The Characteristic Polynomial Uniquely Represents the Topology of a Molecule

YOSHIHIRO KUDO
Japan Electron Optic Laboratory, Tokyo, Japan

TORU YAMASAKI and SHIN-ICHI SASAKI*
Miyagi University of Education, Sendai, Japan

Received July 13, 1973

Chemical structures can be expressed unamibigously with both the atom connectivity matrix and its characteristic polynomial.

Spialter[1-3] has proposed that chemical compounds are topologically expressed by the atom connectivity matrix (ACM) and its characteristic polynomial (ACMCP), and that a specific ACMCP uniquely relates to a specific molecular structure. Balaban[4] and Hosoya,[5,6] on the other hand, have shown that the "ACMCP" does not always correspond to a specific structure. The difference originates in the definition that their "ACMCP" is identical with Spialter's hydrogen (monovalent atom) suppressed ACMCP (HS-ACMCP). Actually, the fact that a cospectral HS-ACMCP was derived from a pair of structures whose ACMCP's are different from each other was described by Spialter himself in 1964,[3,4] and he also emphasized in the paper that the molecular structure should be expressed by such a matrix involving the atom connectivity which completely satisfies the atomic valency to extract minimum and essential information with regard to the structure. Hence, an appropriate collocation is necessary to avoid confusion. The following is suggested to clarify the ACMCP terminology.

Any structure can be unambiguously expressed with both the ACM and the component connectivity matrix (CCM) in which each diagonal element corresponds to its attribute—for example, CH_3, or CH_2, or others. The ACM and CCM then lead to the atom connectivity matrix determinant polynomial (ACMDP) which contains both the ACMCP and the component connectivity matrix determinant polynominal (CCMDP), respectively. The ACM, ACMDP, CCM, and CCMDP are illustrated in Figure 1 for ethanol. If the monovalent atom is hydrogen, the monovalent atom suppressed ACMDP would become HS-ACMCP, and Balaban's and Hosoya's ACMCP's.

The computation method for generating all possible isomeric structures in full agreement with the information on partial structures has already been established by our work on automated analysis of organic compounds.[7,8] We wish to discuss the ACMDP in relation to the method for counting quickly the number of isomers which makes the computation system much more practical and efficient. Our work supports the view that the total number of ACMDP's is equivalent to the total number of structural isomers. For our structures, several sets of "isomorphoric" graphs exemplified by Balaban and Hosoya were chosen.

The results of our evaluation of ACMDP's are shown in Table I, in which the total number of terms in the ACMDP's, and the coefficients which differentiate each from the other ACMDP's, are given for each "cospectral" set cited.[4-6] Table I also shows that the terms consisting of the highest power of monovalent hydrogen atom assigned to $aC^9 + bC^7 + dC^5 + eC^3$, for 2,3,3-trimethylhexane, and equivalent to HS-ACMCP. In this case, a, b, d, and e are equal to 1, −8, 17, and −10, respectively. Thus all the results so far tested, show that ACMDP's and CCMDP's, though the latter are omitted in this paper, for different structures are different from each other. Therefore, as already indicated, neither monovalent atom suppressed ACMDP nor HS-ACMCP are lacking in the explicit information of atomic connectivity. They do represent the molecular structure, and the topological expressions serve as indices for chemical compounds. Our work shows that the ACMDP contains atomic connectivity information, and that the ACMDP uniquely and unambiguously corresponds to a structure.

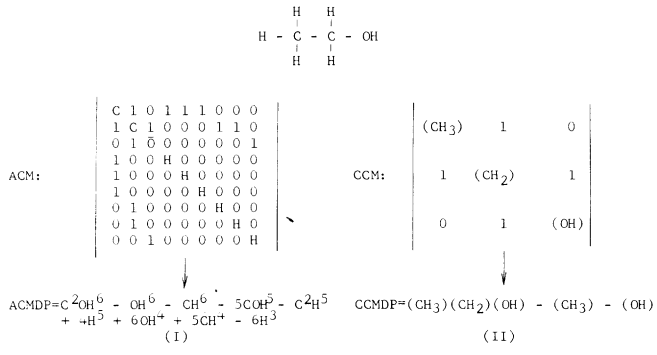

Figure 1. Two expressions for ethyl alcohol derived from either the atom connectivity (I) or the component connectivity (II)

*To whom inquiries should be addressed.

Table I. The Sets of ACMDP Containing Information on Monovalent Atoms

C_9H_{20}

ACMDP: $(aC^9+bC^7+dC^5+eC^3)H^{20} + (fC^8+gC^6+hC^4+iC^2)H^{19} + \cdots\cdots$[a]

Coefficients

Set	a	b	d	e	f	g	h	i	Total terms
2,3,3-trimethylhexane[5,6]	1	−8	17	−10	−20	134	−218	86	27
3-ethyl-2,2-dimethylpentane[5,6]	1	−8	17	−10	−20	134	−218	84	27
2,2-dimethylheptane[5,6]	1	−8	18	−10	−20	132	−228	84	27
2,3,5-trimethylhexane[5,6]	1	−8	18	−10	−20	132	−228	86	28
4,4-dimethylheptane[5,6]	1	−8	18	−12	−20	132	−224	98	27
2,3,4-trimethylpentane[5,6]	1	−8	18	−12	−20	132	−226	100	28

