Ganitam: Frontier Journal of Computational and Applied Mathematics
Vol. 1 No. 1 (June, 2026)

Received: 19th December 2025
Revised: 18th March 2026
Accepted: 20th March 2026

A REVIEW ON MATHEMATICAL CHEMISTRY

A S HARIPRASAD* AND PRUTHVIRAJ R D**

Abstract. Mathematical chemistry entailing the development of novel mathematics for chemical applications is argued to exist, and to manifest an extremely diverse range of applications. Yet further it is argued to have a substantial history of well over a century, though the field has perhaps only attained a degree of recognition with a formal widely accepted naming in the last few decades. The evidence here for the broad range and long history is by way of nu- merous briefly noted example sub-areas. That mathematical chemistry was only recently formally recognized is seemingly the result of its having been somewhat disguised for a period of time – sometimes because it was viewed as just an unnamed part of physical chemistry, and sometimes because the rather frequent applications in other chemical areas were not always viewed as mathematical (often involving somewhat 'non-numerical' mathematics). Mathematical chemistry's relation to and distinction from computational chemistry theoretical chemistry is further briefly addressed.

Keywords: mathematical chemistry, physical chemistry, computational chemistry, theoretical chemistry.

1. Introduction

Chemistry is a rich and complex science, exhibiting a diversity of reproduci- ble and precisely describable predictions. Many predictions are quantitative numerical predictions and also many are of a qualitative (non-numerical) nature, though both are susceptible to sophisticated mathematical formalization. As such, it should naturally be anticipated that there is a 'mathematical chemistry', rather likely with multiple roots and with multiple aims. Mathematical chemistry should focus on mathematically novel ideas and concepts adapted or developed for use in chemistry (this view being much in parallel with that for other similarly named mathematical fields, in physics, or in biology, or in sociology, etc.). This definition distinguishes mathematical chemistry somewhat from simple routine mathematics for chemical problemsand even from rather complex mathematics used repeatedly in some stand- ardized manner (perhaps in the form of a 'canned' computer program). Fur- ther refinement of the idea of 'mathematical chemistry' is then of natural interest.It is perhaps not surprising that 'mathematical chemistry' has come to be so named, two journals inaugurated, and a society founded, all with much research activity having occurred. Indeed much of this activity is evident

---

Key words and phrases. mathematical chemistry, physical chemistry, computational chemistry, theoretical chemistry.

* This research is supported by the Research Students .

