of graph orbits on the basis of the distance matrix. Efforts in this direction, as well as toward applications of the present and further generalizations of the notion of graph center in the fields of chemical nomenclature, computer processing of chemical structures, and synthetic strategy for organic structures are in progress.[25]

ACKNOWLEDGMENT

We thank Dr. M. Randić for his manuscripts prior to publication, and to Mr. A. Zamora for helpful suggestions in revising the paper.

REFERENCES AND NOTES

(1) F Harary, "Graph Theory", Addison-Wesley, Reading, Mass., 1969.
(2) D. Konig, "Theorie der endichen und unendlichen Graphen", Akademieverlagsgesellschaft, m.b.H., Leipzig, 1936, p 64.
(3) R. G. Busacker and T. L. Saaty, "Finite Graphs and Networks. An Introduction with Applications", McGraw-Hill, New York, 1965, p 200.
(4) M. Randić, *Chem. Phys. Lett.*, in press.
(5) M. Randić and C. L. Wilkins, *Chem. Phys. Lett.*, **55**, 547 (1978).
(6) M. Randić, G. M. Brissey, R. B. Spencer, and C. L. Wilkins, *Comput. Chem.*, in press.
(7) M. Randić and D. Bonchev, to be submitted for publication.
(8) D. Bonchev, M. Randić, and A. T. Balaban, *Int. J. Quantum Chem.*, in press.
(9) I. Gutman, M. Ruscić, N. Trinajstić, and C. F. Wilcox, Jr., *J. Chem. Phys.*, **62**, 3399 (1975).
(10) A. T. Balaban, *Theor. Chim. Acta* in press.
(11) C. Shannon and W. Weaver, "Mathematical Theory of Communications", University of Illinois, Urbana, Ill., 1949.
(12) L. Brillouin, "Science and Information Theory", Academic Press, New York, 1956.
(13) A. Katz, "Principles of Statistical Mechanics—The Information Theory Approach", Freeman, San Francisco, 1967.
(14) D. Bonchev, D. Kamenski, and V. Kamenska, *Bull. Math. Biol.*, **38**, 119 (1976).
(15) D. Bonchev and N. Trinajstić, *J. Chem. Phys.*, **67**, 4517 (1977).
(16) D. Bonchev and V. Kamenska, *Croat. Chem. Acta*, **51**, 19 (1978).
(17) D. Bonchev, "Proceedings of the Bremen Conference on Mathematical Structures in Chemistry, Bremen, 1978", *Math. Chem.*, **7**, 65 (1979).
(18) R. F. Muirhead, *Proc. Edinburgh Math. Soc.*, **19**, 36 (1901); **21**, 144 (1903); **24**, 45 (1906).
(19) G. H. Hardy, J. E. Littlewood, and G. Polya, "Inequalities", Cambridge University Press, London, 1934, p 44.
(20) R. C. Read and R. S. Miller, "A New System for the Designation of Chemical Compounds for the Purposes of Data Retrieval. I. Acyclic Compounds", Preprint, University of the West Indies, Jamaica, 1969.
(21) J. Lederberg, G. L. Sutherland, B. G. Buchanan, E. A. Feigenbaum, A. V. Robertson, A. M. Duffield, and C. Djerassi, *J. Am. Chem. Soc.*, **91**, 2973 (1969).
(22) L. Masinter, N. S. Sridharan, J. Lederberg, and D. H. Smith, *J. Am. Chem. Soc.*, **96**, 7702 (1974).
(23) A. T. Balaban and F. Harary, *Tetrahedron*, **24**, 2505 (1968); A. T. Balaban, *ibid.*, **25**, 2949 (1969); *Rev. Roum. Chim.*, **18**, 635 (1973); erratum *ibid.*, **19**, 338 (1974); *Math. Chem.*, **2**, 51 (1976).
(24) A. T. Balaban and P. v. R. Schleyer, *Tetrahedron*, **34**, 3599 (1978).
(25) A. T. Balaban and D. Bonchev, *Tetrahedron*, submitted for publication.

