Evaluation of an Experimental Chemistry Preprint Server†

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A preprint is a research article made publicly available prior to formal publication. A preprint server is a freely available archive and distribution medium for preprints, allowing rapid dissemination and use of multimedia and supporting files. Electronic eprints have been widely adopted in certain fields (notably high energy physics), but, until recently, the preprint concept has not been received with enthusiasm by most chemists. Despite the fact that preprints have the advantage of rapid publication, chemists have been reluctant to produce them because they could be viewed as "unallowable" for research assessment or tenure exercises or for publication in certain prestigious journals. In theory, preprints, together with version control and online discussion, could be a useful compromise: rapid prepublication followed by open peer review, before publication in a traditional journal. This paper constitutes a preliminary evaluation of a Chemistry Preprint Server in its second year of operation and summarizes the lessons that can be learned from the experiment to date.

INTRODUCTION

Before the significant changes that took place in the scientific publishing industry from the 1950s onward, the preprint had a substantial role to play in the dissemination of knowledge. Discoveries were often initially presented in the form of "papers" read to meetings of scientific societies by senior members, who in effect acted as peer reviewers of the articles.[1] (Indeed, preprints of presentations at American Chemical Society National Meetings are still disseminated by several ACS divisions.) With the development of the Internet and particularly the World Wide Web, versions of papers are now exchanged electronically as electronic prints, or eprints. There is a subtle difference between "eprints" and "preprints", the latter term implying that traditional publication may perhaps follow, while the term "postprints" is used for electronic versions of papers that have appeared in print.

A physics eprint server was set up at the CERN laboratory in Geneva in 1994 as an internal document server for papers in the field of high energy physics.[2] Currently, more than 50 000 documents are added to that server annually. Another well-known example is arXiv,[3] set up at the Los Alamos National Laboratory, LANL, by Paul Ginsparg and now run by Ginsparg from Cornell. This eprint server (which is not simply a preprint server) now covers close to 100% of articles in high energy physics and has a growing number of articles in condensed matter physics.[4] There are 17 international mirror sites.

Servers in chemical physics,[5] mathematics, economics, philosophy, education, history, and other disciplines have also been established.[6,7] Many of these servers are run by enthusiastic lone academics or not-for-profit organizations, although the software for the cognitive sciences server (CogPrints)[8] is to be commercialized by Ingenta.

Brown[9] has examined how eprints are cited, used, and accepted in the literature of physics and astronomy. She found that, even though the use of traditional literature has not changed since arXiv began, the number of citations and citation rates to 12 arXiv archives is large and increasing. She concludes that eprints have evolved into an important facet of the scholarly communication of physics and astronomy and will become the major vehicle for physics and astronomy scholarly communication. In a survey of scientists at Oak Ridge National Laboratory (ORNL) carried out in 2000, Tenopir and King[10] found heavy usage of arXiv (75% of scientists, including nearly 100% of physicists) among those readers who had heard of arXiv. However, only 29% of respondents (50% of physicists) were aware of the eprint archive.

While Brown[9] concluded that preprint servers are so successful in physics and astronomy that other disciplines are also likely to adopt the technology, another school of thought suggests that the chemistry community is socially different from the close-knit world of particle physicists.[11] Some authorities[12] are convinced that it is not just a matter of time before all disciplines converge on common ways of using electronic media to support scholarly communication. Speed of publication matters more in some disciplines than others, but there are dangers inherent in premature publication. Nevertheless, Dessy[13] claims that it is a myth that successful eprint servers require an intimate clique of compatriots. Moreover he points out that specialized journals, tightly targeted symposia, and global-village clans are now common, even in chemistry.

ISSUES AND CHALLENGES

Advantages and Disadvantages. An official ACS document[14] lists far more disadvantages than advantages. It states that the advantages of preprint servers are rapid, broad, and generally inexpensive distribution and worldwide access, while the disadvantages include the potential for flooding the literature with trivial and repetitious publications, thus

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making extraction of reliable and valuable information more difficult; absence of peer review; possible premature disclosure with inadequate experimental details or supporting data; premature claims of priority; potential lack of proper references and credit to prior work; abuse of multiple revisions or updates; possible lack of duration; and unreliable long-term archiving. These issues, and others, were discussed at a presidential plenary session at a recent ACS Meeting,[15] and they are considered in more detail below.

Enhanced Chemistry Publication. Articles in electronic form can be enhanced by multimedia features and can include large data sets, computational simulations, and molecular structures for rotating in 3D, for example. Preprint servers are not alone in offering such features: peer-reviewed electronic journals can also do "enhanced chemistry publication". The *Internet Journal of Chemistry*,[16] for example, was launched with several targets including full incorporation of multimedia, promotion of Internet technologies,[17−19] low cost, and liberal copyright policies. It is peer reviewed and covers all areas of chemistry.[20] Publication on the Web can be faster than publication in print but peer review inevitably takes time, so posting an eprint is likely to be the fastest possible way of publishing one's work.