from: Rouvray's editorial forward (1987, for the first issue of the Journal of Mathematical Chemistry); Löwdin's (1990), Mackey's (1997), and Mallion's (2005) commentaries on what 'mathematical chemistry' should become; Trinajstić Gutman's (2002), King's (2000), Haberditzl's (1979), and Bala- ban's (2005) presented 'reviews' of the field; as well as a few briefer com- menting letters (Pauling 1987, Prelog 1987, Karle 1987). And yet further there are related relevant comments (Thomson 1918, Primas 1983, March 1983, Laughlin 2000) on the connection and interaction between chemical theory and physics as well as mathematics. Most all of these earlier works focus on some special recently developed area within mathematical chemis- try, and thereby typically leave a biased view of the field as a whole. A few of the letters or shorter articles, while making a general definition, however describe and illustrate the field so briefly that the full richness of the field is not clearly perceived. And yet further some of the articles seem to indicate that mathematical chemistry has only been born within the last two or three decades.Thence a more comprehensive view of 'mathematical chemistry' seems called for and is here attempted, seeking to indicate the full range and long history. Though the support for this view is found to be difficult to clearly and fully achieve, the current presentation is far more complete than that in the few earlier mentioned articles, which seem often to agree in the formal definition, yet omit mention of sizable portions of the field perhaps giving only a few very narrowly selected examples, often also limited to rather re- cent decades. Here emphasis is placed on the field's breath-taking broadness and long history of well over a century. The contrast to several earlier reviews is evident because the field of mathematical chemistry appears to have been somewhat 'disguised', at least for a period of time, with then huge portions simply unmentioned in several of the earlier reviews. The support for the present view of strength and history is documented here by way of a listing of around two dozen sub-areas of chemical research, each illustrated with a modest (incomplete) selection of representative publications (see Appendix), which are arguably part of mathematical chemistry. Some earlier contributions are merely alluded to by way of a few important names, while the ex- plicitly identified publications are largely focused within the last 100 years. The various identified researchers, books, and articles variously exhibit the use (or proposed use) of novel mathematical ideas in application to chemis- try. Thence a more balanced, a more truthful, and more comprehensive view of the full field of mathematical chemistry is attained.Mathematical Chemistry DetailedAgain, mathematical chemistry focuses on mathematically novel ideas and concepts adapted or developed for chemistry. The mathematics may be from any of many diverse mathematical areas, including: differential equations; partial differential equations; group theory (geometric or not); Lie algebras; combinatorics; graph theory; the theory of partially ordered sets and lattices; linear algebra and matrix theory; probability theory and statistics; number theory; algebraic and combinatorial geometry; topology; functional analysis; Von Neumann and C* algebras; rigged Hilbert spaces; homological category theory; fundamental logic and metamathematics; and more. That is, there is no a priori reason to exclude certain areas of mathematics, though some areas might naturally prove more fruitful for chemistry.Overall there are very many non-trivial chemical applications of novel mathematics from each of the broad chemical 'fields' of analytical, inorganic, organic, biochemical, and physical chemistry. But such work viewed as part of mathematical chemistry is here illustrated at a finer scale of narrower chemical 'areas', as now are listed:Foundational equilibrium thermodynamics was begun long ago in a mathematical mode, e.g., by A. Avogadro and H.L. LeChatelier and most especially by R. Clausius, then also by J.H. van 't Hoff, W. Ostwald, S. Arrhenius, J.W. Gibbs, W. Nernst, F. Haber, and G.N. Lewis. This early work received several Nobel prizes. More recently there are many more examples of mathematical researches, by M.E. Fisher (1972) and B. Widom (1965 and 1974) on critical-point scaling related to critical-point exponents (as further clarified with renormalization-group Nobel-prize- winning arguments of K. Wilson, and others, mostly in physics). Yet also there is F. Weinhold's (1975a,b,c,d) development of a geometric Rie- mannian metric for thermodynamic manifolds, and there are many other results are

(1) Equilibrium statistical mechanics was also begun a little over a century ago by Gibbs and many others (often physicists, like Maxwell and Boltzmann), all in a highly mathematical mode. Later (mathematical) developments arise with J. Mayer's (1938a,b) and others graphical cluster expansions for statistical-mechanical thermodynamic properties, with E. Montroll's (1941) powerful transfer-matrix methodology for the solu-tion of partition functions when interactions are 'local', and with Lars Onsager's (1944) mathematical tour de force (transfer-matrix) solution of the 2-dimensional Ising model. And still there is much further ongoing activity, though there is much more also.

(2) Electrochemistry has an even longer history dating back to H. Davy, M. Faraday and G. Kirchhoff. (Especially Kirchoff's work is accepted as mathematical, while the mathematically uneducated Faraday ended up founding 'field theory'.) More recent mathematical contributions are encountered with P.W. Debye and E. Hückel (1923a,b) in their theory of ionic solutions (and activity coefficients), or with R. M. Fuoss and L. Onsager (1957) and others in the theory of conduction in ionic solutions, or with R. Marcus (1956, 1965, 1977, 1993) in his Nobel-Prize winning work on structure-mediated charge transfer. Yet further there is important work on electrochemical processes, and a recent interest in molecular electronic conduction, particularly for application in nano- devices.

(3) Chemical kinetics dating back to the 19th century has been pursued more recently in terms of many different example cases. Some such are found with the various (mathematical) modelings of the Belousov- Zhabotinsky reaction (as a prototypical complex spatio-temporally oscillatory case), or with Ilya Prigogine's work in this general area, for which there was awarded a Nobel prize. A notable development is M. Eigen (1971) and others mathematical characterization of 'evolution-complicit' hyper-cycles. Also, there is work by L. Peusner (1986) and others on 'network thermo-processes', or Clark's work on reaction-diffusion pro- cesses, or more recent extensive work concerning chaotic reaction dynamics, as reviewed by Scott (1991) and Rice et al. (2005).

(4) Non-equilibrium thermodynamics, beyond chemical kinetics and ordi- nary diffusion, this area has many contributions by physicists, but also includes Lars Onsager's (1931) Nobel-prize winning development of his reciprocal relations amongst thermodynamic response functions. More recently there are various (mathematical) works developing the quantita- tive dynamics of entropy-production particularly in the linear-response regime approaching equilibrium, and there is Prigogine and Henin's (1969, 1973) radical subdynamics, and yet further Ernst Ruch's (1975, 1992) work on his fundamental partial-ordering 'structural principal' which concerns complementarities of distinction/identity and of or- der/disorder.

