Mathematical Chemistry! Is It? And if so, What Is It?

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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 numerous 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 reproducible 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 problems

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and even from rather complex mathematics used repeatedly in some standardized manner (perhaps in the form of a 'canned' computer program). Further 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 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 Balaban's (2005) presented 'reviews' of the field; as well as a few briefer commenting 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 chemistry, 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 recent 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 explicitly 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 chemistry. Thence a more balanced, a more truthful, and more comprehensive view of the full field of mathematical chemistry is attained.

2. Mathematical Chemistry Detailed

Again, 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 meta-mathematics; 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 Riemannian metric for thermodynamic manifolds, and there are many other results. (For references, see Appendix 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. (For references, see Appendix 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. (For references, see Appendix 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 processes, or more recent extensive work concerning chaotic reaction dynamics, as reviewed by Scott (1991) and Rice *et al*. (2005). (For references, see Appendix 4.)
- **Non-equilibrium thermodynamics**, beyond chemical kinetics and ordinary 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 quantitative 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 order/disorder. (For references, see Appendix 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 multi-dimensional spectroscopies (which indeed have garnered a Nobel prize). Further there are different (*e.g.*, mass) spectroscopies based on other than electromagnetic waves. (For references, see Appendix 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. (For references, see Appendix 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 interpretation of molecular or electron scattering may be viewed to be related (and rewarded with a couple Nobel prizes). (For references, see Appendix 8.)
- ***Ab initio* 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 includes 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) powerful 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. (For references, see Appendix 9.)

- **Density functional theory**, which computes from just the electron density, is viewed by many as part of *ab initio* 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. (For references, see Appendix 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. Further there is work on alternancy (or particle-hole) symmetries, on color symmetries, on generalizations thereto, and finally on non-rigid-molecule groups. (For references, see Appendix 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) development 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 hypersurfaces, 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-state

physics. 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) development of solitonic excitations, to be followed up by seminal work on these topics by Su, Schreiffer, and Heeger (1980) (with this work as applied 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. (For references, see Appendix 13.)

- **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 includes 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 prototypical case manifesting the effects of non-classical bonding) and related novel structures. Also there is continuing work with isomers, with molecular geometry characterization, with the Ruch-Schönhofer (1970) chirality characterization, with degrees of achirality and asymmetry, with extensions of chirality characterizations, with molecular shape, and with molecular knottedness. (For references, see Appendix 14.)
- **Polymer statistics** concerns the conformation-mediated and structure-mediated properties of polymers (especially high polymers), with foundational mathematical chemical (Nobel-prize-winning) work both by P.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 other 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 dendrimers, supramolecular structures, and other large-scale morphological characterizations. (For references, see Appendix 15.)
- **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-network

graphs, as of degenerate rearrangements or of substitution reactions (which mathematically form a partial ordering). (For references, see Appendix 16.)

- **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 examples for particular nanostructures, there are considerations of nano-knots, nano-links, nanotubes, their caps, nano-tori, nano-cones, nano-belts, Möbius nano-strips, 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) concerning 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 recent 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 fundamental 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. Fukui'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 chemistry. (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 alternant formulations, subsymmetry classification, reaction-mode enumerations, Balasubramanian's (1981, 1985, 1993) non-identity irreducible-representation enumerations, property characterizations, and comprehensive 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 comprehensive mathematical survey (and a more chemically oriented, more concise survey in a special issue of MATCH). (For references, see Appendix 19.)

- **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 constitutional 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. (For references, see Appendix 20.)
- **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 classifications into: categories of chemical bonding (and its mediation by electronegativities 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 classification can be elegantly viewed mathematically in terms of 'partially ordered sets'. (For references, see Appendix 21, Mislow 1977 in Appendix 14 and Ugi *et al.* 1970 in Appendix 14).
- **Chemo-metrics 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 correlations (*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 invariants) 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 22.)
- **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 chemistry

and function. Further there is intense on-going activity dealing with enzyme conformation and protein folding. (For references, see Appendix 23.)