Speed of Publication. A distinguished academic librarian[21] sees preprints as a symptom of the problems of scholarly publication in the 1990s, not a solution to them. For example, some researchers work at the cutting edge and find preprints meet their speed requirements; preprints have great appeal to these workers. In a metaphor, this authority[21] asked if it is progress if a cannibal eats with a knife and fork.

Speed is more important in some disciplines than others but there are dangers inherent in premature publication. Some authorities feel that patent rights may be more important than speed of publication in chemistry. Bovenschulte, Director of the ACS Publications Division, has asserted that there are many more patenting opportunities in chemical research than in physics and many chemists do not want to release and share information that may be commercially valuable.[22]

For a speed comparison, it is worth noting that for ACS *NanoLetters* and *Organic Letters*, the median time from receipt of the manuscript to Web publication is seven weeks, with a range of 2−17 weeks; 50% of the manuscripts are published in 6−9 weeks. This includes peer review and the editorial production process. The RSC publishes communications (in *Chemical Communications*) in Advance Articles on the Web 60−80 days after receipt. From acceptance to publication on the Web there is a lapse of only 2−3 weeks. It is typically a further 2 weeks before the paper version is produced. RSC publishes full papers within about 4 months. Some learned publishers, such as ACS, have enhanced their journals to the point where the electronic version is considered the version of record.

Peer Review. Stang, current Editor of *Journal of the American Chemical Society*,[23] probably represented the views of most ACS editors when he described how thoughtful peer review and editorial care and handling maintain high standards and the integrity of science. Peer review is stretched to the limit: it is hard, slow work. Stang feels that reviewers are not likely to comment on preprints, and prejudice (for and against) will prevail where reviewing *is* done; public review is less likely to be critical. He wonders whether there will be enough data on a preprint server to validate the publication and he queries who will decide if the data is correct and reproducible. Who will check that others (for example, competitors) get credit for *their* work? Stang admits that his own papers have been improved by thoughtful peer review.

The *ACS Style Guide*[24] has collected comments on peer review from a number of experts. The merits and limitations of classical peer review were discussed in a monograph by Chubin and Hackett.[25] An excellent book devoted to the subject has also been published more recently, but it is mainly concerned with the printed literature.[26] The great majority of peer review studies carried out to date have been in medicine, health, and psychology; it is not known whether the results can be applied to disciplines such as chemistry.

The *British Medical Journal* has carried out randomized, controlled trials of peer review and has shown that the two-reviewer method is only slightly better than random. The researchers inserted eight deliberate errors into a paper about to be published in the journal and sent the paper to 420 potential reviewers, 221 of whom responded. The median number of errors spotted was two, nobody spotted more than five, and 16% did not spot any errors at all.[27] The journal's editor says that peer review is slow, expensive, biased, easily abused, and poor at detecting fraud. On one point, though, he agrees with Stang: what good peer review does achieve is to *improve* a paper.[28] The *British Medical Journal* intends not just to reveal the names of the two reviewers to the authors but to open up peer review to contributors and readers on the Web.[29]

Preprint servers use this nontraditional form of peer review. Once a document is placed on ChemWeb's Chemistry Preprint Server (CPS),[30] for example, readers are able to comment on it, and when the manuscript has been refined by annotation and discussion it can be submitted to a standard journal. The server allows multiple versions of the paper to be stored and dated.

Kling and McKim[31] claim that peer review, whether on paper or electronic, provides valuable functions that are not effectively replaced by self-posting of articles electronically. They have also shown that the common claim that electronic publishing substantially expands access is oversimplified: the interwoven dimensions of publicity, access, and trustworthiness are complex.

In practice, articles that are rejected by a major journal are not necessarily unprinted and forgotten. They go from one journal to a "lesser" one and perhaps even to a third in a process of market selection.[32] Young workers, without an established track record of publication, find it hard to place printed papers in the top tier journals and for them a preprint server can have great advantages.[13]

Wide Dissemination. Dessy feels that, for young scientists, preprints will give quick, inexpensive exposure that can also help spread knowledge.[13] Berry agrees with him concerning the international appeal of a preprint server.[33] In his view, scientists in developing countries will have access to information since access to a preprint server is potentially broader. He also states that, since access is faster, science will move faster and since access is more thorough to the entire archive, the level of scholarship will rise.[33]