Automatic Generation of the Chemical Ringcode from a Connectivity Table

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Received December 10, 1979

A software package is described which generates automatically the General Chemical Ringcode from the connectivity table used by the IDC (Internationale Dokumentationsgesellschaft für Chemie mbH, Fachinformationszentrum Chemie). The conversion package, written for an IBM 370 computer, comprises, in addition to the main program written in Assembler, 35 subroutines of which 33 are written in Fortran, the remaining two in Assembler. The project was induced by the PDR (Pharma Dokumentationsring, e.V.), and supported by the BMFT (Bundesminister für Forschung und Technologie) under the scope of the program of the Federal Government of Germany for the promotion of Information and Documentation 1974 – 1977.

The target of the project was to reach compatibility between two different chemical documentation systems and between connectivity and fragmentary code records, and to create a powerful screen for atom-by-atom searches to optimize chemical structure retrieval.

The Ringdoc. The Pharma Dokumentationsring e.V. (PDR), a union of 18 European pharmaceutical companies and institutions, uses the Ringcode[1] for the encoding of organic chemical structures. The Ringcode, which was developed about 20 years ago by the founder members, is a fragmentary code. Code fragments are, for example, rings, chains, substitutents, functional groups, types of ring-condensation, positions of heteroatoms in a ring, positions of substituents, etc. Each fragment is associated with a defined position in 27 columns of a punched card. This means that all structural information can be coded in 27 × 12 = 324 positions or fragments of the General Chemical Code. Special codes were developed for the coding of steroids, inorganics, carbohydrates, and peptides. Usually one punched card per structure is sufficient. But in some cases additional cards are necessary, e.g., organic salts (separate coding of anion and cation) and adducts. Figure 1 shows the coding sheet for 3-(β-dimethylaminoethyl)indoline.

THE CONNECTIVITY TABLE (CT)

The CT used by the IDC (also known as BASF, main matrix[2]), which is the source for the Ringcode generation, consists of 200 lines and 26 columns. Figure 2 shows the table of the already-mentioned 3-(β-dimethylaminoethyl)indoline.

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Klartext:

1/12 SONDER-SCHLÜSSEL	2/12 1	3/12 ISOLIERT	4/12 ISOLIERT	5/12 LINEAR	6/12 ISOLIERT	7/12 POLY	8/12 POLY	9/12 POLY	10/12 POLY	11/12 POLY	12/12 POLY	13/12 POLY	14/12 POLY	15/12 POLY	16/12 LINEAR
1/11 STEROID	2/11 ~~2~~	3/11 KOND. AROMAT.	4/11 KOND. ALICYCL.	5/11 ANGULAR	6/11 KOND. HET. CYCL.	7/11 MEHR. GL. X i.e. RING	8/11 X ZU MEHR. RING	9/11 ANG.-SUBST.	10/11 ~~HETERO-~~ CYCLUS	11/11 ~~2~~	12/11 >CH3	13/11 -C- -C-,CX,C=Y	14/11 1	15/11 CIS	16/11 GEKREUZT
1/Ø KOHLEN-HYDRAT	2/Ø 3	3/Ø KOND. ALICYCL.	4/Ø KOND. HET. CYCL.	5/Ø ANG.-ANG.	6/Ø ⬡	7/Ø MEHR. UNGL. X i. e. RING	8/Ø ~~α~~	9/Ø GEM. SUBST.	10/Ø HETERO-SUBSTIT.	11/Ø 3	12/Ø -CH	13/Ø C-X C-X	14/Ø 2	15/Ø TRANS	16/Ø KETTE KETTE
1/1 EIWEISS	2/1 4	3/1 ~~KOND. HET. CYCL.~~	4/1 ⬡(1)	5/1 PERI	6/1 ⬡	7/1 ~~1 N~~	8/1 β	9/1 ALICYCLUS	10/1 ALICYCLUS	11/1 4	12/1 -C-	13/1 C-X C-X'	14/1 3	15/1 $A_2C=CA_2$ $A>C=CA_2$	16/1 KETTE RING
1/2 NUCLEIN-SÄUREN	2/2 5	3/2 ~~1~~	4/2 ⬡(2)	5/2 BRÜCKE	6/2 ⬡	7/2 2 N	8/2 1,2	9/2 α	10/2 ~~2~~ 1	11/2 5/10	12/2 CH_3X	13/2 C-Xm C-Xm C-Xn C-X n	14/2 4/6	15/2 >C=CA₂	16/2 KETTE AROMAT.
1/3 AND. NATUR-STOFFE	2/3 ≧6	3/3 2	4/3 ⬡(≧3)	5/3 SPIRO	6/3 ⬡(1)	7/3 3 N	8/3 1,3	9/3 β	10/3 β 2	11/3 11/16	12/3 ~~$-CH_2N$~~ (KETTE)	13/3 C-X C=Y	14/3 ≧7	15/3 $A>C=C<^{A}$	16/3 ~~RING~~ RING
1/4 KUNSTST. U. A. POLYM.	2/4 ISOLIERUNG AUS	3/4 3	4/4 ⬡(1)	5/4 7 MIT 3 F	6/4 ⬡(≧2)	7/4 ≧4 N	8/4 1, ≧4	9/4 1,2	10/4 1,2 3	11/4 ≧17	12/4 $-CH_2X$ (KETTE)	13/4 C-X C=C	14/4	15/4 $>C=C<^{A}$	16/4 BEI ≧6 RINGGL.
1/5	2/5 NACHWEIS	3/5 4	4/5 ⬡(≧2)	5/5 ≧7 UNGES.	6/5 ⬡	7/5 1 0	8/5 ≧3 SYM.	9/5 1,3	10/5 1,3 4	11/5 1	12/5 >CH₂N >CH₂X	13/5	14/5 -C≡C-	15/5 >C=C<	16/5 C≡C
1/6 ANORGAN. SUBSTANZ	2/6 EIGEN SCH	3/6 ≧5	4/6 ⬡	5/6 ≧7 GES.	6/6 ⬡	7/6 ≧2 0	8/6 ≧3 ASYM.	9/6 ≧1,4	10/6 ≧1,4 5	11/6 ~~2~~	12/6 >CHX	13/6	14/6 -C≡CH	15/6 C=C EXO	16/6
1/7 KLARTEXT	2/7 SYNTH. DARST.	3/7 ARYL	4/7 ⬡	5/7 △	6/7 ~~⬡~~	7/7 S	8/7 ≧3 VIC.	9/7 1, 2, 3 1, 3, 5	10/7 1,2,3 1,3,5 6 VIC. SYM.	11/7 3	12/7 >CX	13/7 C=Y C=Y C=Y C-YH	14/7 -C≡CX	15/7 1 X	16/7 GES. ALKYL
1/8 PATENT	2/8 STRUKTUR UNSICHER	3/8 ARALKYL	4/8 ⬡	5/8 □	6/8 ≧7	7/8	8/8 X=C	9/8 1, 2, 4	10/8 1,2,4 ASYM. 7	11/8 4/6	12/8 CH_2X_2 $-CHX_2$ $>CX_2$	13/8 C=Y C=Y C=Y C-YH	14/8 -C=C=C -C=C=Y	15/8 ≧ 2 X ($x_1=x_2$)	16/8 UNGES. ALKYL
1/9 AUS DER LITERATUR	2/9 ALLG FORMEL	3/9	4/9 ⬡	5/9 ALICYCLUS	6/9 △,□	7/9 AND HETERO	8/9 HETERO-CYCLUS	9/9 ≧4 SUBST.	10/9 ≧4 SUBST. ≧8	11/9 ≧7	12/9 CHX_3 $-CX_3$ CX_4	13/9	14/9	15/9 ≧ 2 X ($x_1 \neq x_2$)	16/9