- **Chemo-informatics** is an extension of 'chemo-metrics' (a term popularized in analytical chemistry) and is presently expanding rapidly, and is also related to the area of chemical nomenclature and related classifications. But particularly, it also encompasses topics of chemical data mining, 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. (For references, see Appendix 24.)
- **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 generation, chemo-metrics/QSAR, and chemo-informatics, all already mentioned. But there are numerous other works, *e.g.*, just in the particular area 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 powerful methodology for generating fullerenes (and related structures) (Brinkmann & Dress 1997, 1998, Brinkmann & Greinas 2003, Brinkmann *et al.* 1999 in Appendix 17); characterizations of fullerene transformations (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 references, focused largely just on fullerenes, see Appendix 25.)

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.

3. Comparisons and Qualifications

Comparison to earlier discussions may be made. Primas (1983) (over 2 decades ago) expansively described a quite abstract mathematical view of mathematical chemistry, or at least the part concerned with 'fundamental' quantum mechanics, which might be then taken to indicate that this is all of mathematical chemistry. Trinajstić & Gutman (2002), Balaban (2005), Gutman (2006) and King (2000) discuss mathematical chemistry with a focus on chemical graph theory, though it may be seen that the references quoted in these three articles and in the chemical-graph-theory area here are all more or less disjoint. Hauberditzl's survey (1979) as well as March's (1983) and Laughlin *et al.*'s (2000) comments again focus on quantum chemical aspects. The comments of Mackey (1997), Mallion (2005), Pauling (1987), Prelog (1987), and Karle (1987) each admittedly focus on different special areas (and seemingly do not have the intent of addressing mathematical chemistry in its fullness). Löwdin (1990) illustrates his ideas with very few of the areas in our listing, indicating just two areas, quantum chemistry and chemical graph theory, though this first area is likely intended to include our '*ab initio* quantum chemistry', 'semiempirical quantum chemistry', and 'solid-state chemistry'. Balaban (2005), Rouvray (1987), Löwdin (1990), King (2000), and Klein (1986), perhaps along with Primas (1983), all define mathematical chemistry formally similarly as we have. Yet further seemingly even D'Arcy Thompson (1918) indicates much the same definition (in his visionary 'Growth and Form' where he goes on to focus on his view for mathematical biology). Rouvray (1987) makes no attempt at examples, while perhaps the best attempt to indicate the great broadness is but a brief letter (1986), with only very few examples. As an overall indication of mathematical chemistry the present listing is comparatively very comprehensive and complete. The various works identified in the listings here are generally arguably mathematical.[1]

The present overall view to be taken from the listing here given is that mathematical chemistry is incredibly overwhelming. Some of the indicated areas historically derive more from physics than others, and in some of these areas significant work by physicists has then been referenced in the listing here, though all the listed applications are arguably 'chemical' – applying to chemical systems. Most of the researchers indicated in the listings here are primarily identified as chemists, though some (*e.g.*, Gibbs, Hückel, Jahn, Teller, deGennes, and Wigner) are often identified as physicists, some (Debye, Prigogine, and Fisher) are often identified both as chemists and as physicists, while others (Hauptmann, Pólya, Kerber, Brinkmann, and F. Zhang) are identified as mathematicians, and a few (*e.g.*, MacKay, Shubnikov, and Belov) are perhaps best described as crystallographers (whose field has a long independent tradition between chemistry, physics, and mineralogy). Some

(like K. Ruedenberg or M. Randić) are commonly identified to a field (chemistry in these cases) other than that of their doctoral degree. There is no fundamental reason why mathematical chemistry cannot be done by scientists other than those trained exclusively as chemists. The type of mathematics used can be varied, and even the use of physics should be allowed – indeed even encouraged, as this extends and deepens the results, and interconnects the fields (chemistry and physics). But all such work dealing with (novel) mathematically formalized descriptions of chemical systems is properly part of 'mathematical chemistry', which then reflects the awesome richness and complexity of chemistry itself.

Thus the present view differs notably from earlier announced views of mathematical chemistry, questions remain as to its relation to more traditional areas of chemistry – such as theoretical chemistry, computer chemistry, or physical chemistry.