(5) Spectroscopic theory with a strong mathematical flavor developed enormously during the 20th century, with foundational work on rota-tional, vibrational, rovibrational, vibronic, and electronic spectra, as well as molecular excitonic spectra, electron-spin resonance, and nuclear magnetic resonance. The Nobel prize to G. Herzberg was for (implicitly mathematical) deductions from electronic spectra of features of electronic potential curves or surfaces. With the availability of suitable high- performance electronics there has further followed mathematical (and experimental) development of general Fourier-transform, multi-photon, nonlinear, and multidimensional spectroscopies (which indeed have garnered a Nobel prize). Further there are different (e.g., mass) spectrosco- pies based on other than electromagnetic waves.

(6) Mathematical crystallography developed classically with the identification of the Bravais lattices and crystal classes, followed by the seminal identification of crystallographic space groups by Schoenflies and Fedorov. More recent mathematical work is nicely exemplified by Shubnikov and co-worker's colored crystals (Shubinikov Belov 1964), by the network descriptions of Wells (1954a,b, 1972) and others, and for the theory of quasi-crystals by Mackay (1975, 1982), Penrose (1978), and others (with a Nobel prize going to D. Schectman, for his 'recalcitrant' experimental identification of these). An especially nice (and extremely useful) pure mathematical development is that of J. Karle and P. Hauptmann (1953, 1957a,b, 1960), who shared a Nobel prize for their joint work on the inversion of x-ray scattering data to crystal structures.

(7) Diffractive methods include both electron and x-ray diffraction methodologies, and in application to (the common case of) crystals has much overlap with mathematical crystallography. L. Pauling received a Nobel prize in chemistry for his deduction of the alpha-helix structure of proteins, while earlier (Nobel-prize-winning) work is usually viewed as part of physics, though there have been at least three further Nobel prizes in applications to molecules of biologic importance, with the theoretical (mathematical) deductions here being central. Further work on the in- terpretation of molecular or electron scattering may be viewed to be related (and rewarded with a couple Nobel prizes).

(8) Abinitio quantum chemistry developed following the founding of quantum mechanics (in physics), though ultimately the development of computer technology also played a central role. Mathematical work in- cludes Roothaan's (1951) and Hall's (1951) development of a (discretized) matrix-based SCF theory, many-body perturbation theory building thereon, facile orbital development numerous molecular-integral evaluations, the theory of reduced density matrices (and associated natu-ral orbitals) by P.O. Löwdin (1955) and others, J. Čížek's (1966) power- ful coupled-cluster method, the development of a promising quantum Monte Carlo technology, and rather numerous other developments, with an evident cap-stone in the overall field being extensive program realization, for example, with J. Pople's Nobel-prize-winning efforts.

(9) Density functional theory, which computes from just the electron density, is viewed by many as part of abinitio quantum chemistry, with early work (by L. Thomas, E. Fermi, J. C. Slater, and others) primarily in physics. Work in the field was carried into chemistry in a general formal mathematical mode with Mel Levy's (1979) and many others' proofs and clarifications of fundamental aspects, initiating with the (Nobel-prize- winning) work of W. Kohn and co-workers. But especially significant is a marriage with classically based chemical electronegativity and hardness/softness ideas, all as seminally reviewed in Parr and Yang's (2000) text. Again there is a cap-stone of extensive program development.

(10) Group-theoretic methodology, mostly following the advent of quantum mechanics (detailed in early summary works of Weyl (1928), Wigner (1931), and Yutsis et al. (1962)) includes work on the symmetric group (of permutations) by F.A. Matsen (1964), I.G. Kaplan (1975), and others, then work on the unitary group by J. Paldus (1974, 1975) and others, and yet further work on general Lie group (or Lie algebraic) uses by C. Wulfman and others. With a more classical geometric scope there is much work on point groups, indicated in F.A. Cotton's (1963) popular text, and also note the extensive development of ligand-field theory. Fur- ther there is work on alternancy (or particle-hole) symmetries, on color symmetries, on generalizations thereto, and finally on non-rigid- molecule groups.