17/12 POLY	18/12 POLY	19/12 POLY	20/12 POLY	21/12 POLY	22/12 POLY	23/12 POLY	24/12 POLY	25/12 POLY	26/12 H	27/12 D, T	Sp. 28	Sp. 29	30/12
17/11 GRUPPE AN F	18/11 GRUPPE AN F	19/11 GRUPPE AN F	20/11 GRUPPE AN F	21/11 H	22/11 GRUPPE AN F	23/11 GRUPPE AN F	24/11 GRUPPE AN F	25/11 GRUPPE AN F	26/11 R	27/11 C*			30/11
17/Ø F	18/Ø 1 (4) OH	19/Ø $R-NH_2$	20/Ø >S=Y	21/Ø R	22/Ø -N=N-	23/Ø -C-C	24/Ø H	25/Ø >=Y	26/Ø OH, OM, OR SH, SM, SR	27/Ø ANDERE RADIO-AKTIVE			30/Ø
17/1 Cl	18/1 2 (5) OH	19/1 R-NHT	20/1 >S	21/1 Sp. 17 Sp. 20	22/1 =N≡N	23/1 -C-C	24/1 OH, OM, OT SH, SM, ST	25/1	26/1 NH_2	27/1 Na Li 1			30/1
17/2 Br	18/2 3 (≧6) OH	19/2 R-NHR	20/2 >P-	21/2 OH	22/2 -N≡N	23/2 -C OH(SH)	24/2 OR, SR	25/2	26/2 NHR	27/2 Mg Hg 2			30/2
17/3 J	18/3 $-OCH_3$	19/3 $R-NT_2$	20/3 >P	21/3 OR	22/3 KETTE	23/3 C OM(SM OT, ST)	24/3 NT_2	25/3 Y=⬡=Y	26/3 NR_2	27/3 Al B 3			30/3
17/4 NO_2	18/4 -OR	19/4 R-NRT	20/4 >Si	21/4 SH, SR	22/4 NT_2	23/4 -C OR(SR)	24/4 =NT	25/4	26/4 OX, NX, SX	27/4 Si 4			30/4
17/5 NO	18/5 -OT	19/5 $R-NR_2$	20/5 >B-	21/5 OM, SM OT, ST	22/5 OH, OM OR, OT	23/5 -C NT_2	24/5 Sp. 17	25/5	26/5 Sp. 17,20	27/5 P 5			30/5
17/6 C≡N	18/6 ONIUM	19/6 ~~$R-N(CH_3)_2$~~	20/6 GRUPPE I. RING	21/6 NT_2	22/6 ANDERE HETERO	23/6 -C X=Sp. x 17, 20 ABHYDR. PERS.	24/6 Sp. 20	25/6	26/6 R^+X^-	27/6 S 6			30/6 SCHABLONE
17/7 N=C	18/7 S	19/7 $-NR_3^+$	20/7 Y=O	21/7 -OP--SP- -OS--SS-	22/7 N→O	23/7 Y=O	24/7 Y=O	25/7 Y=O	26/7 R^+R^-	27/7 HAL 7			30/7 SPUREN-ELEMENTE
17/8 GRUPPE AN C	18/8 O/S	19/8 N^+ CYCLISCH	20/8 Y=S	21/8 -O-Si	22/8 SONSTIGE	23/8 Y=S	24/8 Y=S	25/8 Y=S	26/8 KOMPLEX ADD. VERB.	27/8 Fe, Ni Co 8			30/8 SUBSTANZ BEEINFLUSST
17/9 SUBST. ALLG.	18/9 HOMOLOGE	19/9 OZONID AZID	20/9 Y=NT	21/9 HOMOLOGE	22/9 HOMOLOGE	23/9 Y=NT	24/9 Y=NT	25/9 Y=NT	26/9 METALLORG. RADIKAL	27/9 ANDERE			30/9 SUBSTANZ WIRD BEEINFLUSST

Figure 1. Coding sheet for 3-(β-dimethylaminoethyl)indoline.

