STRUCTURE OF MATTER
AND QUANTUM CHEMISTRY

Graph Theory in Structure−Property Correlations[1]

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Abstract—The possibilities of the theoretical graph approach to the construction and interpretation of additive schemes for calculation and prediction are discussed. Working formulas are derived for calculating the thermodynamic properties of alkanes and their substitutes. The obtained algorithms are used to calculate thermodynamic properties of chloroalkanes that correspond to experimental values.

INTRODUCTION

Topological indices (TIs) are widely used in studying structure−property correlations. Some of them were considered in [1−6]. The aim of this work was to study theoretical graph−based structure−property correlations of alkanes and their substitutes.

GENERATION AND SYSTEMATIZATION OF ISOMERS

The study of a class of chemical compounds benefits from initially categorizing these objects. It is important to know not only the total number of species of the class (a list), but the type and number of isomers.

Methods of the theory of graph enumeration are used to investigate chemical isomers as combinatorial graphical objects. The number of isomeric alkanes and alkyl monoradicals (alcohols) was first counted by A. Keli [3] (on the basis of his theory of trees). His calculations were later refined and extended to other classes of compounds.

Graph theory describes C_nH_{2n+2} alkanes in the form of trees. The enumeration theory of graphs (using derived functions or numbered lists) allows us to calculate

(1) the total number of trees with n vertices (t_n);

(2) the number of chemical trees (N_n) whose vertex degrees do not exceed 4 (the number of structural isomers of alkanes[2] (Table 1));

(3) the number of root trees with the selected vertex (root), and the number of root trees with restrictions

on nonroot vertices (isomeric alkyl monoradicals) and so on.

Table 1 shows that six trees with six vertices can be constructed, but five isomeric hexanes are identified; 11 trees with seven vertices can be constructed, but nine isomeric heptanes exist; and so on.

PHENOMENOLOGICAL THEORY

From a phenomenological point of view, a molecule acts as a system of interacting atoms. Accepting this physical model of a molecule naturally assumes that some (extensive) property of substance P can be represented as the sum of the properties attributable to individual atom−atom interactions: single-centered

Table 1. Number of trees (t_n) and tree alkanes (N_n)

n	t_n	N_n	N	t_n	N_n
1	1	1	13	1301	802
2	1	1	14	3159	1858
3	1	1	15	7741	4347
4	2	2	16	19320	10359
5	3	3	17	48629	24894
6	6	5	18	123867	60523
7	11	9	19	317955	148284
8	23	18	20	823065	366319
9	47	35	21	2144505	910726
10	106	75	22	5623756	2278658
11	235	159	23	14828074	5731580
12	551	355	24	39299897	14490245
			25	104636890	36797588

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[1] This article was translated by the authors.
[2] For higher alkanes [7].

