>2</sub> H	4.347	66.3	66.5
	13	CBrClH <sub>2</sub>	4.013	55.0	54.3
	14	CCl <sub>3</sub> F	4.143	58.7	59.1
	15	CCl <sub>2</sub> F <sub>2</sub>	3.726	52.2	43.8
	16	CFH <sub>3</sub>	3.205	17.8	24.8
	17	CF <sub>2</sub> ClH	3.417	38.6	32.5
	18	CFCl <sub>2</sub> H	3.817	48.8	47.2

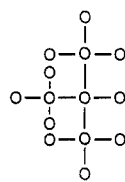
regression equation:  $-\chi_M = -89.575 + 35.930 \times 10^6 H_1$   
 correlation coefficient: 0.961; deviation max: 8.5; av: 4.3

**Table 3.**  $H_1$ 's and  $\chi_M$ 's (Unit: 10<sup>6</sup> cgs) of Halogen Substituted Ethanes

molecular graph	no.	compd	$H_1 (\times 10^{-6})$	$-\chi_M^{\text{exp},21}$	$-\chi_M^{\text{calcd}}$
	1	CHCl <sub>2</sub> CHCl <sub>2</sub>	12.71	89.8	90.7
	2	CH <sub>2</sub> ClCH <sub>2</sub> Cl	11.57	59.6	64.6
	3	CHCl <sub>2</sub> CCl <sub>3</sub>	13.30	99.1	104.2
	4	CCl <sub>3</sub> CCl <sub>3</sub>	13.90	112.7	117.9
	5	CH <sub>2</sub> BrCH <sub>2</sub> Br	11.93	78.8	72.9
	6	CBr <sub>3</sub> CBr <sub>3</sub>	15.10	148.0	145.4
	7	CClBrHCClBrH	13.09	108.6	99.4
	8	CBrCl <sub>2</sub> CBrCl <sub>2</sub>	14.29	126.0	126.8

regression equation:  $-\chi_M = -199.97 + 22.87 \times 10^6 H_1$   
 correlation coefficient: 0.980; deviation max: 9.2; av: 4.3

**Table 4.**  $H_1$ 's and  $\chi_M$ 's (Unit: 10<sup>6</sup> cgs) of (CH<sub>3</sub>)<sub>3</sub>MX

molecular graph	no.	compd	$H_1 (\times 10^{-6})$	$-\chi_M^{\text{exp},6}$	$-\chi_M^{\text{calcd}}$
	1	Me <sub>3</sub> SiCl	31.76	79.0	81.4
	2	Me <sub>3</sub> SiBr	22.19	91.3	91.3
	3	Me <sub>3</sub> SiI	32.75	104.1	104.7
	4	Me <sub>3</sub> GeCl	31.99	90.3	86.7
	5	Me <sub>3</sub> GeBr	32.42	98.5	97.0
	6	Me <sub>3</sub> SnCl	32.67	101.1	102.9
	7	Me <sub>3</sub> SnBr	33.15	112.5	114.1
	8	Me <sub>3</sub> SnI	33.80	130.7	129.4
	9	Me <sub>3</sub> GeI	33.01		110.8

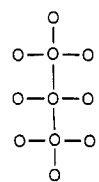
regression equation:  $-\chi_M = -668.338 + 23.603 \times 10^6 H_1$   
 correlation coefficient: 0.991; deviation max: 3.6; av: 1.6

equally important in the formation of a bond. Though such a postulate does not always hold, the effectiveness has been proven in the previous investigations.

## RESULTS AND DISCUSSION

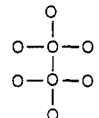
Diamagnetic susceptibilities of various alkanes and aliphatic alcohols have been investigated using the connectivity indices by Kier et al.<sup>11</sup> In most of the cases, up to seven different kinds of indices have been employed for a good

**Table 5.**  $H_1$ 's and  $\chi_M$ 's (Unit: 10<sup>6</sup> cgs) of (CH<sub>3</sub>)<sub>2</sub>MX<sub>2</sub>

molecular graph	no.	compd	$H_1 (\times 10^{-6})$	$-\chi_M^{\text{exp},6}$	$-\chi_M^{\text{calcd}}$
	1	Me <sub>2</sub> SiCl <sub>2</sub>	21.22	81.3	82.8
	2	Me <sub>2</sub> SiI <sub>2</sub>	22.85	131.8	125.6
	3	Me <sub>2</sub> GeCl <sub>2</sub>	21.44	91.6	88.7
	4	Me <sub>2</sub> GeBr <sub>2</sub>	22.16	107.0	107.5
	5	Me <sub>2</sub> GeI <sub>2</sub>	23.13	138.2	133.0
	6	Me <sub>2</sub> SnCl <sub>2</sub>	22.13	102.8	106.8
	7	Me <sub>2</sub> SnBr <sub>2</sub>	22.92	121.3	127.5
	8	Me <sub>2</sub> SnI <sub>2</sub>	24.00	153.5	155.7
	9	Me <sub>2</sub> SiBr <sub>2</sub>	21.9		101.0
	10	Me <sub>2</sub> SiClBr	21.56		91.8
	11	Me <sub>2</sub> SiBrI	22.38		113.3
	12	Me <sub>2</sub> SiClI	22.03		104.1
	13	Me <sub>2</sub> GeClBr	21.80		98.1
	14	Me <sub>2</sub> GeClI	22.28		110.7
	15	Me <sub>2</sub> GeBrI	22.64		120.1
	16	Me <sub>2</sub> SnClBr	22.52		117.0
	17	Me <sub>2</sub> SnClI	23.06		131.1
	18	Me <sub>2</sub> SnBrI	23.46		141.6