Atom number	Element symbol	Linkage value	Ring value	Number of hydrogen atoms	Number of ligands	Charge indication	Hetero orientation	Complex bonds	Screen coordinates (f. struct. Diagr.)	1.Lig. Type of linkage	1.Lig. Ligand address	2.Lig. Type of linkage	2.Lig. Ligand address	3.Lig. Type of linkage	3.Lig. Ligand address	4.Lig. Type of linkage	4.Lig. Ligand address	5.Lig. Type of linkage	5.Lig. Ligand address	6.Lig. Type of linkage	6.Lig. Ring No.	Ring No.	Ring No.	Ring No.	Ring No.	Area indication
main matrix MAT																										
MAT	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26
1	5	1	5	1	2	0	0	0	41	3	2	3	3	0	0	0	0	0	0	0	0	15	0	0	0	0
2	5	1	5	1	2	0	0	0	42	3	1	3	4	0	0	0	0	0	0	0	0	15	0	0	0	0
3	5	1	5	1	2	0	0	0	52	3	5	3	1	0	0	0	0	0	0	0	0	15	0	0	0	0
4	5	1	25	0	3	0	0	0	54	1	6	3	2	3	7	0	0	0	0	0	0	15	16	0	0	0
5	5	1	5	1	2	0	0	0	64	3	7	3	3	0	0	0	0	0	0	0	0	15	0	0	0	0
6	7	0	20	1	2	0	0	0	55	1	4	1	8	0	0	0	0	0	0	0	0	16	0	0	0	0
7	5	1	25	0	3	0	0	0	65	3	5	1	9	3	4	0	0	0	0	0	0	15	16	0	0	0
8	5	1	20	1	2	0	0	0	67	1	6	5	9	0	0	0	0	0	0	0	0	16	0	0	0	0
9	5	1	20	0	3	0	0	0	78	1	7	5	8	0	10	0	0	0	0	0	0	16	0	0	0	0
10	5	0	0	2	2	0	0	0	89	0	11	0	9	0	0	0	0	0	0	0	0	0	0	0	0	0
11	5	0	0	2	2	0	1	0	100	0	10	0	12	0	0	0	0	0	0	0	0	0	0	0	0	0
12	7	0	0	0	3	0	0	0	111	0	13	0	14	0	11	0	0	0	0	0	0	0	0	0	0	0
13	5	0	0	3	1	0	1	0	123	0	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	5	0	0	3	1	0	1	0	122	0	12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15	4	3	5	0	0	0	6	0	53	0	0	0	0	0	0	0	0	0	0	0	17	16	0	0	0	0
16	3	2	20	0	0	0	5	0	16	0	0	0	0	0	0	0	0	0	0	0	18	15	0	0	0	0
17	160	15	1	2	4	7	5	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
18	160	16	4	6	8	9	7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Figure 2. Master connectivity table with redundant dates for 3-(β-dimethylaminoethyl)indole (simplified presentation).

It is possible to store the table either in half-words (2 bytes) or in words (4 bytes) per entry. The conversion programs described here use the half-word format. All figures of the table are integers and do not exceed the value of 255. The first step in creating the CT for a given compound is the numbering of all atoms except hydrogen.[3] The description of each atom, e.g., symbol, number of ligands, number of linked hydrogen atoms, etc., is stored in the 26 columns either using code numbers or the exact figures. Besides the structural information some additional figures are necessary for an unambiguous description, for example, ring-member characteristics. Columns 1–25 contain information about linkage value (col. 2), ring value (col. 3; alicycle = 1, benzene ring = 5, heterocycle = 20), number of ligands (col. 5), hetero orientation (col. 7), etc. Column 1 contains code numbers for the element symbols, e.g., 5 for C atoms, 7 for N atoms.