(11) Molecular dynamics concerns the quantum mechanical characterization of the motion of nuclei, as in Wilson et al.'s seminal book (see Appendix 5), and it is further nicely exemplified with the Jahn-Teller (1937) effect, with H.C. Longuet-Higgins' phase (more often termed the 'Berry' phase), and with A.D. Liehr's (1963a,b) related elegant characterizations. More recently there is R.D. Levine and R.B. Bernstein's (1973) develop- ment of very broadly useful information-theoretic 'surprisal' methods. There is much work with conceptual import (as of reaction paths or of semi-classical ideas), related characterizations of potential energy hyper- surfaces, and much work on molecular scattering, as well as some work on 'chaotic' dynamics. (For references, see Appendix 12.)Solid-state chemistry has much

overlap with crystallography and further is perhaps dominated by the enormous amount of work in solid-statehysics. Still there are numerous mathematical chemical articles (by chemists) including H.C. Longuet-Higgins (1959) and L. Salem's work on Peirels distortions, and J.A. Pople and S.J. Walmsley's (1962) devel- opment of solitonic excitations, to be followed up by seminal work on these topics by Su, Schreiffer, and Heeger (1980) (with this work as ap- plied to further experimental work on polyacetylene and other organics associated to a Nobel prize for A.J. Heeger, H. Shirakawa, and A.G. MacDiarmid). There is further mathematical work on molecular excitons, on Burdett's characterizations of band structure, and on yet other notable aspects of solid-state theory.

(12) Stereochemistry has a long history back beyond Van 't Hoff and LeBel, and is related closely to some previous noted areas. But also this area in- cludes Pauling's (1931) fundamental molecular geometric hybridization rules, informative analyses of inversions or internal rotations or pseudorotations (as in cyclopentane), and Lipscomb's (1958, 1973) Nobel- prize winning work as well as that of others treating boranes (as a proto- typical case manifesting the effects of non-classical bonding) and related novel structures. Also there is continuing work with isomers, with mo- lecular geometry characterization, with the Ruch-Schönhofer (1970) chi- rality characterization, with degrees of achirality and asymmetry, with extensions of chirality characterizations, with molecular shape, and with molecular knottedness.

(13) Polymer statistics concerns the conformation-mediated and structure- mediated properties of polymers (especially high polymers), with foun- dational mathematical chemical (Nobel-prize-winning) work both byP.J. Flory (1953, 1969) and by P.G. DeGennes (1979), particularly as to the manner of polymer size-scaling as a function of their length, and oth- er control parameters. Monte-Carlo methods have been developed and have proved useful. But there are many further mathematical approaches. Also, the field has further blossomed with the development of den- drimers, supramolecular structures, and other large-scale morphological characterizations.

(14) Chemical reaction-network analysis, though long around in an informal mode in synthetic organic chemistry, has systematically (and thence mathematically) been developed to elucidate organic synthetic strategies in the work of the groups of E.J. Corey (Corey et al. 1974, 1977), J.E. Dubois (1973), T. Wipke (Wipke Rogers 1984, Wipke Vladutz 1990), J.B. Hendrickson (1976, 1986), I. Ugi (Ugi Gillespie 1971, Dugundji Ugi 1973), N.S. Zefirov et al. (2002), S. Fujita (2001), P.J. Stadler et al. (1995, 1996), and of several others. Recently there is rather intense effort toward a general theory of 'complex networks'. And there is work on the mathematical characterization of special reaction-networkgraphs, as of degenerate rearrangements or of substitution reactions (which mathematically form a partial ordering).

(15) Chemical nanotechnology has recently emerged as an interesting and greatly burgeoning separate field, following the development of carbon nanotubes