regression equation:  $-\chi_M = -473.112 + 26.203 \times 10^6 H_1$   
 correlation coefficient: 0.984; deviation max: 6.2; av: 3.6


**Table 6.**  $H_1$ 's and  $\chi_M$ 's (Unit: 10<sup>6</sup> cgs) of MeMX<sub>3</sub>

molecular graph	no.	compd	$H_1 (\times 10^{-6})$	$-\chi_M^{\text{exp},6}$	$-\chi_M^{\text{calcd}}$
	1	MeSiCl <sub>3</sub>	12.79	87.45	88.71
	2	MeSiBr <sub>3</sub>	13.60	115.5	111.2
	3	MeGeCl <sub>3</sub>	13.00	95.1	94.5
	4	MeGeBr <sub>3</sub>	13.84	120.5	117.7
	5	MeGeI <sub>3</sub>	15.00	158.25	150.04
	6	MeSnCl <sub>3</sub>	13.64	107.7	112.1
	7	MeSnBr <sub>3</sub>	14.57	129.8	138.0
	8	MeSnI <sub>3</sub>	15.88	172.1	174.1
	9	MeSiI <sub>3</sub>	14.73		142.4
	10	MeSiCl <sub>2</sub> I	13.42		106.2
	11	MeSiCl <sub>2</sub> Br	13.06		96.2
	12	MeSiClBrI	13.69		113.6
	13	MeSiBr <sub>2</sub> Cl	13.33		103.7
	14	MeSiBr <sub>2</sub> I	13.97		121.4
	15	MeSiClI <sub>2</sub>	14.06		123.9
	16	MeSiBrI <sub>2</sub>	14.35		131.9
	17	MeGeCl <sub>2</sub> Br	13.27		102.0
	18	MeGeCl <sub>2</sub> I	13.65		112.5
	19	MeGeClBrI	13.93		120.3
	20	MeGeBr <sub>2</sub> Cl	13.55		109.8
	21	MeGeBr <sub>2</sub> I	14.22		128.3
	22	MeGeClI <sub>2</sub>	14.32		131.1
	23	MeGeBrI <sub>2</sub>	14.61		139.1
	24	MeSnCl <sub>2</sub> Br	13.94		120.6
	25	MeSnCl <sub>2</sub> I	14.36		132.2
	26	MeSnClBrI	14.68		141.0
	27	MeSnClBr <sub>2</sub>	14.26		129.4
	28	MeSnBr <sub>2</sub> I	15.00		149.9
	29	MeSnClI <sub>2</sub>	15.11		153.0
	30	MeSnBrI <sub>2</sub>	15.43		161.82

regression equation:  $-\chi_M = -265.455 + 27.691 \times 10^6 H_1$   
 correlation coefficient: 0.984; deviation max: 8.3; av: 4.0

linear fitting of the experimental data. But the large families of variables used in the correlation need more experimental  $\chi_M$  values, which may not be the cases in practice. On the other hand, until now, the method is only limited to the organic compounds. As for the organometallics, intrinsic difficulty arises. But on our indices, no confinement is imposed at the point.