Table 2. Topological indices of the first 40 alkanes

№	Compound	p_1	p_2	p_3	p_4	p_5	p_6	R	W	Z	χ	MTI
1	Methane	0	0	0	0	0	0	0	0	1	0	0
2	Ethane	1	0	0	0	0	0	0	1	2	1.000	4
3	Propane	2	1	0	0	0	0	0	4	3	1.414	16
4	*n*-butane	3	2	1	0	0	0	0	10	5	1.914	38
5	2-Methylpropane	3	3	0	0	0	0	1	9	4	1.732	36
6	*n*-Pentane	4	3	2	1	0	0	0	20	8	2.414	74
7	2-Methylbutane	4	4	2	0	0	0	1	18	7	2.270	68
8	2,2-Dimethylpropane	4	6	0	0	0	0	4	16	5	2.000	64
9	*n*-Hexane	5	4	3	2	1	0	0	35	13	2.914	128
10	2-Methylpentane	5	5	3	2	0	0	1	32	11	2.770	118
11	3-Methylpentane	5	5	4	1	0	0	1	31	12	2.808	114
12	2,2-Dimethylbutane	5	7	3	0	0	0	4	28	9	2.561	106
13	2,3-Dimethylbutane	5	6	4	0	0	0	2	29	10	2.643	108
14	*n*-Heptane	6	5	4	3	2	1	0	56	21	3.414	204
15	2-Methylhexane	6	6	4	3	2	0	1	52	18	3.270	190
16	3-Methylhexane	6	6	5	3	1	0	1	50	19	3.308	182
17	3-Ethylpentane	6	6	6	3	0	0	1	48	20	3.346	174
18	2,2-Dimethylpentane	6	8	4	3	0	0	4	46	14	3.061	170
19	2,3-Dimethylpentane	6	7	6	2	0	0	2	46	17	3.181	168
20	2,4-Dimethylpentane	6	7	4	4	0	0	2	48	15	3.126	176
21	3,3-Dimethylpentane	6	8	6	1	0	0	4	44	16	3.121	162
22	2,2,3-Trimethylbutane	6	9	6	0	0	0	5	42	13	2.943	156
23	*n*-Octane	7	6	5	4	3	2	0	84	34	3.914	306
24	2-Methylheptane	7	7	5	4	3	2	1	79	29	3.770	288
25	3-Methylheptane	7	7	6	4	3	1	1	76	31	3.808	276
26	4-Methylheptane	7	7	6	5	2	1	1	75	30	3.808	272
27	3-Ethylhexane	7	7	7	5	2	0	1	72	32	3.846	260
28	2,2-Dimethylhexane	7	9	5	4	3	0	4	71	23	3.561	260
29	2,3-Dimethylhexane	7	8	7	4	2	0	2	70	27	3.681	254
30	2,4-Dimethylhexane	7	8	6	5	2	0	2	71	26	3.664	258
31	2,5-Dimethylhexane	7	8	5	4	4	0	2	74	25	3.626	270
32	3,3-Dimethylhexane	7	9	7	4	1	0	4	67	25	3.621	244
33	3,4-Dimethylhexane	7	8	8	4	1	0	2	68	29	3.719	246
34	2-Methyl-3-ethylpentane	7	8	8	5	0	0	2	67	28	3.719	242
35	3-Methyl-3-ethylpentane	7	9	9	3	0	0	4	64	28	3.682	232
36	2,2,3-Trimethylpentane	7	10	8	3	0	0	5	63	32	3.481	230
37	2,2,4-Trimethylpentane	7	10	5	6	0	0	5	66	19	3.417	242
38	2,3,3-Trimethylpentane	7	10	9	2	0	0	5	62	23	3.504	226
39	2,3,4-Trimethylpentane	7	9	8	4	0	0	3	65	24	3.553	236
40	2,2,3,3-Trimethylpentane	7	12	9	0	0	0	8	58	17	3.250	214

Symbols: p_l is the number of paths of length l = 1, 2, 3, 4, 5, 6; R is the number of triples of adjacent edges with a common vertex; W is the Wiener number; Z is the Hosoyi index; χ is the Randič connectivity index; and MIT is the Schultz molecular topological index. In [5, 6], these indices were given for all 35 nonanes and all 75 deans (a broader set of TIs was given for lower alkanes).

(p_α); two-centered or paired $(p_{\alpha\beta})$; three-centered or triple $(p_{\alpha\beta\gamma})$; and so on [3]:

$$P = \sum_n p_\alpha + \sum_{\alpha,\beta} p_{\alpha\beta} + \sum_{\alpha,\beta,\gamma} p_{\alpha\beta\gamma} + \ldots \quad (1)$$

N	N_n
30	4111846763
40	62481801147341
50	1117743651746953270
60	22158734535770411074184
70	471484798515330363034639871
80	10564476906946675106953415600016
90	2462451502428214396323044759956113295
100	5921072038125809849884993369103538010139

(a mathematical model). Summation is performed along all the atoms, their pairs, triples, and so on. The interactions between atoms in a molecule are separated into valence and nonvalence.