and focused on organic syntheses of novelly interconnected nanostructures; there being notable theoretical work and different mathematically oriented articles, some concerning general theory. As exam- ples for particular nanostructures, there are considerations of nano- knots, nano-links, nanotubes, their caps, nano-tori, nano-cones, nano- belts, Möbius nanostrips, and various negatively curved structures, and yet further there are more elaborate molecular devices, such as molecular motors. Most recently there is incredible activity (with reviews) concern- ing graphene (including a Nobel prize). (For references, see Appendix 17, Sumners 1988 in Appendix 15, and Flapan 2000 in Appendix 14).Semi-empirical quantum chemistry includes Pauling and Wheland's classically related resonating valence-bond theory, with many more re- cent developments, as reviewed in various chapters by Klein Trinajstić (1990), Cooper (2001), and Shaik Hiberty (2007). Also there is the 'alternative' molecular-orbital approach with much mathematical work by E. Hückel (1931), Charles Coulson, H.C. Longuet-Higgins (1974a,b,c,d,e), E. Heilbronner, and many colleagues achieving funda- mental Hückel-model-based theorems for the case of conjugated pi- electron networks. Besides ligand-field theory already mentioned (under group theory) there is Woodward and Hoffmann's Nobel-prize winning orbital-symmetry conservation rules for concerted reactions (Woodward Hoffmann 1965a,b, 1970, Hoffmann Woodward 1965), and K. Fu- kui's (Nobel-prize-winning) work concerning frontier orbitals, though also there are many other important results. Parr's (1964) survey book nicely reveals a gradation between this field and ab initio quantum chem- istry. (For references, see Appendix 18 and Coulson 1940 in Appendix 11).Structure generation and enumeration is addressed in G. Pólya's (1937) foundational combinatorial theory of enumeration under group-mediated equivalences – all, in fact, developed to enumerate chemical isomers. Now there are various refinements and extensions, regarding al- ternant formulations, subsymmetry classification, reaction-mode enu- merations, Balasubramanian's (1981, 1985, 1993) non-identity irreduci- ble-representation enumerations, property characterizations, and com- prehensive structure generations. It is argued by Bytautas Klein (1998) that this field relates intimately to the idea of chemical nomenclature. Much of the mathematics (up to about 1986) is reviewed in Read's dis-cussion (Pólya Read 1987), and A. Kerber makes a more comprehen- sive mathematical survey (and a more chemically oriented, more concise survey in a special issue of MATCH).

(16) Physical organic theory is typically defined in terms of the ('physical') measurements considered, but it might arguably be better defined as the area dealing with the quantification of the idea of 'functional groups' in organic chemistry. Work goes back over a century to deal with constitu- tional additivities for enthalpies, magnetic susceptibilities, and other (physical) properties. There is also extensive theoretical work on 'linear free energy relationships', and the area overlaps extensively with a few others already mentioned.

(17) Chemical classification includes the long-standing area of chemical nomenclature, with cap-stone formalizations (which then are implicitly mathematical) available from IUPAC. But there are also the classifica- tions into: categories of chemical bonding (and its mediation by electro- negativities and hardnesses); different functional-group classes; different isomer classes; families of elements in Mendeleev's periodic chart; classes of 'acid' and 'base'; and different classes of 'aromaticity'. Much of this merges into chemical nomenclature. Also note that much of this classifi- cation can be elegantly viewed mathematically in terms of 'partially or- dered sets'.

(18) Mislow 1977 in Appendix 14 and Ugi et al. 1970 in Appendix 14).Chemometrics and QSAR have roots back into the 19th century, though these namings are more recent. The field has recently extensively developed with systematic statistical methodology in drawing correla- tions (e.g., with consideration of a variety of multivariate regression techniques, sometimes developed in a purely chemical context). There has been an immense development of a diversity of different sorts of available quantities (which can be other experimental properties, quantum-chemically computed characteristics, or simply molecular graph in- variants) so as to make structure/property or structure/activity correlations, such as involved in toxicity evaluations, and particularly in drug design. (For references, see Appendix

(19) Molecular biology extends classical biochemistry to deal with larger molecules: enzymes, proteins, DNAs, and RNAs. There are then many fundamental theoretical works dating back over half a century, with a few Nobel prizes in recognition of them. Following Watson and Crick's Nobel-prize-winning seminal decipherment of the DNA-double-helix structure, there have been numerous quite mathematical works dealing with molecular sequence codes. But also there are many other aspects to this general area, concerning prebiotic evolution immunochemistry, protein chemistry, cell chemistry, and neurochemistry, as well as brain chemistryand function. Further there is intense on-going activity dealing with enzyme conformation and protein folding.

(20) Chemo-informatics is an extension of 'chemometrics' (a term popular- ized in analytical chemistry) and is presently expanding rapidly, and is al- so related to the area of chemical nomenclature and related classifications. But particularly, it also encompasses topics of chemical data min- ing, molecular similarity comparisons, molecular pattern recognition, (virtual or theoretical) combinatorial chemistry and biomimetics, as well as of various theoretical aspects of the immense rapidly expanding related frontier areas of molecular biology, genomics, proteomics, and general bio-informatics – all deserving of a separate extensive discussion.

