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The Journal of Mathematical Chemistry: A Bibliometric Profile

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Abstract

This paper describes the bibliometric characteristics of 2,398 articles published in the Journal of Mathematical Chemistry in the period 1987-2015. These articles have been analysed using data from the Web of Science Core Collection and demonstrate the contribution of the journal not only to mathematical chemistry but also to science more generally.

1 Introduction

The Journal of Mathematical Chemistry (hereafter JMC) was first published in 1987 by J.C. Baltzer AG, then in 2000 by Kluwer and since 2004 by Springer in both printed and electronic forms. In the very first issue, the founding editor, Dennis Rouvray, noted that "Mathematics and chemistry make excellent partners. Cross-fertilization of mathematical theory with chemical concepts has been responsible for the growth of major areas of chemistry over the past two centuries" [1] and the journal supports this by publishing (as the website at http://www.springer.com/chemistry/physical+chemistry/journal/10910 states) "original, chemically important mathematical results which use non-routine mathematical methodologies often unfamiliar to the usual audience of mainstream experimental and theoretical chemistry journals. Furthermore JMC publishes papers on novel applications of more familiar mathematical techniques and analyses of chemical problems which indicate the need for new mathematical approaches".

For many years, each volume consisted of three or four issues (or occasionally of a single, very large issue) with one or more volumes a year; this changed in 2011 to the current format with a single, ten-issue volume each year. In this brief note, we provide a bibliometric profile of JMC, based on the articles that have appeared in the journal and that have been indexed in the Clarivate Analytics

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(formerly Thomson Reuters) Web of Science Core Collection database (hereafter WoS), which provides coverage of the journal since the very first issue. A search of WoS in August 2016 showed a total of 2,543 contributions to the journal up to and including the final issue of volume 53 at the end of 2015. The discussion that follows is based on the 2,398 articles that remained after the removal of reviews, editorial material, corrections and the like.

2   Publication data

The dark bars in Figure 1 demonstrate the increase in contributions to the journal over the years, with the height of each column denoting the total number of articles in each four-year period (and similar comments apply to the citation counts discussed in the next section). The first three years saw a total of 57 articles appearing, but the numbers soon increased to 40-50 a year and remained at this level (albeit with some degree of variation) until about 2005, since when there has been a marked increase so that there are now typically about 150 articles a year (these covering 2,213 pages in 2015's volume 53 as against just 421 pages in 1987's volume 1).

These 2,398 articles are the work of 2,603 different authors. As would be expected, there is a highly skewed distribution with no less than 2,172 of these individuals being associated with just one or two articles. Conversely, as is common with most academic specialisms, there are some individuals who have made very substantial contributions to the journal. For JMC, the ten most productive authors are R. Carbó-Dorca (with 69 publications), T.E. Simos (59), P.G. Mezey (40), M. Demiralp (36), R.F. Nalewajski (35), E. Besalu and I.I. Guseinov (both 31), I. Gutman (30), S. Fujita and N. Trinajstić (both 29). Of these, Carbó-Dorca, Simos and Trinajstić are current members of the editorial board and Mezey is the current editor of the journal (having become joint editor with Trinajstić in 1990 and then sole editor in 1994). After taking account of a few joint publications, these ten authors have jointly contributed no less than 15.5% of the total number of JMC articles.

The distribution for the 92 distinct nations of origin is comparably skewed with the USA contributing 468 articles, followed by the People's Republic of China (PRC) (345), Spain (252), Canada (185), Turkey (149), UK (136), Germany (101), Hungary (99), Poland (97) and India (93). The strong showing of the PRC is a recent one, with only 26 of its 345 articles having been published prior to 2001; in like vein, just 13 of India's and 10 of Turkey's articles pre-date 2001, demonstrating the increasing interest that is being taken in mathematical chemistry world-wide.