Some introductory remarks for the Ringcode conversion from the CT described above follow: (a) one CT can stand for more than one compound; (b) one CT can contain one or more fragments of a compound which are described separately; (c) several identical components in one compound are coded only once according to the rules for the General Chemical Ringcode; (d) in the case of keto/enol and imino/amino tautomerism, heterocycles are coded in the most unsaturated ring form.

For an explanation, see the examples in Figure 3: Compound 2 contains three identical organic anions; only one can be coded (c).

Compound 3 consists of three parts: the two organic cations and the inorganic metal containing anion. Only one cation is coded and on an additional coding sheet the hexachloroplatinic acid, H_2PtCl_6 (c).

The CTs for examples 4–8 contain two components each (b). These two and the three components of example 3 are described separately. The CTs do not contain information concerning the type of linkage. For example, the number of ligands in examples 4 and 5 for the oxygen ions is 1, and for the NH_4^+ and the Bi^{3+} cation 0 (hydrogen atoms are not regarded as ligands). In such cases the cations must be linked

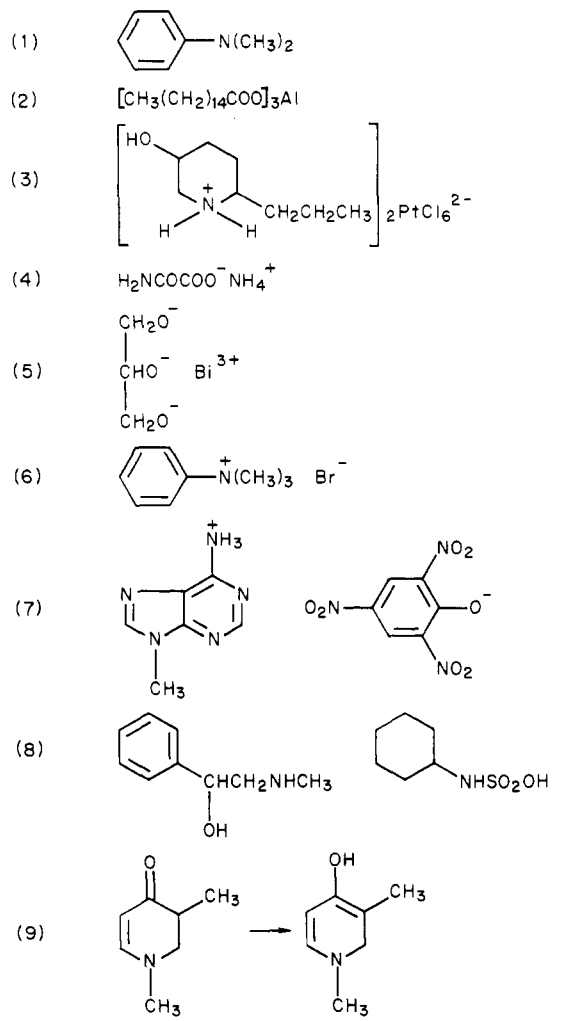

Figure 3. Examples for connectivity tables with different numbers of components.

with their anions, and the CTs have to be corrected as, according to the rules of the General Chemical Code, these ions are not compounds, as is the case in examples (b and c) and 7 (b). This leads to two coding sheets for each ion.

In example 6 the Br^- ion must be blocked for conversion. The coding of the salt is carried out in column 26 of the Ringcode. The same occurs in examples 3 and 7.

Example 8 is an adduct of two compounds. The CT contains the information of both under the same registry number. Two Ringcode codings with the same registry number are necessary.

Heterocycles, such as the one shown in example 9a, must be coded only in their enolized form (9b).

To consider remarks a–d accordingly, a structure analysis has to be undertaken before conversion. This will be carried out by some subroutine programs required.

THE PROGRAMS

The basis for the conversion programs was the newest edition of the Ringcode coding rules. Because the program cannot distinguish between general chemical structures and special compounds, as steroids, peptides, carbohydrates, and inorganic compounds, all these are converted into the general chemical code.