(21) Chemical graph theory has come to be so identified over the last few decades, and significantly overlaps with polymer statistics, stereochemistry, semi-empirical quantum-chemistry, nanotechnology, structure gen- eration, chemo-metrics/QSAR, and chemo-informatics, all already mentioned But there are numerous other works, e.g., just in the particular ar- ea of

fullerenes (yet again involving a Nobel prize, to Kroto, Smalley, and Curl) including: combinatoric methodology to apply the conjugated- circuits scheme (Herndon 1974, Randić 1977a,b); Manolopolous Fowler's (1992) important development of 'topological coordinates' for a simple geometric realization of fullerene structures; Brinkmann's pow- erful methodology for generating fullerenes (and related structures) (Brinkmann Dress 1997, 1998, Brinkmann Greinas 2003, Brink- mann et al. 1999 in Appendix 17); characterizations of fullerene trans- formations (Brinkmann Fowler 2003, Brinkmann et al. 2003); and numerous other theorematic and algorithmic fullerenic results. For a more embracing (older) overview of chemical graph theory see Trinajstić 1992 (or more briefly several earlier reviews (Trinajstić Gutman 2002, King 2000, Balaban 2005) or an intended follow up article). (For refer- ences, focused largely just on fullerenes,

(22) Note that certainly there are many more examples within the frequently overlapping listed areas, likely with very important examples missing. Yet there is quite a variable degree of importance for the articles collected in the Appendix, and sometimes just secondary sources (reviews or books) are quoted – and undoubtedly biases of this reviewer are manifested. Much more could be said about mathematical results for very many of these areas – such incompleteness should not be construed as indicating exclusions of various results from mathematical chemistry, but rather as an indication of the great difficulty of making a comprehensive review. Each one of the areas are often only sparsely sampled and could be extensively expanded upon.

2. Mathematical Chemistry Detailed

Mathematical chemistry focuses on mathematically novel ideas and concepts adapted or developed for chemistry[cite: 26]. The mathematics may be from many diverse areas, including:

- Differential equations and partial differential equations.
- Group theory, Lie algebras, combinatorics, and graph theory.
- Linear algebra, matrix theory, probability theory, and statistics.
- Topology, functional analysis, and fundamental logic.

Mathematical Foundations in Mathematical Chemistry Summary of Mathematical Frameworks

3. Quantum Chemistry and Matrix Theory

The article identifies **linear algebra and matrix theory** as fundamental to quantum chemistry . A cap-stone development is the matrix-based **Self-Consistent Field (SCF) theory**, represented by the Roothaan-Hall equations:

$$FC = SC\epsilon \tag{3.1}$$

Where:

- F is the Fock matrix
- C is the matrix of expansion coefficients for molecular orbitals

- S is the overlap matrix
- ϵ is the diagonal matrix of orbital energies

4. Statistical Mechanics

A "mathematical tour de force" noted in the text is the solution of the **2-dimensional Ising model** The interaction energy is defined by the Hamiltonian:

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \tag{4.1}$$

This involves the use of **transfer-matrix methodology** to solve partition functions.

5. Non-Equilibrium Thermodynamics

The field includes Nobel-prize winning work on **reciprocal relations** amongst thermodynamic response functions. These relations describe the linear response regime:

$$J_i = \sum_j L_{ij} X_j \quad \text{where} \quad L_{ij} = L_{ji} \tag{5.1}$$

Here, J_i represents thermodynamic flows and X_j represents conjugate forces.

6. Structure Enumeration (Pólya's Theory)

The article cites G. Pólya's (1937) foundational **combinatorial theory of enumeration** used to count chemical isomers. This utilizes the Cycle Index polynomial $Z(G)$:

$$Z(G; x_1, x_2, \ldots, x_n) = \frac{1}{|G|} \sum_{g \in G} \prod_{k=1}^{n} x_k^{c_k(g)} \tag{6.1}$$

This formula allows for structure generation under **group-mediated equivalences**.

