

fast computer scanning, is the "truncated" ACMCP. This is obtained by considering only the first three of four terms of the ACMCP for indexing and then hand-sorting for further selection. This approximation method is particularly convenient because, with techniques described elsewhere,²⁵ it is possible to compute the value of the first few coefficients by simple inspection of the molecular pictograph without the necessity of constructing the ACM and reducing it to the polynomial. This visual computation technique is rapid, screens a large quantity of data efficiently, and yet maintains a close discernible rapport between the chemical and the mathematical concepts of the ACM-ACMCP nomenclature. As such it lends itself to personal filing systems, commercial chemical catalog listing, and the like.

It must be emphasized that most of the specific details of formulation and procedure discussed above need not be the concern of the average chemist. He is free to converse with his colleagues by means of molecular pictographs, as

he now does, even in abstracts,³⁰ or by compound names, systematic or trivial, but he leaves most of the literature searching and data retrieval—particularly that related to specific compounds—to computer-based systems. His link to and from the computer is the pictograph, but the ACM-ACMCP concept is suggested as providing the working language within the storage-retrieval system.

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(30) Note, for example, the publication "Index Chemicus," Institute for Scientific Information, Philadelphia, Pa.

The Atom Connectivity Matrix Characteristic Polynomial (ACMCP) and Its Physico-Geometric (Topological) Significance*

By LEONARD SPIALTER

Chemistry Research Laboratory, ARL, Wright-Patterson Air Force Base, Ohio

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INTRODUCTION

The concept of the Atom Connectivity Matrix (ACM) and its characteristic polynomial (ACMCP) as a computer-oriented nomenclature for chemical pictographs has been described elsewhere.^{1,2} The ACM is an array in which symbols for the constituent atoms or vertices of a pictograph (chemical or otherwise) are placed as mathematical elements in the main diagonal, and values or symbols for the respective connectivities for pairs of atoms are entered at appropriate off-diagonal column-row intersections. The ACMCP is derivable from the ACM by any of a number of algebraic processes.³

The ACM is clearly directly relatable, datum-by-datum, to its pictographic progenitor. However, it appeared initially that, in the process of transforming the ACM into the ACMCP, any physical significance would be lost and the ACMCP would be simply a collection of mathematical artifacts, exceedingly useful but physically and chemically meaningless. Such proved *not* to be the case.

The Homoatomic ACMCP.—If one takes a homoatomic⁴ ACM of completely general connectivity, such as the fifth-order symmetric ACM⁵

$$\begin{vmatrix} X & p & q & r & s \\ p & X & t & u & v \\ q & t & X & w & y \\ r & u & w & X & z \\ s & v & y & z & X \end{vmatrix}$$

(where X represents the homoatom; i and j are running indexes (from 1 to 5) to identify row and column, respectively; and p, q, r, \dots, w, y, z represent the appropriate connectivity between the X_i and X_j atoms) and determines the coefficients of each degree in X, in the related ACMCP, the following results are obtained.

$$\begin{aligned} \text{Coeff. of } X^5: & 1 \\ \text{Coeff. of } X^4: & 0 \\ \text{Coeff. of } X^3: & -(p^2 + q^2 + r^2 + s^2 + t^2 + u^2 + v^2 + w^2 + y^2 + z^2) \\ \text{Coeff. of } X^2: & +2(pqt + prv + psu + qrv + qsv + rsz + tuw + tvy + \\ & \quad uwz + wyz) \\ \text{Coeff. of } X: & -[2(pquw + pqvy + prt v + prvz + psty + psuz + \\ & \quad qrut + qryz + qstv + qsuw + rsuv + rsvy + tvyz + \\ & \quad twvz + uvwy) - \\ & \quad (p^2w^2 + p^2y^2 + p^2z^2 + q^2u^2 + q^2v^2 + q^2z^2 + r^2t^2 + \\ & \quad r^2v^2 + r^2y^2 + s^2t^2 + s^2u^2 + s^2w^2 + t^2z^2 + u^2y^2 + \\ & \quad v^2w^2)] \\ \text{Constant term:} & +2[(pqvyz + pqvuz + prtyz + prvuy + pstwz + \\ & \quad psuwy + qrtvz + qruvy + qstuz + qsuwv + rstuy + \\ & \quad rstvw) - (p^2wyz + q^2uwz + r^2tvz + s^2twv + t^2rsz + \\ & \quad u^2qsv + v^2qrw + w^2psv + y^2pru + z^2pqt)] \end{aligned}$$

* A portion of this subject material was presented before the Chemical Abstracts Research and Development Division, Columbus, Ohio, Aug. 15, 1963, and before the Chemical Information and Data System (CIDS) Phase IV Workshop, U. S. Army Missile Command, Huntsville, Ala., Nov. 12-14, 1963.

(1) L. Spialter, *J. Am. Chem. Soc.*, **85**, 2102 (1963).

(2) L. Spialter, *J. Chem. Doc.*, **4**, 261 (1964).

(3) Methods and mathematical nomenclature herein used are to be found in any text or reference on matrix algebra, matrix calculus, or determinants. For the sake of brevity and concentration on the newer concepts introduced in this work, standard operations will not be detailed.

(4) For the sake of simplicity in understanding the initial development, it is preferable that all atoms in the diagonal be made equivalent. Extension to heteroatomic systems will be presented later.

(5) The symmetric case is representative of a molecule or transition state.⁶