Equation (1) includes different physical properties: scalar (e.g., enthalpies of formation), vector (electric dipole moments), and tensor (polarizability, magnetic susceptibility) in both the gas and liquid phases, and in the solid state. It has a quantum mechanical and statistical basis [8−10] and actually allows direct calculations, which are very time-consuming.

In the phenomenological approach to alkanes (1), it follows that [3, 4]

$$P_{C_nH_{2n+2}} = a + bn + x_{cc_1}\Gamma_{cc}$$
$$+ x_{ccc_1}\Delta_{ccc} + x_{cc_2}\tau_{cc} + x_{cc_3}\omega_{cc} \quad (2)$$
$$+ x_{cc_4}\nu_{cc} + x_{cc_5}\mu_{cc} + x_{cc_6}O_{cc} + \ldots$$

where a and b represent valence; Γ_{cc} and Δ_{ccc} are effective nonvalent remote interactions between a pair and a trio of C atoms next to a single carbon atom; respectively; τ_{cc}, ω_{cc}, ν_{cc}, μ_{cc}, O_{cc}, are effective nonvalent remote interactions between pairs of C atoms at a distance of two, three, four, five and six carbon atoms, and so on; and x_{cc_1}, x_{ccc_1}, x_{cc_2}, and x_{cc_3} are the numbers of the relevant interactions. Equation (2) summarizes the familiar schemes of Fajan, Zahn, Allen et al.

TOPOLOGICAL INDICES

Many TIs have been proposed, including the familiar indices of Wiener (1947), Hosoya (1971), Randič (1975), Balaban (1982), Schultz (1989), Harare (1991), and others. Not all of these have a clear physical meaning and are equal in their ability to correlate with properties.

The most important TIs are p_l, the number of paths of length $l = 1, 2, 3, \ldots$ (in other words, the number of pairs of vertices, separated by l edges); R is the number of trios of adjacent edges with a common vertex; and so on (see. Table 2). Let us note other TIs:

1. The Wiener number (W), defined as half the sum of the elements of the distance matrix in a graph:

$$W = (1/2)\sum_{\sigma,\rho=1}^{n} d_{\sigma\rho} + p_1 + 2p_2 + 3p_3 + \ldots.$$

2. The Hosoya index (Z) is defined as the number of ways k edges without mutually common ends can be selected in graph G:

$$Z = \sum_k P(G,k).$$

By definition, $P(G, 0) = 1$, $P(G, 1) = m$ is the number of edges.

3. The Randič index (χ), known as the first-order ($^1\chi$) molecular connectivity index, can be expressed as

$$\chi = \sum_{\sigma,\rho}^{n} (r_\sigma r_\rho)^{-1/2}.$$

Where r_σ and r_ρ are the degrees of vertices σ and ρ that form an edge.

4. The molecular topological Schultz index (MTI), defined as the sum of matrix elements

$$v(A + D),$$

where A and D are the adjacency matrix and distance, and v is a matrix row of vertex degrees.

The number of interactions of skeletal atoms in (2) can be expressed in terms of topological indices p_l and R as

$$x_{cc_0} = p_1, \quad x_{cc_1} = p_2, \quad x_{ccc_1} = R,$$
$$x_{cc_2} = p_3, \quad p_4 = x_{cc_3}, \quad \ldots$$

An important feature of TIs is their discriminatory ability (capability for distinguishing isomers).

Carbon number n and indices expressed in terms of n (e.g., $p_1 = n - 1$) thus have little discriminating ability (high-degeneration), since they cannot differentiate isomeric alkanes (Table 2).

Indices p_2 and R partly distinguish between isomeric butanes and pentanes: hexanes, heptane, octane, and so on. However, they do not distinguish between 2-methylpentane and 3-methylpentane; 2,3-dimethylpentane and 2,4-dimethylpentane; and so on (Table 2). Indices p_3 or χ, distinguish between isomeric pentanes, hexanes, and heptanes; octanes, nonanes, and so on, partially. However, they do not distinguish between 3-and 4-methylheptane methylheptane; 3,4-dimethylhexane and 2-methyl-3-etilpentan; and so on. (Table 2). Indices p_4, p_5 ..., distinguish between isomeric alkanes more fully.