7. Spectroscopy and Diffraction

The mathematical development of **Fourier-transform spectroscopies** [cite: 52] and the inversion of X-ray scattering data to crystal structures [cite: 56] rely on the Fourier Transform:

$$F(\omega) = \int_{-\infty}^{\infty} f(t) e^{-i\omega t} dt \tag{7.1}$$

8. Chemical Kinetics

The text addresses the mathematical modeling of complex spatio-temporally oscillatory reactions, such as the **Belousov-Zhabotinsky reaction**. These are characterized by systems of non-linear differential equations:

$$\frac{d\mathbf{c}}{dt} = \mathbf{f}(\mathbf{c}, \mathbf{k}) \tag{8.1}$$

Where $\mathbf{c}$ represents the vector of concentrations of chemical species.

8.1. Key Chemical Areas. The field is illustrated through various chemical "areas" as listed below:

- **Equilibrium Thermodynamics:** Begun by Clausius, Gibbs, and others; includes recent work on critical-point scaling and Riemannian metrics for thermodynamic manifolds[cite: 33, 34, 35].
- **Statistical Mechanics:** Includes graphical cluster expansions (Mayer), transfer-matrix methodology (Montroll), and the solution of the 2D Ising model (Onsager).
- **Electrochemistry:** Dating back to Davy and Faraday; includes the Debye-Hückel theory and Marcus's work on charge transfer.
- **Chemical Kinetics:** Includes modeling of the Belousov-Zhabotinsky reaction, Prigogine's Nobel-prize work, and chaotic reaction dynamics.
- **Quantum Chemistry:** Involves matrix-based SCF theory (Roothaan and Hall), coupled-cluster methods (Čížek), and density functional theory.
- **Chemical Graph Theory:** Overlaps with nanotechnology, stereochemistry, and chemo-metrics; includes studies on fullerenes and topological coordinates.

9. Conclusion

To answer the question in the title, it is concluded that mathematical chemistry certainly 'is', which is to say that 'it exists', and moreover that it properly is an extremely broad field, with even a long and incredibly rich history of over a century of developments. Here it is argued that often many of the older mathematical developments are elsewhere categorized in other man- ners, so that often the field has been somewhat disguised. A substantial part of mathematical chemistry has been embedded in physical chemistry (where the connection to physics rather than mathematics has been emphasized), and other substantial portions of mathematical chemistry have been embed- ded in chemical structure, notation, and concepts – where often the non- numerical and non-geometrical nature of the relevant mathematics has led many to view such ideas as non-mathematical. Again, the present grand view has notable difference in comprehensiveness as compared to several previous presumably general commentaries (Rouvray 1987, King 2000, Haberditzl 1979, Balaban 2005),4 while the present definition of 'mathematical chemis- try' is quite similar to other earlier commentaries (Rouvray 1987, Löwdin 1990, Thompson 1918),4 which however provide very much less overall detail than with the documentation presently marshalled here. Mathematical chem- istry is seen to contact all 'classical' chemical fields: inorganic, organic, ana- lytical, biochemical, and physical. Evidently some areas of mathematical chemistry have much contact with chemical physics, physics, mathematical physics, or even with biology or mathematical biology. At the same time computational chemistry has here and elsewhere (Mackey 1997, Haberditzl 1979, Coulson 1960) been distinguished from mathematical and theoretical chemistry.Some historical questions remain to be clarified, e.g., as to why it has tak- en so long to make an explicit recognition of the field of mathematical chem- istry. This and other questions relating to the manner of its development and to the areas of mathematics naturally distinctively close to classical chemical structure theory (such as graph theory) are to be addressed in a second arti- cle, building from the presently established broad view. As a plausible con- clusion, one could argue that university curricula include mathematical chem- istry – say as indicated in the Figure 1.The curriculum could plausibly encompass computer chemistry as part of mathematical chemistry – most especially the part involving program devel- opment.Especially mathematical and theoretical chemistry reflect the overall rich- ness and complexity of chemistry itself.

10. References

(1) Balaban, A.T.: 2005, 'Reflections on mathematical chemistry', Foundations of Chemistry, 7, 289-306[cite: 141].

(2) Karle, J.: 1987, 'Welcoming letter', Journal of Mathematical Chemistry, 1, v-vii[cite: 155].

(3) Löwdin, P-O.: 1990, 'Mathematics in chemistry and in mathematical chemistry', Journal of Mathematical Chemistry, 4, 3-14[cite: 161].

(4) Balaban, A.T.: 2005, 'Reflections on mathematical chemistry', Foundations of Chemis- try, 7, 289-306.

(5) Baxter, R.J.:1969, 'F model on a triangular lattice', Journal of Mathematical Physics, 10, 1211-6.