Prior Publication. ACS editors have policies on prior publication and on prevention of multiple publication and proliferation of papers.[14] These policies may deter people

who want to publish fast, although publishers vary in their attitude to prior publication. Under the editorship of Franz Ingelfinger, the *New England Journal of Medicine* adopted a policy of declining to referee or publish research that had been previously published or publicized elsewhere. Other biomedical journals, as well as broad-spectrum journals such as *Science*, have since adopted this "Ingelfinger rule".[34] In one camp are the *New England Journal of Medicine*, *Science*, and ACS Publications who will not publish any paper if it has appeared previously on the Web. (However, it should be noted that, in practice, ACS editors are allowed a certain amount of personal discretion.) In the other camp are the RSC, *Nature*, and *Physical Review*. Stevan Harnad, an outspoken proponent of nontraditional academic publishing, has expressed strong opposition to the Ingelfinger Rule.[35]

Copyright. This is not the place for a lengthy discussion on copyright (the reader may care to read the ACS learning module on the Web[36]), but the issue of prior publication involves, to some extent, the question of transgressing the intellectual property rights of the copyright holder on the first publication. Most traditional publishers require authors to assign copyright to the publisher, whereas the owners of preprint servers (and the *Internet Journal of Chemistry*) usually allow the author to retain copyright while asking for a license to reproduce the material. A committee of scientists, attorneys, legal scholars, and publishers, convened by the American Association for the Advancement of Science (AAAS), recently issued a report on intellectual property rights in the information age.[37]

Tenure and Promotion. Steve Heller has put this in a nutshell in more than one oral presentation: "*You don't get tenure at Harvard by publishing in the* Internet Journal of Chemistry". As long as the established system of promotion and tenure depends on a record of publishing in "quality" journals, it is difficult to persuade chemical research workers that it is safe, or advisable, to publish in nontraditional sources. Not only are they influenced by the opinions of those who judge them but also many chemists themselves really believe that a chemistry preprint server would be the "*Journal of Not Very Good Science*". Indeed, this author started on the current study with such a prejudice.

Butterworth[38] has reported an anecdote concerning the online-only section of *Pediatrics*. Both standard and online sections have identical peer review procedures, and the editor selects items for the online section at random. The two sections are remarkably similar yet scientists perceive the online-only one as being of less high quality.

Boyce[39] does not think self-publication will count much toward tenure and promotion, but he concedes that peer pressure from colleagues has kept the quality of submissions to preprint servers higher than might have been anticipated. Dessy believes that no harm, except to incautious authors, would result from electronic preprints, and promotion and tenure committees and evaluation panels would have the advantage of Web access to the open criticism and positive responses of *all* interested peers, helping them to analyze a candidate fairly.[13]

Lawrence[40] has shown that there is a clear correlation between the number of times an article is cited and the probability that the article is online. He recommends that for greater impact and faster scientific progress, authors and publishers should aim to make research easy to access.

Measures of Quality. The concept of the most cited, high impact journal and its impact factor is well established in the measurement of "quality". An example of the value of this measure is the recent announcement by The Scholarly Publishing and Academic Resources Coalition, SPARC,[41] that ACS' *Organic Letters* has exceeded Elsevier's *Tetrahedron Letters* in impact factor. According to the 2000 ISI Journal Citation Reports, *Organic Letters* is seventh in impact factor, while *Tetrahedron Letters* is number 13. When *Organic Letters* is evaluated with respect to journals publishing more than 100 articles in 2000, it rises to number two in impact factor, second only to ACS' *The Journal of Organic Chemistry*. Stang[23] believes that preprint servers will be cited infrequently, because they are unreliable and inaccessible. He suspects that they will thus have little long-term value.

However, there are those in the information science community who feel that different measures of quality also need to be considered. In suggesting a different range of objects on which bibliometricians may work, Cronin[11] has said the following: "*...the units of analysis will be messy, slippy, evanescent and promiscuous...what are the kinds of indicators of perceived quality that we're going to want to rely upon or invoke when dealing with multi-modal, promiscuous output from publishing?*". He predicts a future for "indicator mining", with facilities well beyond the studies he and others have done of acknowledgments and citation counts, giving richer, multidimensional pictures of an individual's presence and impact on the peer community.

Signal and Noise. While improving access to information, preprints can also contribute to information overload. There are those who feel that lowering barriers to information access makes information less valuable. Separating the reliable, good, and valuable results can be a problem, i.e., extracting the signal from the noise.[23] However, as the deluge of information on the Web increases, so does the availability of new tools for filtering it. Modern search engines and database structuring make it possible to select finely the subset of preprints offered to a researcher.[13] Cronin[11] predicts that in future we will see a battery of tool sets and engines that go beyond today's search engines and allow us to carry out "prospect mining". Meanwhile, CAS has added preprints as a document type and is indexing articles from CPS.