Table 3. Parameters of schemes and results from calculating the thermodynamic properties of chloroalkanes

Parameter	$\Delta_f H°(g, 298\ K)$, kJ/(mol K)	$S°(g, 298)$, J/mol	$\Delta_f G°(g, 298)$, kJ/mol	$C_p°(g, 298)$, J/(mol K)
a_0	−16.178	44.553	−14.314	6.903
b	10.413	−28.374	46.413	9.946
C	−33.904	99.081	−16.970	20.044
Γ_{CC}	1.492	−21.490	−3.207	0.715
Γ_{CX}	−6.473	−18.674	−16.836	−0.927
Γ_{XX}	4.676	−15.620	−7.002	−2.035
Δ_{CCC}	−5.741	−5.084	−2.263	0.038
Δ_{CCX}	−4.732	9.892	1.118	1.160
Δ_{CXX}	−0.223	7.284	9.145	2.431
Δ_{XXX}	2.730	1.715	13.721	3.877
τ_{CC}	1.805	−1.287	0.618	−1.517
τ_{CX}	−1.486	13.929	−7.415	−2.725
τ_{XX}	6.517	−0.930	6.945	0.084
ω_{CC}	−2.136	5.689	−8.826	−0.049
ω_{CX}	−2.778	−12.566	−7.170	−0.667
ω_{XX}	−1.388	−15.306	−0.835	4.792
$|\overline{\varepsilon}|$	1.3	2.1	1.9	0.7
ε_{max}	−6.0	8.9	−5.0	±2.8

The Wiener number (see Table 2) does not distinguish between the two pairs of heptanes (numbers 17, 20 and 18, 19) and the two pairs of octanes (28, 30, 32, 34); the Hosoya index does not differentiate between the four pairs of octanes (24, 33; 28, 38; 31, 32, 34, 35); the Randič index does not distinguish between the two pairs of octanes (25, 26 and 33, 34); and the Schulz index does not distinguish between two pairs octanes (26, 27 and 34, 37).

Along with topological (two-dimensional) indices, three-dimensional (topographic) indices are used that allow for the spatial structure of molecules.

METHODOLOGY OF STUDYING THE STRUCTURE–PROPERTY RELATIONSHIP

This methodology is based on the theoretical graph approach and includes the following steps [3–6].

1. Selecting objects of study (trial samples) and analyzing numerical data on the properties of *P* for this range of compounds.

2. Selecting TIs in light of their discriminating ability, ability to correlate with properties, and so on.

3. Studying the graphic dependences of property *P* on a TI of the molecular graph, e.g., of *P* on *n*, the number of skeletal atoms; and so on.

4. Establishing the functional (analytical) relationship $P = f(TI)$; in a more general case, $R = f(TI_1, TI_2,$

...) and defining (through optimization) parameters in these equations.

5. Numerical calculations of *P*, and comparing the calculated values to experimental values.

6. Predicting the properties of compounds not studied or even not synthesized (i.e., not included in the sample).

GRAPH THEORY AND ADDITIVE SCHEMES

Additive schemes of calculations can have a theoretical graph interpretations. In such algorithms, topological indices are used as the number of parameters.

In the theoretical graph approach, formula (2) takes the form

$$P_{C_nH_{2n+2}} = a + bn + p_2\Gamma_{CC}$$
$$+ R\Delta_{CCC} + p_3\tau_{CC} + p_4\omega_{CC}$$
$$= a_0 + p_1b + p_2\Gamma_{CC} + R\Delta_{CCC} + p_3\tau_{CC} + p_4\omega_{CC}$$

$(a_0 = a + b,\ a = -p_{C-C} + 2p_{C-H} = 2p_H,\ b = p_{CC} + 2p_{C-H} = p_C + 2p_H)$ и т.д.