The content of the 2,398 JMC articles is summarised in the two word-clouds (produced using Wordle at http://www.wordle.net/) shown in Figure 2. Here, the size of each word in a word-cloud is proportional to its frequency of occurrence within the titles, after the removal of stop-words and the conflation of obvious word variants, e.g., "bond" and "bonds", to the singular form. Figure 2(a)

covers the 659 articles published in 1987-2000 and Figure 2(b) the 1,739 articles published in 2001-2015. A comparison of the two plots demonstrates some considerable differences, in particular a substantial reduction in the use of the words 'chemical', 'graph' and (albeit to a lesser extent) 'matrix' during 2001-15 when compared to the earlier period. However, words such as 'method' and 'model' have retained their importance, with 'Schrodinger', 'reaction' and 'equation' being some of the words in Figure 2b that have come into greater prominence. This would suggest a transition from discrete mathematics, with graph theory and matrices being used to study molecular structure, to greater application of continuous mathematics oriented to problems in quantum chemistry. The increase in the use of 'Schrodinger' is particularly notable: it had just five appearances in the first period (with 0.8% of the titles of that period contained that word) but no less than 85 appearances in the second period (corresponding to 5% of the titles).

3   Citation data

The 2,398 JMC articles had attracted citations from a total of 11,988 distinct articles up to the end of 2015, i.e., a mean of 5.0 citations per article. The growth in citations is illustrated by the lighter bars in Figure 1, and the eleven articles that have attracted over 100 citations are listed in Table 1; the reader should note that these citations are total counts, and there is hence an obvious bias toward the older articles, since they have had a longer period in which to accrue citations. This bias is reflected in the fact that six of the articles in the table involve applications of graph theory to chemistry (with five of these having to do with the generation of molecular descriptors), a topic that Figure 2 shows was of much greater prominence in the earlier days of the journal. That said, the articles cover a broad range of subject matter including, e.g., modelling ionic solutions and liquid crystals, catacondensed benzenoid hydrocarbons, and the relationship between molecular energy and numbers of electrons.

Table 1 also lists the journal, or journals, that provided the greatest number of citations for each of the eleven articles. The presence of MATCH Communications in Mathematical and in Computer Chemistry (hereafter just MATCH) and of the Journal of Chemical Physics are unsurprising, while the prominence of the Journal of Chemical Information and Modeling is accounted for by this being a journal that has had a long-standing interest in both chemical graph theory and molecular descriptors. There is, however, one exceptional article, viz that by Turanyi. This attracted the fourth largest total number of citations with many of these coming from the engineering literature, in particular from journals related to various aspects of combustion. The range of citing sources for this article provides a striking example of the behaviour discussed further below, where we consider the influence of JMC outside of the most obviously related subject fields.

The most-cited article, that by Klein and Randić, was one of three papers in Table 1 (the others are those by Plavsic et al. and by Ivanciuc et al.) that appeared in 1993 in a special issue of the journal that was dedicated to Frank Harary, a pioneer in the development of graph theory, on the occasion of his 70th birthday. Despite being now almost one-quarter of a century old, the article continues to attract an increasing number of citations, rising from just two in 1993, the year of publication, to 52 in 2015. A similar pattern of behaviour is seen for the next two papers in the table, viz those by Rabitz and Alis and by Cances and Mennucci. Rabitz and Alis are two of the four authors (the others are Randić and Trinajstić) who appear twice in Table 1. Other articles in Table 1, however, show a more conventional citation profile, with the citations slowly rising (albeit often with variations from year to year) to a maximum value and then becoming of less importance as the years go by. For example, the 2008 article by Ayers received its largest number of citations in 2012 but these are now dropping off; while the 1992 paper by Mihalić et al. received the largest number of citations (12) as long ago as 1997 but has continued to attract a few citations year-on-year to the present day.