Role of Learned Societies. Preprints of conference presentations are being produced by the Fuel Chemistry, Polymer, Polymer Materials: Science and Engineering, and Petroleum Divisions of ACS. These preprints are not free of charge; they are a member benefit and a revenue stream for the divisions in question. For 2 years, the ACS Publications Division did consider setting up a preprint server for journal articles, though responses to a survey of ACS members and journal subscribers ranged "from condemnation to enthusiasm", according to Robert D. Bovenschulte.[42] A supporter of the idea[43] reasoned as follows. An unsupervised preprint system could corrupt the chemistry literature. An unmanaged preprint literature could neglect the linkage of preprints to the formal chemical literature, whereas a preprint literature has the potential of capitalizing upon the Internet's potential. The ACS is well positioned to lead in a manner that will preserve the integrity of the chemistry literature. In summary, "*ACS should be pioneering this or someone less noble will do it*".[43]

The RSC also maintains that its members are, on balance, not in favor of RSC's mounting a preprint server. Since the peer-review process equates to a cost of about $600 per submitted (not accepted) paper,[44] RSC does not actively seek to commission papers from any source where the paper may not yet be of an anticipated adequate standard, although it has published, in its learned journals, a small number of papers from CPS. ACS and RSC have, however, launched "fast-track", but more traditional, publications in conjunction with SPARC,[41] which claims that one of these journals, ACS' *Organic Letters*, has also created price moderation in the field.

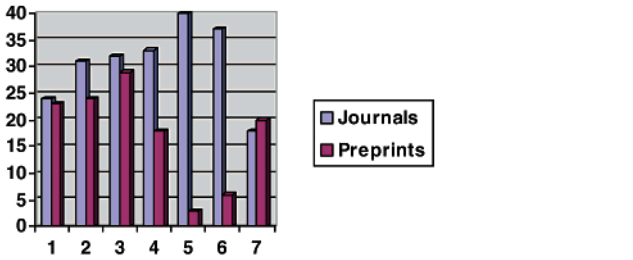
Economics. Since the 1990s, there has been a trend toward "self-publishing", but it is not clear how sustainable such ventures will be and who will continue to finance them. Many preprint servers are run by academics on a voluntary basis, and publishers maintain that such amateur ventures are doomed to failure. The CEO of Elsevier Science, for example, has stated that publishers need to be well funded and in the business for the long term. Publishing is tedious, hard work and also intellectually challenging. The scientist who says, "let's do it ourselves" underestimates the work, funds, and perseverance needed.[45]

Commercial firms offer one method of funding; governments, academic institutions, and professional organizations may also provide the infrastructure and funding to support preprints. Various initiatives have advocated the concept of the institutional archive, which is rather different from that of the preprint server devoted to one discipline. The best known example is DSpace[46] at the Massachusetts Institute of Technology (MIT), supported by a $1.8 million grant from Hewlett-Packard Company, but other institutions such as California Institute of Technology have followed suit.[47] It is estimated that DSpace could cost $250 000 a year to maintain. The availability of metadata codes from the Open Archives initiative[48] and free software from MIT[49] and the University of Southampton, England[50] may reduce costs for other institutions.

Some initiatives such as the Public Library of Science propose to impose the publishing costs on authors, or the organizations with which they are affiliated, rather than on libraries and readers,[51] yet page charges levied by journals are another economic reason some authors are choosing to publish in preprints rather than in journals.

So, how will CPS pay for itself? For example, will the operators of the server expect to receive first-refusal e-journal rights and copyright? There are those who suspect that ChemWeb (a division of Elsevier Science, albeit a service which tries to be publisher-neutral) does not host the Chemistry Preprint Server for wholly altruistic reasons.

Tracing, Tracking, and Version Control. A document in the prepublication stages undergoes many revisions. Without a reliable tracking mechanism it can be almost impossible to tell the lineage of an electronic document. A seamless integration of all e-publishing is required. One solution is to track a preprint through the publication process, so that it can automatically be identified with the published paper using meta-tags and URL pointer/resolvers. The search system returns the URL of the preprint until the paper is published and the URL of the electronic journal article afterward. At that point the preprint may be dismounted from the preprint server.[13]



1. Priority stamping
2. Building a collective knowledge base
3. Distribution and communication of research findings
4. Enabling citation of articles
5. Quality control
6. Reward and recognition
7. Building a community of interest.

Figure 1. Results of Keller's Delphi survey.