**Table 7.**  $H_1$ 's and  $\chi_M$ 's (Unit:  $10^6$  cgs) of  $MX_4$ 

molecular graph	no.	compd	$H_1 (\times 10^6)$	$-\chi_M^{\text{exp.6}}$	$-\chi_M^{\text{calcd}}$
	1	SiCl <sub>4</sub>	6.484	87.4	95.2
	2	SiBr <sub>4</sub>	7.266	123.3	119.8
	3	GeCl <sub>4</sub>	6.655	99.0	100.6
	4	GeBr <sub>4</sub>	7.469	129.2	126.2
	5	GeI <sub>4</sub>	8.630	170.9	162.7
	6	SnCl <sub>4</sub>	7.188	117.3	117.3
	7	SnBr <sub>4</sub>	8.105	148.8	146.2
	8	SnI <sub>4</sub>	9.424	195.6	187.7
	9	SiCl <sub>3</sub> Br	6.675		101.2
	10	SiCl <sub>3</sub> I	6.935		109.4
	11	SiCl <sub>2</sub> Br <sub>2</sub>	6.869		107.3
	12	SiCl <sub>2</sub> BrI	7.133		115.6
	13	SiCl <sub>2</sub> I <sub>2</sub>	7.401		124.0
	14	SiClBr <sub>3</sub>	7.066		113.5
	15	SiBr <sub>3</sub> I	7.537		128.3
	16	SiBr <sub>2</sub> I <sub>2</sub>	7.812		137.0
	17	SiClBr <sub>2</sub> I	7.333		121.9
	18	SiClI <sub>3</sub>	7.882		139.2
	19	SiBrI <sub>3</sub>	8.093		145.8
	20	SiClBrI <sub>2</sub>	7.605		130.5
	21	GeCl <sub>3</sub> Br	6.854		106.8
	22	GeCl <sub>3</sub> I	7.124		115.3
	23	GeCl <sub>2</sub> Br <sub>2</sub>	7.056		113.2
	24	GeCl <sub>2</sub> BrI	7.331		121.8
	25	GeCl <sub>2</sub> I <sub>2</sub>	7.610		130.6
	26	GeClBr <sub>3</sub>	7.261		119.6
	27	GeBr <sub>3</sub> I	7.752		135.1
	28	GeBr <sub>2</sub> I <sub>2</sub>	8.039		144.1
	29	GeClBr <sub>2</sub> I	7.540		128.4
	30	GeClI <sub>3</sub>	8.112		146.4
	31	GeBrI <sub>3</sub>	8.332		153.4
	32	GeClBrI <sub>2</sub>	7.823		137.3
	33	SnCl <sub>3</sub> Br	7.412		124.4
	34	SnCl <sub>3</sub> I	7.718		134.0
	35	SnCl <sub>2</sub> Br <sub>2</sub>	7.640		131.6
	36	SnCl <sub>2</sub> BrI	7.951		141.4
	37	SnCl <sub>2</sub> I <sub>2</sub>	8.268		151.3
	38	SnClBr <sub>3</sub>	7.571		138.8
	39	SnBr <sub>3</sub> I	8.426		156.3
	40	SnBr <sub>2</sub> I <sub>2</sub>	8.752		166.6
	41	SnBr <sub>2</sub> ClI	8.186		148.8
	42	SnClI <sub>3</sub>	8.836		169.2
	43	SnBrI <sub>3</sub>	8.508		158.9

regression equation:  $-\chi_M = -108.965 + 31.484 \times 10^6 H_1$   
 correlation coefficient: 0.988; deviation max: 8.2; av: 4.3

$H_1$  and the calculated  $\chi_M$ 's of several halogenated methanes are listed in columns 4 and 6, respectively, and good correlation coefficients ( $r = 0.961$ ) are found. The maximum and average deviation of the calculated  $\chi_M$ 's from those observed is  $8.5 \times 10^6$  cgs. As to the halogen substituted ethanes (Table 3), a good linear relation is also held with correlation coefficient  $r = 0.980$ , maximum deviation  $9.2 \times 10^6$  cgs. It can be seen that, for the organic halides, our topological index  $H_1$  derives a relationship as good as the others.

Up to date, no quantitative structure property relationship (QSPR) analysis has been made in the sense of topology for the organometallic compounds. The attempts to correlate the diamagnetic susceptibilities of  $(CH_3)_nMX_{4-n}$  ( $M = \text{Si, Ge, Sn; } n = 0-4$ ;  $X = \text{halogen}$ ) with  $H_1$ 's seem to be promising. For each set of compounds, no matter what kinds of central atoms (e.g., Si or Sn) are involved, only one linear relationship is observed for the same graphic representation, as listed in column one of Tables 4–7, with the least square fitting equations, correlation coefficients, calculated  $\chi_M$ 's, and the maximum as well as average deviations subsequently. It can be seen that the coefficients are generally larger than 0.98, while the maximum deviations demonstrate that the calcu-

lated  $\chi_M$ 's are within the reasonable accuracy compared with the experimental ones, which provides us confidence to the further estimation of the unknown  $\chi_M$ 's of various compounds. Accordingly, our estimated diamagnetic susceptibility values of various sets of organometallics are shown in Tables 4–7, which are subject to the future experimental test, especially for the organometallic mixed halides.

The success of the topological index  $H_1$  may not seem too surprising, if one express the eq 1 as follows:

$$H_1 = \sum_i h_i^2 + \sum_{i \neq j} h_i h_j \quad (3)$$

where the first term is the summation over all edges, which may be considered as contributions from each bond, while the last term is the summation over all pairs of edges, which may be considered as contributions from pairs of bonds, i.e., pairwise contributions. Hence, our topological index  $H_1$  has already combined two kinds of contributions together.

## CONCLUSION

In summary, our topological index  $H_1$  is proved to be quite simple and effective in the correlation with the diamagnetic susceptibility  $\chi_M$ 's of alkyl-group IV organometallic halides. The method is a powerful tool for the estimation of  $\chi_M$ 's with reasonable accuracy. Further exploring of its applications are in progress.

## ACKNOWLEDGMENT

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