For X-substituted alkanes (wherein X = F, Cl, Br, ...), we have

Table 4. Results from calculating the enthalpies and entropies of the formation of chloroalkanes

№	Molecule	$\Delta_f H°$(g, 298 K), kJ/mol		$S°$(g, 298), J/(mol K)	
		Experiment	Calculation	Experiment	Calculation
1.	CH_3Cl	−81.9 [11]	−82.4	234.6 [11]	232.7
2.	CH_2Cl_2	−95.4 [11]	−95.5	270.3 [11]	271.6
3.	$CHCl_3$	−102.7 [11]	−101.1	295.7 [11]	296.7
4.	CCl_4	−95.7 [11]	−96.6	309.9 [11]	309.5
5.	CH_3CH_2Cl	−112.1 [11]	−110.9	275.8 [11]	274.8
6.	CH_3CHCl_2	−127.7 [11]	−130.6	305.1 [11]	302.3
7.	CH_3CCl_3	−144.6 [11]	−143.2	323.1 [11]	323.2
8.	CH_2ClCH_2Cl	−126.4 [11]	−128.5	308.4 [11]	309.7
9.	$CH_2ClCHCl_2$	−144.7 ± 1.9 [12]	−141.8	337.1 [11]	336.3
10.	CH_2ClCCl_3	−149.4 [11]	−147.8	355.9 [11]	356.3
11.	$CHCl_2CHCl_2$	−149.2 [11]	−148.5	362.7 [11]	362.0
12.	$CHCl_2CCl_3$	−142.0 [11]	−148.0	381.5 [11]	381.0
13.	CCl_3CCl_3	−143.6 [11]	−141.0	398.7 [11]	399.1
14.	$CH_3CH_2CH_2Cl$	−131.9 [11]	−132.8	319.1 [11]	328.0
15.	$CH_3CHClCH_3$	−144.9 [11]	−142.5	304.2 [11]	305.3
16.	$CH_3CHClCH_2Cl$	−162.8 [11]	−161.7	354.8 [11]	354.1
17.	$CH_3CCl_2CH_3$	−173.2 [11]	−173.7	326.0 [11]	331.3
18.	$(CH_2Cl)_2CH_2$	−159.2 [11]	−159.9	367.2 [11]	362.4
19.	$(CH_2Cl)_2CHCl$	−182.9 [11]	−182.2	382.9 [11]	387.7
20.	$CH_3CCl_2CH_2Cl$	−185.8 [11]	−186.3	382.9 [11]	379.2
21.	$CH_3(CH_2)_2CH_2Cl$	−154.6 [11]	−154.2	358.1 [11]	353.4
22.	$CH_3CHClCH_2CH_3$	−161.2 [11]	−162.6	359.6 [11]	357.1
23.	$(CH_3)_2CHCH_2Cl$	−159.4 [11]	−159.0	355.0 [11]	354.6
24.	$(CH_3)_3CCl$	−182.2 [11]	−183.2	322.2 [11]	319.0
25.	$CH_3(CH_2)_3CH_2Cl$	−175.0 [11]	−175.0	397.0 [11]	397.0
26.	$(CH_3)_2CHCH_2CH_2Cl$	−179.7 [11]	−179.9	349.8 [13]	352.2
27.	$(CH_3)_2CClCH_2CH_3$	−202.2 [11]	−201.5	368.4 [13]	369.6

$$P_{C_nH_{2n+2}X_n} = a_0 + p_1 b + p_1' c + p_2 \Gamma_{CC}$$
$$+ p_2' \Gamma_{CX} + p_2'' \Gamma_{XX} + R\Delta_{CCC} + R'\Delta_{CCX} + R''\Delta_{CXX}$$
$$+ R'''\Delta_{XXX} + p_3 \tau_{CC} + p_3' \tau_{CX} + p_3'' \tau_{XX} + p_4 \omega_{CC}$$
$$+ p_4' \omega_{CX} + p_4'' \omega_{XX}.$$

Here, a_0 represents the number of C–H bonds; p_l is the number of paths of length 1, 2, ...; R, R', R'', R''' is the number of trios of adjacent edges; b and c are the numbers of C–C and C–X; and Γ_{CC}, Γ_{CX}, Γ_{XX}, Δ_{CCC}, Δ_{CCX}, Δ_{CXX}, Δ_{XXX}, τ_{CC}, ...are the effective interactions between pairs and trios of the considered atoms over one, two, ..., atoms along the chain of a molecule.