Through the Open Archives initiative,[48] search across multiple archives is possible. ArXiv, CPS, CogPrints, and "ancestral" in computer science[52] comply with the open archiving standard. Reliability, durability, and reference tracking are challenges. Librarians find it hard enough tracking gray literature, let alone preprints. Other problems are the relationship to finding aids, access, secure archiving, a permanent identifier for linking, and affordability.[21] There is considerable debate at present about who can be trusted to archive the electronic scientific literature and who will pay for the resource required.

Other Issues. It has been claimed that preprints will be cheaper than traditional publications (at least for libraries and readers) and that they are environmentally friendly, since less paper is used. On the other hand, there are issues of security, plagiarism, and privacy that need to be addressed.

The Role of Preprints. Boyce[39] lists five functions of traditional journals: status (keeping the community up-to-date), news (disseminating the latest research results), information (providing a repository of knowledge), author evaluation (judging the competence of authors), and historical (maintaining a record of the progress of science). He feels that preprint servers fill the status and news roles well but do not, and may perhaps never, fill the other three, more important roles.

The opinion of the panel in a Delphi survey carried out by Keller[53] was that preprint archives will be the main competitors of traditional journals during the next decade. Experts were asked to consider how suitable peer-reviewed journals and preprint archives will prove to be for different functions. Their answers are illustrated diagrammatically in Figure 1.

Keller states that these results might cause some to question whether it is appropriate that academic and research libraries spend up to 80% of their acquisitions budget on one publication type that is superior to another, much cheaper publication channel, in only two or three areas. However, although most respondents thought it desirable that all major subject areas be served by large preprint servers, there were many reservations. Some experts consider peer review a prerequisite for publication. Others mention that speed of availability and maximum accessibility are not equally important in all disciplines. Some felt that preprint archives

do not have a potentially sound commercial basis and depend too much on voluntary involvement of interested individuals. It was concluded that, due to their deficiencies in quality control, preprint archives may be less successful and widespread in the long term than is sometimes assumed. Keller's article draws some clear conclusions about the decline of the print journal, but there was no agreement on whether preprint archives are desirable for all subject areas or not. Digital archiving was also an issue.

Another paper[54] identifies the growing importance of electronic preprints in the published literature and addresses several areas of concern regarding the future role of electronic preprints in scientific communication. Because of the timeliness of these papers as well as the increasing demand for current research, physicists and astronomers have found it necessary to cite these preprints in their research articles rather than wait until they appear in print.

CHEMISTRY PREPRINT SERVER

Functionality of CPS. The first preprint server devoted to all areas of chemistry was set up by ChemWeb in July 2000.[42,55−56] It was seen as a means for chemists to exchange ideas before they are in a final form that is ready for publication. The site accepts any document about chemistry. Preprint drafts are submitted in standard word-processing format; additional files such as chemical structures or graphics can also be included.

To submit a preprint, an author would upload the main article, any number of supplementary files, and also the metadata for the preprint. Metadata fields on the CPS are author name, additional author names, affiliation address, author e-mail address, article title, the chemistry classification to which the preprint was submitted, and a chemistry "technique" relevant to the preprint. The main article may be submitted in a wide variety of formats, including Portable Document Format (.pdf), Microsoft Word for Windows (.doc), PostScript (.ps), Rich Text Format (.rtf), and HTML (.html). All articles are automatically converted to PDF on the server.

The article is screened by a CPS editor to ensure that it does contain genuine chemistry content. However, there is no formal peer review for acceptance of articles to the CPS. There are 10 primary classifications to which the preprint may be submitted. Each category contains a number of subcategories so that the article may be classified more precisely. The 10 primary classifications are as follows:

- Analytical Chemistry
- Biochemistry
- Chemical Engineering
- Environmental Chemistry
- Inorganic Chemistry
- Macromolecular Chemistry
- Medicinal Chemistry
- Organic Chemistry
- Physical Chemistry
- Miscellaneous.

It is also possible to classify the preprint further as a Conference Proceeding.

Every article accepted for the CPS is given a unique identifier of the form category/YYMMNNN, where "category" is the classification to which the preprint was submitted, "YY" represents the year, "MM" the month, and "NNN" the number in relation to the number of articles submitted to the category in that month. The article may be cited as "CPS: category/YYMMNNN", for example as CPS: physchem/0102001, the citation for the first preprint submitted to the physical chemistry classification in February 2001. The citation is used to form a "friendly URL" for each article of the format http://preprint.chemweb.com/category/YYMMNNN. When a user accesses this URL, he or she is taken directly to the relevant article, without having to browse and search through all the preprints to locate it on the server.

Once a document is placed on the server, readers can comment on it, in a nontraditional form of peer review. Each article has its own online discussion group where users can rank the article (allocating it one to five "stars") and comment on its content. It is also possible to recommend the preprint to a colleague, by e-mail.