(6) Baxter, R.J.:1970, 'Three colorings of the square model', Journal of Mathematical Physics, 11, 3116-24.

(7) Baxter, R.J.:1972. 'Partition function of the eight-vertex lattice model', Annals of Physics, 70, 193-228.

(8) Bethe, H.A.: 1931, 'Zur Theorie der Metalle. I. Eigenwerte und Eigenfunktionen Atomkette', Zeitschrift für Physik, 71, 205-26.

(9) Biggs, N.L.: 1977, Interaction models, Cambridge: Cambridge University Press, pp. 5- 9.

(10) Coulson, C.A.: 1960, 'Present state of molecular structure calculations', Review of Modern Physics, 52, 170-7.

(11) Fulton, W. Harris, J.: 1991, Representation theory, Berlin: Springer, pp. 1-566. Galilei, G.: 1623, Il saggiatori. Appresso G. Mascardi, Roma. English translation in

(12) Galilei, G.: 1957, The assayer. In: Galilei, G. Discoveries and opinions of Gali- leo, New York: Doubleday Company, pp. 1-320.

(13) Gutman, I.: 2006, 'Chemical Graph Theory – The Mathematical Connection', Ad- vances in Quantum Chemistry, 51, 125-138.

(14) Haberditzl, W.: 1979, '100 Jahre 'Mathematische Chemie' und 50 Jahre Theorie der

(15) Chemischen Bindung: Versuch einer Bilanz', MATCH Communications in Mathematical and in Computer Chemistry, 7, 197-215.

(16) Harary, F. Palmer, E.G.:1973, Graphical enumeration, New York: Academic Press, p. 236.

(17) Kant, I.: 1900-2000, Akademieausgabe von Immanuel Kants Gesammelten Werken, vol. 4, p. 470

(18) Karle, J.: 1987, 'Welcoming letter', Journal of Mathematical Chemistry, 1, v-vii. King, R.B.: 2000, 'The role of mathematics in the experimental/theoretical/ computa- tional trichotomy of chemistry', Foundations of Chemistry, 2, 221-36.

(19) Laughlin, R.B.; Pines, D.; Schmalian, J.; Stojković, B. P. Wolynes, P.: 2000, 'The middle way', Proceedings of the National Academy of Sciences, 97, 32-7.

(20) Lieb, E.H.:1969a, 'Residual entropy of square ice', Physical Review, 162, 162-71.

(21) Lieb, E.H.:1969b, 'Two-dimensional ice and ferroelectric models', in: K.T. Mahantap- pa W.E. Brittin (eds.), Lectues in Theoretical Physics, volume XI, New York: Gordon and Breach, pp. 329-54.

(22) Lossers, O.P.: 2005, 'Integral by Mellin transform', The American Mathematical Monthly, 112, 843-4.

(23) Löwdin, P-O.: 1990, 'Mathematics in chemistry and in mathematical chemistry', Journal of Mathematical Chemistry, 4, 3-14.

(24) Mackey, A.: 1997, 'Lucretius on the philosophy of chemistry', Colloids and Surfaces A: Physicochemical and Engineering Aspects, 129/130, 305-10.

(25) Mallion, R.B.: 2005, 'An autobiographical account of chemical graph theory in the years surrounding the launch of MATCH: an Oxford participant's highly per- sonal and parochial reminiscence about the period 1969-1976', MATCH Communications in Mathematical and in Computer Chemistry, 53, 15-52.

(26) March, N.H.: 1983, "Quantum mechanics has accounted for a large part of physics and the whole of chemistry'. true or false?', Contemporary Physics, 24, 373-87. March, N.H.: 2002, Private communication.

(27) Metropolis, N.; Rosenbluth, A.W.; Rosenbluth, M.N.; Teller, A.H. Teller, E.: 1953,

(28) 'Equations of state calculations by fast computing machines', Journal of Chem- ical Physics, 21, 1087-92.

(29) Onsager, L. Samaras, N.N.T.: 1934, 'The surface tension of Debye-Huckel electro- lytes', Journal of Chemical Physics, 2, 528-36.

* DEPARTMENT OF MATHEMATICS, RAJARAJESWARI COLLEGE OF ENGINEERING, BANGALORE , India

** DEPARTMENT OF CHEMISTRY , RAJARAJESWARI COLLEGE OF ENGINEERING, BANGALORE, India