The 11,988 citing articles appeared in 2,194 different publications (mainly journals but also including over a thousand conference proceedings together with reviews, book chapters, editorial material and the like), with JMC itself providing 1,219 journal self-citations (i.e., articles in a journal that cite other articles in the same journal). Apart from JMC, the following twelve journals have cited JMC at least 100 times: MATCH (549 citations), Journal of Chemical Physics (460), Journal of Chemical Information and Modeling (446), International Journal of Quantum Chemistry (333), Journal of Physical Chemistry A (221), Journal of Computational Chemistry (165), Chemical Physics Letters (164), Croatica Chemica Acta (163), AIP Conference Proceedings (145), Discrete Applied Mathematics (139), Journal of Molecular Structure: THEOCHEM (121), and Physical Chemistry Chemical Physics (100). The appearance of MATCH at the head of this list as the journal that cites JMC the most mirrors the fact that a bibliometric analysis of that journal shows JMC to be the publication that cites MATCH the most [2]; and it is noteworthy that the top three journals here are the ones that provided the greatest numbers of citations for the most-cited JMC articles in Table 1.

The remaining journals in the list of heavily-citing journals are hardly unexpected given the sorts of topic that they cover, and moving down to journals providing less than 100 citations to JMC one comes across many other mathematical and chemical journals of various sorts. However, consideration of some of the other citing journals reveals a surprising breadth of interest in the material that is published in the journal. For example: an article in Acta Alimentaria entitled "Extrusion of corn grits with native or modified starch addition - influence on starch digestibility fractions, shear stress-at-break, and expansion ratio" [3] cites a JMC article on the use of Markov chains to model non-homogeneous flows [4]; and an article in Desalination entitled "Recent

applications of nanomaterials in water desalination: A critical review and future opportunities" [5] cites a JMC article modelling the transportation of sodium and chloride ions [6].

Similar behaviour is observed if one analyses the citing publications in terms of the WoS subject category to which they belong. The 2,194 publications represent 157 different subject categories of which the largest contributions come from categories representing the areas of chemistry, mathematics and physics: for example, the five categories contributing most citations were Chemistry Multidisciplinary, Chemistry Physical, Mathematics Interdisciplinary Applications, Physics Atomic Molecular Chemical, and Computer Science Interdisciplinary Applications. Many less obvious categories are also included in the 157. For example, an article in Social Networks (in the Anthropology category) entitled "Resistance distance, closeness, and betweenness" [7] cites the paper by Klein and Randić that is listed in Table 1 as having received the greatest number of citations for any JMC article; and a chapter in the book Chaos Theory in Politics (in the International Relations category) entitled "Large spatial and temporal separations of cause and effect in policy making - Dealing with non-linear effects" [8] cites a JMC paper on first-order autonomous ordinary differential equations [9]. One could quote many further such examples that, taken together, demonstrate clearly the influence and importance of the journal not just for its core subjects but also for a much wider range of less cognate disciplines.

4 Discussion and Conclusions

Thus far, this paper has presented the publication and citation characteristics of JMC. To put this data in context, the journal needs to be compared with other journals that cover the same, or related, subject fields.

Whilst there are many journals that publish articles on the computational aspects of chemistry (such as the Journal of Chemical Information and Modeling, the Journal of Computational Chemistry, and the Journal of Computer-Aided Molecular Design inter alia) there is only one, MATCH, that shares the detailed mathematical focus of JMC. We hence compare some of the results above with those that were obtained in a recent, entirely analogous study of MATCH that covered the articles published there during the period 1995-2014 [2]. The two journals have similar foci, as evidenced by a comparison of the MATCH mission statement ("publishes papers of original research as well as reviews on chemically important mathematical results and non-routine applications of mathematical techniques to chemical problems. A paper acceptable for publication must contain non-trivial mathematics or communicate non-routine computer-based procedures AND have a clear connection to chemistry") with that for JMC noted in the Introduction (vide supra). This being so, it is hardly surprising that they share several features in common. For example, as noted previously, MATCH is the journal that cites