Authors have the option of replacing the original submission with a revised version. Version control and open archive standards[48] add value. CPS complies with the open archiving standard, allowing users to search through the data hosted on other compliant preprint servers, such as the arXiv preprint server. In a similar manner, users of those servers will be able to access the information stored on the CPS. After open review, "good" manuscripts may be submitted to a standard journal.

Shortly after the current study was carried out, ChemWeb announced a new feature facilitating submission to a print journal. The Journal Finder presents an author with a selection of relevant journals, based on the classification given to a preprint at the time of submission. Authors can also choose from a list of other journals and publishers. Next, the author is taken to the relevant page on the external publisher's Web site, from where the preprint can be submitted for consideration for publication. This submission process is external to the CPS.

Readers of CPS can perform both "quick" and "advanced" searches within a particular chemistry classification or across all fields. They can access the preprints for free and can browse them using a variety of filtering mechanisms, i.e., they can access the most recent, most viewed, most discussed, and highest ranked articles. Articles in this last group are ranked by readers' evaluation of their significance. Users can request automatic notification, by e-mail, concerning relevant articles. It is possible to be alerted when an article is uploaded that contains a particular word or phrase, when a new article is submitted to a particular classification, or when a new thread is uploaded into a discussion group.

Criteria for Evaluation. Patrick S. Jackson, Publishing Director, Elsevier Science, gave these criteria for judging the success of CPS (approximately in descending order of importance): the total number of preprints published, geographic spread, the number of people who access CPS, and the number of articles going on to be published. He also noted that the "progressive" nature of the publication process seems to be working well, in terms of the number of papers that have been revised at least once. Other issues that this author decided to investigate were the submission of supplementary files, the type of author who submits a paper to CPS, quality of the papers, the views of authors and the scientific advisory board, and browsing and search features.

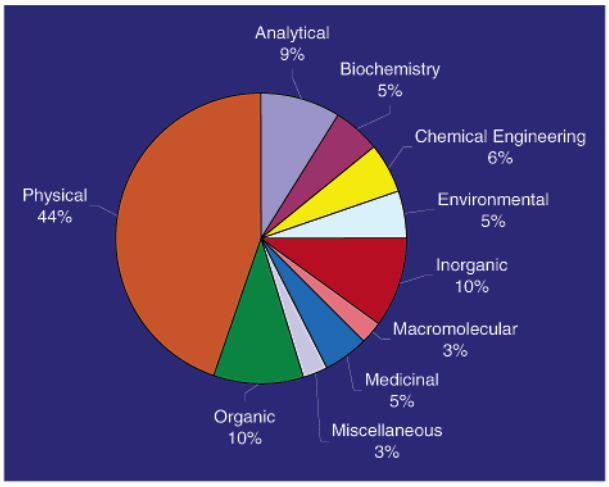


Figure 2. Categories into which CPS papers fall.

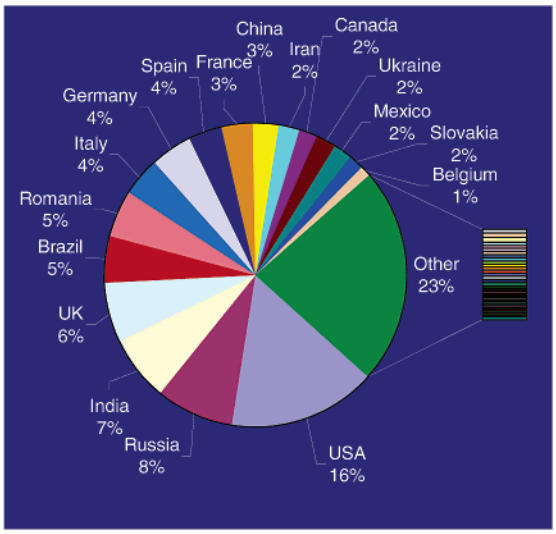


Figure 3. CPS submissions by country.

PAPERS PUBLISHED AND ACCESSED

This evaluation is based on 466 preprints published by the end of May 2002. By October 11, the number had risen to 539. The number of submissions each month shows no sign of falling. For comparison, note that RSC receives some 10 000 papers *per annum*;[44] ACS receives close to 40 000 per annum. CPS, however, has attracted far more submissions than the *Internet Journal of Chemistry*,[16] judging from the latter's acceptance after peer review of 38 articles in 1998, 25 in 1999, 14 in 2000, and 12 in 2001.