C_9H_{20}

ACMDP: $(aC^9+bC^7+dC^5+eC^3+fC^1)H^{20} + (gC^8+hC^6+iC^4+jC^2+kC^0)H^{19} + \cdots\cdots$

Coefficients

Set	a	b	d	e	f	g	h	i	j	k	Total terms
3,3-dimethylheptane[5,6]	1	−8	18	−12	2	−20	132	−224	94	−6	29
2,3,4-trimethylhexane[5,6]	1	−8	18	−12	2	−20	132	−226	96	−6	30
2,3-dimethylheptane[5,6]	1	−8	19	−14	2	−20	130	−232	110	−6	30
3-ethyl-5-methylhexane[5,6]	1	−8	19	−14	2	−20	130	−232	108	−6	30

$C_{10}H_{22}$

ACMDP: $(aC^{10}+bC^8+dC^6+eC^4+fC^2)H^{22} + (gC^9+hC^7+iC^5+jC^3+kC^1)H^{21} + \cdots$

Coefficients

Set	a	b	d	e	f	g	h	i	j	k	Total terms
2,3-dimethyloctane[5,6]	1	−9	26	−27	8	−22	164	−370	270	−44	35
3-ethyl-2-methylheptane[5,6]	1	−9	26	−27	8	−22	164	−370	268	−42	35

$C_{10}H_{22}$

ACMDP: $(aC^{10}+bC^8+dC^6+eC^4+fC^2)H^{22} + \cdots + (gC^8+hC^6+iC^4+jC^2+kC^0)H^{20} + \cdots$

Coefficients

Set	a	b	d	e	f	g h	i j	k	Total terms
4,5-dimethyloctane[5,6]	1	−9	26	−28	9	215 − 1292	2144 − 1007	64	35
3-ethyl-2-methylheptane[5,6]	1	−9	26	−28	9	215 − 1292	2144 − 1007	63	35

X_6Y_{16}[b]

ACMDP: $(aX^6+bX^4+dX^3+eX^2+fX^1+fX^0)Y^{16} + (hX^5+iX^3+jX^2+kX^1+mX^0)Y^{15} + \cdots$

Coefficients

Set	a	b	d	e	f	g	h	i	j	k	m	Total terms
G1[2]	1	−7	4	7	−4	−1	−16	84	−40	−44	16	21
G2[2]	1	−7	4	7	−4	−1	−16	80	−40	−40	16	22

W_7Y_{20}[b]

ACMDP: $(aW^7+bW^5+dW^4+eW^3+fW^2)Y^{20} + (gW^6+hW^4+iW^3+jW^2+kW^1)Y^{19} + \cdots$

Coefficients

Set	a	b	d	e	f	g	h	i	j	k	Total terms
G3[2]	1	−11	10	16	−16	−20	164	−130	−136	100	26
G4[2]	1	−11	10	16	−16	−20	164	−136	−128	104	26
G5[2]	1	−11	10	16	−16	−20	168	−136	−140	96	25

X_8Y_{26}[b]

ACMDP: $(aX^8+bX^6+dX^4)Y^{26} + (eX^7+fX^5+gX^3)Y^{25} + (hX^5+iX^4+jX^2)Y^{24} + \cdots$

Coefficients

Set	a	b	d	e	f g	h i	j	Total terms
T1[2]	1	−7	9	−26	150 − 144	289 − 1320	864	21
T2[2]	1	−7	9	−26	150 − 144	289 − 1328	816	20

(Continued)

Table I Continued

	$C_{12}H_{26}$										
	ACMDP: $(aC^{12}+bC^{10}+dC^{8}+eC^{6}+fC^{4})H^{26} + (gC^{11}+hC^{9}+iC^{7}+jC^{5}+kC^{3})H^{25} + \cdots$ Coefficients										
Set	a	b	d	e	f	g	h	i	j	k	Total terms
$T3^2$	1	−11	40	−55	21	−26	250	−768	848	−232	44
$T4^2$	1	−11	40	−55	21	·	·	·	·	−240	44

[a] Each dot means the coefficient uncounted.
[b] W = pentavalent element; X = hexavalent element; Y = monovalent element.

LITERATURE CITED

(1) Spialter, L., *J. Amer. Chem. Soc.* **85,** 2012 (1963).
(2) Spialter, L., *J. Chem. Doc.* **4,** 261 (1964).
(3) *Ibid.*, **4,** 269 (1964).
(4) Balaban, A. T., and Harary, F., *Ibid.*, **11,** 258 (1971).
(5) Mizutani, K., Kawasaki, K., and Hosoya, H., *Natur. Sci. Rep. Ochanomizu Univ.* **22,** 39 (1971).
(6) Hosoya, H., *J. Chem. Doc.* **12,** 181 (1972).
(7) Sasaki, S., Kudo, Y., Ochiai, S., and Abe, H., *Mikrochim. Acta* **1971,** 726.
(8) Sasaki, S., Kudo, Y., Ochiai, S., and Fujioka, I., *Jap. Anal.* **22,** 25 (1973).