NUMERICAL CALCULATIONS

Numerical calculations of the enthalpy of formation, entropy, heat capacity and Gibbs energy are performed according to this algorithm. Table 3 shows the values of the relevant properties, the mean absolute error of calculation $|\bar{\varepsilon}|$, and the maximum deviation ε_{max}. Table 4 presents the results from calculating the enthalpy and entropy of formation of chloroalkanes, while Table 5 contains the Gibbs energies and heat capacities.

The calculated values are consistent with experimental values and have a high degree of accuracy (within the experimental error) in predicting the missing values for the properties of this class of compounds.

Table 5. Results from calculating the Gibbs energies and heat capacities of chloroalkanes

№	Molecule	$\Delta_f G°$(g, 298). kJ/mol		$C_p°$(g, 298). J/(mol K)	
		Experiment	Calculation	Experiment [11]	Calculation
1.	CH_3Cl	−58.5 [11]	−59.1	40.8	40.8
2.	CH_2Cl_2	−68.9 [11]	−69.6	51.0	51.9
3.	$CHCl_3$	−76.0 [11]	−72.5	65.7	64.8
4.	CCl_4	−53.6 [11]	−55.0	83.4	83.5
5.	CH_3CH_2Cl	−60.5 [11]	−59.0	62.6	63.6
6.	CH_3CHCl_2	−73.8 [11]	−76.3	76.2	76.2
7.	CH_3CCl_3	−76.2 [11]	−77.8	93.3	93.1
8.	CH_2ClCH_2Cl	−73.9 [11]	−71.5	78.7	75.9
9.	$CH_2ClCHCl_2$	−77.5 [11]	−81.9	89.0	88.6
10.	CH_2ClCCl_3	−80.3 [11]	−76.5	102.7	105.5
11.	$CHCl_2CHCl_2$	−85.6 [11]	−85.4	100.8	101.3
12.	$CHCl_2CCl_3$	−70.3 [11]	−73.0	118.1	118.4
13.	CCl_3CCl_3	−54.9 [11]	−53.6	136.7	135.5
14.	$CH_3CH_2CH_2Cl$	−50.7 [11]	−51.8	84.6	85.3
15.	$CH_3CHClCH_3$	−62.5 [11]	−60.1	87.3	88.3
16.	$CH_3CHClCH_2Cl$	−83.1 [11]	−80.1	98.2	97.8
17.	$CH_3CCl_2CH_3$	−84.6 [11]	−84.0	105.9	103.5
18.	$(CH_2Cl)_2CH_2$	−82.6 [11]	−79.5	99.6	99.6
19.	$(CH_2Cl)_2CHCl$	−97.8 [13]	−100.9	–	112.2
20.	$CH_3CCl_2CH_2Cl$	−97.8 [11]	−97.0	112.2	113.2
21.	$CH_3(CH_2)_2CH_2Cl$	−38.8 [11]	−43.8	107.6	107.6
22.	$CH_3CHClCH_2CH_3$	−53.5 [11]	−52.3	108.5	108.5
23.	$(CH_3)_2CHCH_2Cl$	−49.7 [11]	−50.1	108.5	107.8
24.	$(CH_3)_3CCl$	−64.1 [11]	−65.6	114.2	114.9
25.	$CH_3(CH_2)_3CH_2Cl$	−37.4 [11]	−37.4	130.5	130.5
26.	$(CH_3)_2CHCH_2CH_2Cl$	−43.7 [13]	−41.2	–	130.6
27.	$(CH_3)_2CClCH_2CH_3$	−56.5 [13]	−57.2	–	133.6

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