The number of papers in each CPS category is shown in Figure 2. Some 44% of all submissions have been made into the physical chemistry classification. A possible explanation may be the popularity of the arXiv preprint server for mathematics and physics. The number of unique authors who contributed the 466 papers was 251. The authors' geographic distribution (across 54 countries) is shown in Figure 3. If the distribution is done on the basis of 466 papers, rather than on 251 authors, Argentina becomes the country of greatest significance after the United States (with 11% of papers as opposed to 18% from the United States), because one author from Argentina has submitted many papers. The distribution based on authors (Figure 3), in which Argentina is accounted for among "other" countries, seems more useful.

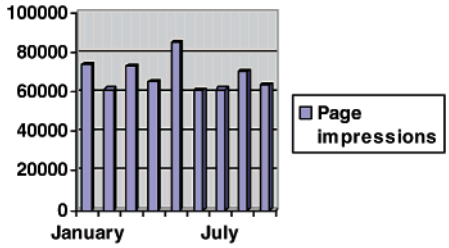


Figure 4. CPS page impressions (page views) per month in 2002.

The geographic spread of arXiv papers is rather different: U.S. .edu 25.3% (plus 0.7% .com and 0.2% .mil); Germany 11.1%; Italy 6.2%; UK 6.1%; Japan 5.7%; France 5.0%; Russia 3.0%; and Switzerland 3.0% (distribution according to e-mail domain of the submitting author of all 134 945 physics submissions received during the 5 year period 1997−2001).[57] Compared with arXiv, the CPS distribution reflects a greater influence of countries with a much lower GDP than the United States. It will be interesting to see if the distribution becomes more like that of arXiv in future.

In July 2001, ChemWeb stated that CPS was attracting more than 100 000 page impressions every month. The viewing figures have now settled at a rather lower level but remain steady (see Figure 4).[58] In October 2002, the most viewed paper had been viewed 3171 times. This figure may be somewhat meaningful from the point of view of measuring the number of visitors and the popularity of the page, but it should not be used as an absolute measure of the quality of the most visited papers since the "most viewed" concept tends to be self-perpetuating: new and casual readers are tempted to go to this page, in a phenomenon similar to the so-called "slashdot effect".[59]

AUTHORS

Who publishes in CPS? Are they cranks, young authors in the developing world, full professors in the United States, Nobel Laureates, or a complex mixture? One paper is indeed coauthored by a Nobel Laureate, but he (Lehn, at CPS: inorgchem/0107001) has Brazilian co-workers and has a known interest in third world issues.[60] An article by Schreiber et al., of Harvard (CPS: orgchem/0009004), was sent to CPS at the same time as it was submitted via the TetSubmit service to *Tetrahedron Letters*. The first version of the paper is still on CPS; there is no pointer to the version that finally appeared in print. The following have also appeared: one preprint from the University of Oxford, England (CPS: physchem/0103011) and three from the University of Cambridge, England (CPS: orgchem/0009006; CPS: biochem/0009001; and CPS: biochem/0009002). Two papers listed under a Cornell affiliation (CPS physchem/0202001 and CPS: physchem/0203012) are from an author who completed his Ph.D. at Cornell some years ago and has submitted preprints with a variety of affiliations and e-mail ids.

At the other extreme is the possibility of attracting papers from authors with outlandish or eccentric views or papers with little supporting evidence. Although preprint servers do not carry out peer review before posting an article they do not necessarily post every manuscript submitted. Ginsparg says of the physics arXiv: *"We still think it's important to have a minimal level of screening, to keep the material at least "of refereeable quality", and avoid material that is*

manifestly irrelevant, offensive, or silly. ArXiv was set up for an elite research community; there was never a pretense of Jeffersonian democracy".[61] ChemWeb, too, screens submissions to ensure they do contain genuine chemistry content. CPS has suffered from one crank in particular, but there has been no evidence of his extravagances since ChemWeb tightened up the submission procedure in summer 2001. Despite the fact that ChemWeb monitors only for the presence of chemical content and the existence of an appropriate affiliation and the normal organization of a valid learned paper, the CPS has been remarkably free of papers by cranks.

It has been pointed out that chemists who have already gained eminence beyond simple tenure may be more comfortable with publishing preprints.[10] This would seem logical, but, in a study of the increase in the number of papers published nowadays, Bachrach[62] has shown that the full professors are not responsible for the proliferation of papers: it is people lower down the ladder. There is some evidence (from discussions and e-mail responses) that CPS is used by graduate and postdoctoral students.

OPEN PEER REVIEW

Peer review in terms of useful online discussion has not been a great success so far. ChemWeb agrees that online discussion is not currently used to a great extent, but as evidence that its use is starting to accelerate mentions CPS: physchem/0201007, where there is useful discussion, CPS: orgchem/0107002 which shows that offline discussion has taken place and now an online statement has aided the researchers, and CPS: analchem/0008002 where a reader has asked whether the researcher has looked at something similar, the author gives references and, from that, clearly received many offline comments and so has posted more research.