4. Where Does Mathematical Chemistry Fit?

Though mathematical chemistry is seemingly widespread with a long history, it is also evident that there must be intimate relations to 'theoretical chemistry' and 'computer chemistry'. Particularly, the distinction between mathematical, theoretical, and computational chemistry might be deemed a delicate matter. But (in common with typical usages in physics and biology) one may look upon these distinctions as involving the three-way interplay of:

- the degree of adherence to mathematical formalism (say with explicit theorems and proofs in mathematical chemistry);
- the use of 'scientific induction' in theoretical chemistry, with the associated immediacy of general chemical predictions;
- the extent of usage of the computer.

Especially Coulson in 1960, but also later Primas (1983), Löwdin (1990), Roberts (1996), and King (2000) emphasized the distinction of 'mathematical chemistry' from 'computational chemistry'. Perhaps Coulson's (1960) description is clearest and most dramatic, with 'computational chemistry' being (in some sense) ascribed as somewhat like experimental chemistry – just involving seemingly ever more complicated computer 'experiments', with the 'experimental apparatus' being the computer.[2] That is, an experiment often seeks to test a theory with there often being much effort using extensive apparatus to draw forth the numerical data – while also computational chemistry makes much the same effort with extensive apparatus (namely the computer, and associated software) to draw forth data – and neither the experimentalist nor the computer chemist need understand the underlying theory

or mathematics. As a related incidental point, the leaving of H.C. Longuet-Higgins and J.S. Griffith from theoretical (or mathematical) chemistry is said to have been born of their aversion to an ever more dominating view that theoretical chemistry was to evolve to naught but computational chemistry (March 2002). One point of some possible confusion concerns the development of novel computer algorithms[3] (Metropolis *et al*. 1953), which proceed by way of (mathematical) derivation (though their use is by way of computation), so that the derivation is properly part of mathematical chemistry. Again once the algorithm is in hand, there remains a problem of programming it, and at a yet later stage running it in production runs, with this last stage having evolved out of what is here argued to be mathematical chemistry. In further support of the view of computational chemistry's experimental aspects, Coulson (1960) (as well as John Roberts (1996)) emphasized that after a 'computer experiment' which has generated great tabulations of numbers, there typically still remains a need of theoretical (perhaps mathematically refined) interpretation and understanding. Presumably now with ever more voluminous computer data to interpret, there is a consequent ever increasing need of theory (and mathematics) – there surely being a useful mathematics concerning 'data mining'. Overall in its developmental stage it is deeply mathematical, while in 'production runs' a program's use is more like that of an instrument in an experimental lab. Moreover, the data so generated only adds to the need for theoretical and mathematical chemistry.

The question as to the distinction between 'mathematical chemistry' and 'theoretical chemistry' is delicate, with a large degree of overlap. In fact perhaps even half the articles noted in the preceding listings of different mathematical chemistry areas may be reasonably argued to belong more to theoretical chemistry than mathematical chemistry – though still the quoted articles and books may be seen to have some (often strong) novel mathematical component. Again a difference with 'computational chemistry' is that it tends to deal more with individual cases (such as also does experimental chemistry), while 'mathematical chemistry' generally adheres more to 'mathematical deduction' (perhaps even with formal theorems and proofs) often of wide generality, while 'theoretical chemistry' uses more 'scientific induction'. Here 'mathematical deduction' is understood to be by way of strict logic, while 'scientific induction' is by way of analogy and repeated agreements of individual predictions with experimental measurements. Of course, there are always articles which partake of more than one of these aspects – *e.g.*, computations which are then interpreted and perhaps a novel theoretical explanation given, or theoretical articles which introduce novel mathematics but further rely on experimental interpretation or fitting to cement the relevance. For an article with different parts each closer to a different area (mathematical, theoretical, or computer chemistry), it may be proper to classify it to more than

one of these areas. And some articles classifiable to one or more of these areas might also involve experimental chemistry.