JMC most frequently, and vice versa; and there are two further journals (Croatica Chemica Acta and Discrete Applied Mathematics) that have provided at least 50 citations to both journals. In like vein, there is a fair degree of overlap in the authors that publish in the two journals: not only are I. Gutman and S. Fujita two of the ten most frequent contributors to JMC (vide supra), but they are also among the ten top contributors to MATCH; and there are another seven authors (A.T. Balaban, M.V. Diudea, T.E. Simos, N. Trinajstic, D. Vukicevic, H.P. Zhang and B. Zhou) who have published at least ten times in both journals. There is, however, at least one aspect of the journals that is now rather different, whereas this was not the case previously. In the early days, as exemplified by the prominence of the word "graph" in Figure 2a, JMC carried many articles on applications of graph theory to chemistry (with, as noted above, six of the highly-cited articles in Table 1 being of this sort). This was also the case with MATCH since it published large numbers of articles about graph theory, in particular its use for the calculation of a range of different types of topological index. However, JMC, as we have noted above, now publishes a greater proportion of quantum chemistry articles, whereas graph-based articles continue to appear on a very regular basis in MATCH right up to the present day with, for example, the latest issue (Vol. 77, No. 2) containing two articles on the comparison of chemical structures using maximum common subgraph isomorphism algorithms. In this respect, then, there has been some divergence in the precise focus of the two journals.

In conclusion, this paper has reported a bibliometric analysis of the articles appearing in JMC from 1987 to 2015. It has grown steadily over this period and now publishes ca 150 articles a year. There has been a shift from applications of discrete mathematics (chemical graph theory in particular) to continuous mathematics (as evidenced by the increased importance of quantum chemistry papers than previously). The citation analysis demonstrates clearly the widespread impact of the journal since it attracts large numbers of citations, with these coming not just from obvious, cognate areas such as chemistry, mathematics and physics but also from many other disciplines. In this sense, it can be seen as an important example of a knowledge exporter using the intellectual trading metaphor of Yan et al. [10].

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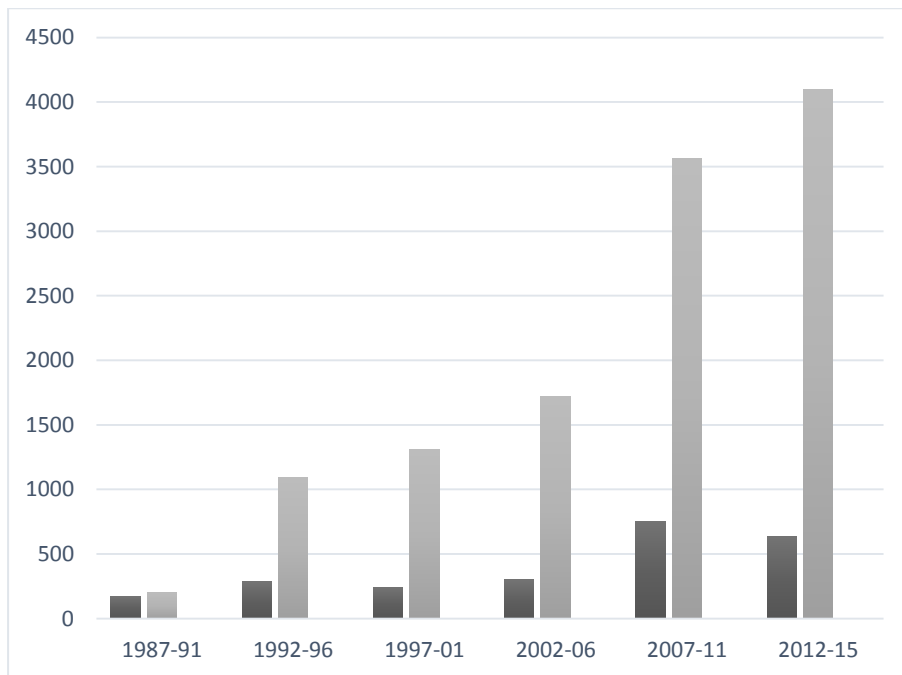10.   E. Yan, Y. Ding, B. Cronin, L. Leydesdorff, J. Informetrics 7, 249 (2013).