The program cannot handle compounds with more than nine-membered rings. These compounds are, according to the GREMAS rules[5] which are applied to the CT generation, not assigned to a so-called ring center. Without an atom-by-atom search, such compounds cannot be identified as rings and are handled as noncyclic structures. The conversion of ring systems with several endo bridged sometimes will lead to faulty codings in columns 2–10 and 25, the reason for this again being the different rules for ring definitions of Ringcode and GREMAS. Figure 4a shows the compound adamantane which contains according to GREMAS rules seven rings; according to Ringcode rules, only three rings. The compound shown in Figure 4b contains nine rings according to the first code and six according to the second.

If such codings are converted, the program prints, besides a warning message, the converted Ringcode positions additionally with the CT and the corresponding structure diagram.

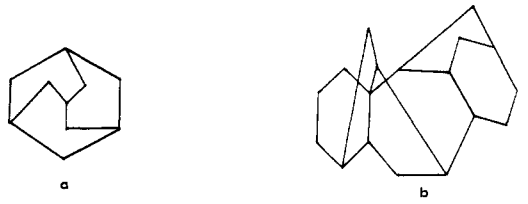

Figure 4.

A further coding error should be indicated. To determine the number of heteroatoms in rings, four counters are used: one for oxygen, one for nitrogen, one for sulfur, and one for the remaining heteroatoms. If a heterocyclic ring contains no N, O, or S-atoms but two other different heteroatoms, the fragment for "several-like X in rings" (pos. 7/11) is erroneously converted, instead of the fragment for "several different X in rings" (pos. 7/0). Because of the rareness of such structures, this error may be acceptable.

Another inaccuracy occurs during the conversion of the keto groups of tetracyclines. According to the Ringcode rules, the fragment "POLY" (pos. 25/12) for cyclic keto groups is not allowed. The described program cannot consider this, and generates pos. 25/12.

In consideration of the aforementioned details, there are probably no further restrictions for the application of this program package. Several error and warning messages are provided in the different subroutines which will lead to the printout of CTs, Ringcodes, and structure diagrams to cover those possibilities not considered during the programming work.

REFERENCES AND NOTES

(1) W. Nübling and W. Steidle, *Angew. Chem.*, **82**, 618 (1970).
(2) E. Meyer, Aufbau der BASF-Hauptmatrix, Ludwigshafen, BASF, 1969. BASF = Badische Anilin & Soda-Fabrik AG.
(3) E. Meyer, *Angew. Chem.*, **82**, 605 (1970).
(4) Ringcode, General Chemical Code, 5th ed., April, 1977, Pharma Dokumentationsring e.V. and Derwent Publications Ltd.
(5) S. Rössler and A. Kolb, *J. Chem. Doc.*, **10**, 128 (1970).

Algorithms for Unique and Unambiguous Coding and Symmetry Perception of Molecular Structure Diagram. I. Vector Functions for Automorphism Partitioning†

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Received June 4, 1979; Revised Manuscript Received January 21, 1980

Several vector functions which are useful for automorphism partitioning of the set of vertices in a chemical graph are proposed on the basis of mathematical theorems. Proofs are given for the theorems used and details of the methods to employ these functions are described. The present approach provides more systematic and powerful methods for a partitioning procedure than existing algorithms (Morgan, Corneil–Gotlieb).

INTRODUCTION

Problems such as unique and unambiguous coding,[1-11] automorphism partitioning,[12] and computation of symmetry groups[11,14] often require preliminary partitioning of vertices of a chemical graph. Morgan's connectivity value[5] approach and Corneil–Gotlieb's Algorithm I[12] are two well-known methods which can be used. These existing methods, however, are entirely ineffective for partitioning of the vertices of regular graphs and poorly effective for several types of graphs.

In this paper, a matrix method[7] has been applied to the partitioning problem, and a general equation useful for de-

† Presented at the Division of Chemical Information, ACS/CSJ Congress, Honolulu, Hawaii, April 3, 1979.

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