That there is overlap between theoretical, mathematical, computational, and experimental chemistry should not be taken as a criticism of these distinctions. These simply correspond to different activities of which different scientists partake, and some may partake of two or more, perhaps intimately intermixed – while others may focus almost entirely on one of these aspectual activities. That is, the distinction of these aspects gives a more complete characterization of what goes on in chemistry in a quite different manner than the categorization into the various chemical divisions and fields of the preceding section. Notably this categorization of theoretical, mathematical, computational, and experimental cuts across all of science much outside of chemistry.

The relations of mathematical chemistry to the different main fields of chemistry and especially to physical chemistry and chemical physics bear further examination. But these relations have much to do with broad historical trends of development not only in chemistry, but also in physics and in mathematics. This then entails extensive further discussion, all as is to be addressed in a future separate article.

It seems that some of the previous articles on mathematical chemistry have sought to exclude or preclude mathematics mediated by physics (or by physical chemistry). But no 'substantive' reason has been made for such an exclusion – the exclusions being introduced by way of definitional *fiat*, or more subtly by way of quoted examples of mathematical chemistry. It is certain that many of the exemplary physical-chemistry-related (or chemical-physics-related) articles noted in the preceding listing here are highly mathematical and often of a novel character, while revealing very interesting things about chemical systems (*e.g.*, as judged in several cases by awards of Nobel prizes). That such often beautiful work comes from physical chemistry should not count against the work as being part of mathematical chemistry.

Somewhat similarly, that mathematicians do not immediately pick up on much mathematical chemistry should not necessarily discount it either. Mathematical fundamentalness can be obscured due to the chemical context and applications, so that even if something is mathematically very fundamental, it may take some time to be so recognized. As an example, note Lars Onsager's solution (1944, in Appendix 2) of the 2-dimensional Ising model, which mathematicians seem not to have noted for some decades, till especially following work by E. Lieb (1969a,b), Yang & Yang (1966a,b), and R.H. Baxter (1969, 1970, 1972) (and by many others) combining Onsager's work with further early ideas of H.A. Bethe (1931), where-after it was seen (*e.g.*, Biggs 1977, Takhtadzhan & Fadeev 1979) as entailing novel fundamental mathematics. Another example is Ruch & Schönhofer's (1970, in Appendix

14) symmetry chirality characterizations, which was later recognized by Dress (1979, in Appendix 14), Fulton & Harris (1991), and Kerber (Gugisch *et al*. 2000, Kerber 1999, in Appendix 19) to entail novel fundamental mathematics. Another more minor case is that of Eyring & Polanyi's ideas (1931, in Appendix 12) about 'navigation' (or reaction) on complex potential-energy hyper-surfaces, as has recently been seen (Porter & Critanovic 2005) to be mathematically fundamental in a general theory of dynamical systems. Sometimes it can be just an incidental albeit challenging integral evaluation (Onsager & Samaras 1934) only much later done (Lossers 2005) in pure mathematics. Again the view here is that mathematical chemistry includes novel mathematical results for chemistry, regardless of whether the results are mediated by way of physics. It seems that often the mathematical novelty is recognized in mathematics only after some individual recognized mathematician makes a point of this, so that without such a stimulus, the recognition in mathematics might even take much longer.

A mirror attitude to that of excluding physical-chemical mathematical articles is that mathematical and theoretical chemistry are entirely subsumed within physical chemistry (and chemical physics). And though one finds physical chemists or chemical physicists that seem to think this, this attitude is comparably inappropriate. That is, there is no reason to imagine that novel mathematical (and again often beautiful) work from other subdivisions of chemistry should not be counted as theoretical or mathematical. Indeed the example (of the preceding paragraph) concerning Ruch and Schönhofer's work (1970, in Appendix 14) can be argued to come more from organic (or general) chemistry than from physical chemistry. Moreover many of the ideas identified in the listing of different mathematical chemistry areas are not generally viewed as part of physical chemistry. As a related point it is here suggested that the disguise of the field of mathematical chemistry has been fed by the (misguided) attitude that mathematical chemistry is subsumed within physical chemistry and chemical physics. This is taken up in a follow-up article – especially as regards chemical graph theory.