Figure 1: Numbers of articles (darker) published in JMC over the period 1987-2015, with the lighter bars denoting the numbers of citations to those published articles.

polyhexes concept hamiltonian vertical orbital aspect comparison geometric chiral numbers coefficients electron random oscillator electronic condition elements order

perturbation representation quantum property general hexagonal atomic isospectral asymptotic polymer reduced

lattice new equation chirality integral analysis generalized network case calculation basis waves

structure model function measure solution approach index algebra conformational approximation variational

symmetry operator study number nonorthogonal

field interactions s-n formulation using similarity chemistry set potential related distance analytic nonlinear density

local distances mathematical polymers geometry algebraic based reaction theory surface global state

functional topological invariants bond benzenoid procedure effect

polynomial linear autocatalytic kekule shape chain group spin analytical problem

enumeration principle eigenvalue calculations characteristic space technique perfect nuclear multiple

dynamical internal indexes transformations results thermodynamics theorem molecular

quantitative matrix energy kinetics classification nmr correlation topology application

graph chemical method system molecule

(a)

(b)

Figure 2: Word-clouds based on title words extracted from articles published in JMC over the periods (a) 1987-2000; (b) 2001-2015.

Authors	Title	Reference	Citations	Citing journal
D.J. Klein, M. Randić	Resistance distance	J. Math. Chem. 12, 81 (1993)	396	MATCH Communications in Mathematical and in Computer Chemistry
H. Rabitz, O.F. Alis	General foundations of high-dimensional model representations	J. Math. Chem. 25, 197 (1999)	344	Journal of Chemical Physics
E. Cances, B. Mennucci	New applications of integral equations methods for solvation continuum models: ionic solutions and liquid crystals	J. Math. Chem. 23, 309 (1998)	306	Journal of Chemical Physics
T. Turanyi	Sensitivity analysis of complex kinetic systems - tools and applications	J. Math. Chem. 5, 203 (1990)	263	Combustion and Flame; Reliability Engineering and System Safety
D. Plavsic, S. Nikolic, N. Trinajstić, Z. Mihalic	On the Harary index for the characterization of chemical graphs	J. Math. Chem. 12, 235 (1993)	187	Journal of Chemical Information and Modeling
O. Ivanciuc, T.S. Balaban, A.T. Balaban	Design of topological indexes. 4. Reciprocal distance matrix, related local vertex invariants and topological indexes	J. Math. Chem. 12, 309 (1993)	177	Journal of Chemical Information and Modeling
M. Randić	Generalized molecular descriptors	J. Math. Chem. 7, 155 (1991)	153	Journal of Chemical Information and Modeling

Z. Mihalić, D. Veljan, D. Amić, S. Nikolić, D. Plavšić, N. Trinajstić	The distance matrix in chemistry	J. Math. Chem., 11, 223 (1992)	132	Journal of Chemical Information and Modeling
P.W. Ayers	The dependence on and continuity of the energy and other molecular properties with respect to the number of electrons	J. Math. Chem. 43, 285 (2008)	128	Journal of Chemical Physics
O.F. Alis, H. Rabitz	Efficient implementation of high dimensional model representations	J. Math. Chem. 29, 127 (2001)	114	Journal of Chemical Physics
P.V. Khadikar, P.P. Kale, N.V. Deshpande, S. Karmarkar, V.K. Agrawal	Novel PI indices of hexagonal chains	J. Math. Chem. 29, 143 (2001)	106	MATCH Communications in Mathematical and in Computer Chemistry

Table 1: JMC articles with more than 100 citations