Though the broadness of mathematical chemistry should be clear from our detailed listings of areas, this broadness of view is in (often sharp) contrast to most of the earlier mentioned reviews of mathematical chemistry (Rouvray 1987, Löwdin 1990, Mackey 1997, Mallion 2005, Trinajstic & Gutman 2002, King 2000, Haberditzl 1979, Balaban 2005, Pauling 1987, Prelog 1987, Karle 1987, Primas 1983, March 1983), which end up often making a tight focus on the areas which are to comprise mathematical chemistry. Again mathematical chemistry is seen to overlap with all the traditional fields of chemistry.

5. 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 manners, 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 embedded 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 chemistry' 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 chemistry is seen to contact all 'classical' chemical fields: inorganic, organic, analytical, 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 taken so long to make an explicit recognition of the field of mathematical chemistry. 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 article, building from the presently established broad view. As a plausible conclusion, one could argue that university curricula include mathematical chemistry – 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 development.

Especially mathematical and theoretical chemistry reflect the overall richness and complexity of chemistry itself. Evidently the general philosophical aim in science in making precise and unambiguous statements (of fact, of theory, or of prediction) is to implement a mathematical framework. Indeed

this is somewhat a tautology – if one grants that mathematics is the realm of precision and clarity of statement (with numerics being just one form in which to so cast such statements). Notably this view of science is in complete concert with Leonardo da Vinci's statement (White 2001): "No human investigation can be called true science which has not passed through mathematical demonstrations". And also note Galileo's statement (1623): "The great book of nature is written in the mathematical language, ... without whose help it is impossible to comprehend a single word of it". And in a similar vein Immanuel Kant wrote (1900-2000, vol. 4, p. 470): "I believe that one may ascribe to every study of nature only so much scientific character as it contains mathematics".

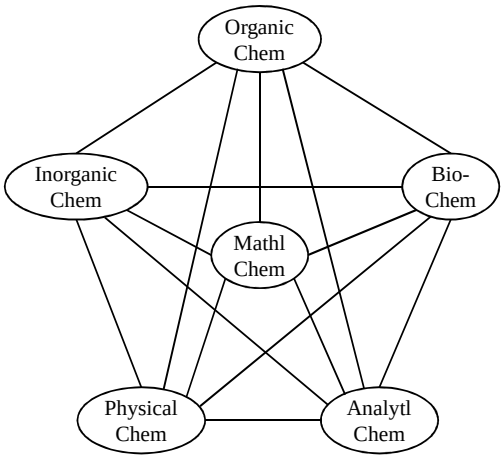

Figure 1: Inclusion of mathematical chemistry in university curricula

Thence it is emphasized that mathematics is an integral part of fundamental science in general, and chemistry in particular, so that a subdiscipline such as mathematical chemistry[5] is naturally anticipated – or perhaps even demanded. Reflecting chemistry as a whole, it is not surprising that the field is rich and diverse. Mathematical and theoretical chemistry are seen to be at the foundation of the science of chemistry. Indeed, as indicated in our discussion of the appearance of mathematical chemistry in different chemical fields, the general relevance of mathematical chemistry is well recognized in terms of the numerous examples of associated Nobel prizes awarded.

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Notes

[1] Sometimes it seems likely that some of the quoted articles might be argued to be non-mathematical. Some such further discussion of just what is 'mathematical' is taken up in a synoptic history, where for example, there is discussion of an early article of Crum Brown (1864) on chemical notation, which many at the time considered fundamental chemistry but not mathematical, whereas we argue that it is mathematical – just not numerical. Of the quoted articles in the present exemplar section, articles which many might consider not so mathematical include those concerning acids and bases (Brønsted 1923, Lewis 1923, 1938, Usanovich 1939 in Appendix 21), which nevertheless here are argued to manifest a fundamental mathematical germ. Lewis (1938, p. 302, in Appendix 21) enunciates his ideas in terms of four formal definitional (arguably axiomatic) conditions. He allows the idea of degree of acidity, but notes (on page 299) "how impossible it is to arrange our acids in any single monotonic order", so that one perceives an indication of a 'partial ordering', such as is elaborated in a more formally mathematical framework (Klein 1995, Klein & Babic 1997, in Appendix 21). Overall, if something of a concrete or substantive nature has been enunciated, then it should be susceptible to mathematical formalization. Or perhaps the converse statement is better to make, that if it is not susceptible to mathematical formalization, then it is not really substantive. Perhaps it would be appropriate to leave a few of the articles out of the listing of mathematical articles, though the position taken here is that the foundational work which is being formalized has some element of the mathematical content. Another area which many might question as mathematical concerns 'classification' (*e.g.*, as complicit in the mentioned chemical nomenclature). But classification is fundamentally mathematical, if made precise – this often entailing not only equivalence classes, but also various hierarchical orderings of these classes. Such matters are neatly (and often deeply) considered in isomer classification (as in Mislow 1977, in Appendix 14), substance classification, and nomenclature.

[2] In addition to computer chemistry having similarities to experiment, there are sharp differences. In computational chemistry the 'real world' of chemistry is substituted by a 'virtual computer world' controlled by the theoretical model employed. Still in either case the 'studied world' is itself so complex that it is often studied by a rather explicitly trial and error method, *e.g.*, perhaps involving Monte Carlo sampling. Often significant guidance from theory is non-trivially employed, though this may be done in the usual experimental context also. Indeed techniques for guidance in one field (computer chemistry or experimental chemistry) might often be profitably transferred to the other field.

[3] A nice example here is the development of the Metropolis Monte-Carlo algorithm (Metropolis *et al.* 1953) for sampling state 'configurations' to appear in a statistical-mechanical partition function (and then entering into different statistical mechanical expectations). In fact there are numerous other examples involving derivations of 'unbiased' Monte-Carlo sampling techniques, *e.g.*, Wall's 'slithering

snake' algorithm (Wall & Mandel 1975, in Appendix 15), or various constrained-diffusion algorithms for quantum Monte-Carlo electronic structure (Reynolds *et al*. 1982, Ceperley 1991; ten Haaf *et al*. 1995, in Appendix 9).

[4] King (2000) seems to imagine a wide range to mathematical chemistry when in passing he ascribes the development of quantum mechanics in the early 20th century as a development in mathematical chemistry. In the current article here a less extreme, more pragmatic (more conventional) view is taken: when both experiment and theory are done primarily by physicists (*i.e.*, scientists in physics departments) who think that they are doing physics, this is identified as physics. Ambiguities remain (*e.g.*, with thermodynamics or statistical mechanics), but so it is. Returning to King's review, once past the comment about quantum mechanics, it is quite lop-sided in an opposite way, in illustrating mathematical chemistry such that there is essentially no mention of most of the areas detailed in the present article. Perhaps 90% of his discussion is drawn from 'chemical graph theory', and then almost all from within a special sub-area of this – without clearly indicating this narrow focus.

[5] Again it is noted that there is some qualification in that it is demanded that mathematical chemistry involve *novel* mathematics. The general argument expounded for the development of science demands only that mathematics be part of (substantive) science, without the demand that the mathematics be novel. But granted mathematics appearance in science, it seems that extensive scientific development should ultimately lead to some novel mathematics arising at some point along the way. Again in chemistry much of the more evident less trivial mathematics has often been perceived to be filtered through physics, though in principle this is something that is independent of the novelty. In some of our examples the mathematics might be argued not to be so novel – but here we let our idea of 'novelty' be colored by its chemical application. For instance, in the discussion of physical organic theory, various 'linear free-energy relationships' were identified as mathematical chemistry (thence with some novelty), though this mainly involves expressing logarithms of quantities (equilibrium constants or rate constants) as a linear combination of structural characteristics. What is novel in this case is not so much the logarithms or linear combinations, but rather the manner in which the (graph-theoretic) structural features are treated. That is, though the 'intrinsic' mathematics might not be novel, the area or manner of its application might be novel – perhaps so much so that some fundamental mathematics is reinvented (in a new context). Indeed such a phenomenon may be seen to occur even within mathematics proper, and an even standard sort of *modus operandi* in mathematics is to borrow (or more colloquially 'steal') from one area to build in another.

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