There is some evidence that *offline* discussion could well be contributing to quality improvement and revised versions. This issue is considered in more detail later in this paper, but it is worth mentioning here the comments of one author (whose name is withheld, despite his willingness to stand up and be cited): *"Of all the papers whose abstracts I've read (perhaps about 50), none has had an online discussion with contributions about scientific issues, even several months after appearing at the CPS. The online "discussion" is a complete joke (you may cite me on this one...)*".

He supports his views with reference to the list of "most discussed" papers as of May 2002. The three most discussed items at that stage were speculative contributions from a nonscientist, and the discussion is essentially an attempt to explain some undergraduate level chemistry to the author. Of the remaining 17 papers on the list of most discussed papers, only seven contain contributions dealing with scientific issues, while 10 "discussions" consist of author comments, reprint requests, etc. The last item on the list, the 20th most discussed paper on the CPS, has four contributions to the discussion, all four of them coming from the author.

One is forced to sympathize with these comments. A discussion count of seven messages is high, and rare, and it usually means messages from two people at maximum. If "crank" submissions and duplicate entries in the discussion forums were removed, online discussions would perhaps seem more credible. However, *offline* discussion is also an issue to be considered.

QUALITY CONTROL

Peer Review. To compare the quality of CPS with that of a traditional journal in a rigorous study, one would have had to review all 466 CPS papers according to the same standards as those applied in the traditional journal. This would not have been feasible, even if there were a traditional journal, covering the whole field of chemistry, which could be used as a control. Such a study would also not take into account the fact that CPS deliberately caters for some papers that are "works in progress".

Instead, this author used two trusted reviewers to comment on the quality of a selection of papers. One of these reviewers looked at the most recent 20 papers in the CPS medicinal chemistry category. He concluded that five were all very solid, mainline medicinal chemistry papers; one was not mainline medicinal chemistry, but could be useful if the data were reliable (and it did seem to be so); two were not medicinal chemistry papers but chemometric papers and were of limited interest to the medicinal chemistry community (and of mediocre quality); two were very speculative toxicology (not medicinal chemistry) papers where the author had minimal evidence to support major claims; two were good papers, but in toxicology, not medicinal chemistry; and the remaining eight papers were medicinal chemistry papers average in both content and quality. This preliminary review must be very encouraging news for proponents of CPS: 2 awful papers (neither of which would appear in CPS under the new guidelines), 8 good ones, and 10 average is not a bad count for submissions even to a learned journal.

As an aside, the reviewer queried whether toxicological and chemometric papers should be included in this category. Since CPS has only 10 major categories, there will inevitably be a wide variety of papers in each class. The subcategories available in CPS have limited usefulness at present; browsing can be done only by major category. Minor inconsistencies in classification have also been noted.

The second reviewer had problems analyzing the papers assigned to him. He had problems displaying PDF files, encountered another problem with long URLs in Microsoft Internet Explorer 5, and was not able to respond in time. More importantly at least one of the papers he was asked to read was inaccessible because it had already been published.

This requires some explanation. The original plan for CPS was that the final version of a published paper would be removed from the preprint server and replaced with a pointer to the publisher's Web site. This linking (which is heavily dependent upon the authors' notifying CPS of publication details) was to have been carried out using MDL's LitLink technology.[63] However, for reasons not explained to this author, ChemWeb did not continue to run the LitLink server, leaving links that point only to a page with an apology and a promise. Eventually, a different, proprietary technology from Elsevier Science will be implemented, but until then it is not possible to read the final version of some of the preprints that have gone on to be published in the traditional literature. Since many papers have been rendered unreadable, and since it could well be that these papers are among those of the highest quality, carrying out a traditional peer review

exercise of any statistical value was quite impossible and the author was forced to abandon this line of work.

One other reviewing issue that was of interest was the possibility that authors will use CPS as a depository for papers that have been rejected by traditional journals. There is, in fact, little evidence that CPS is serving that function. In the discussion sections on CPS there are four papers that the authors admit have been rejected elsewhere. In a survey (detailed below) of the authors of about 55 papers, only four papers could be detected as rejects. In addition, one other paper is known to have been rejected, according to a communication from a journal editor. Not one author mentioned offering a paper to a "lesser" journal after the journal of choice had rejected it. Clearly it is not going to be easy to study rejected papers,[32] but the fact that only nine rejects in the 466 have been positively identified came as a surprise to this author.

Citations. A good scientific paper often has a long list of citations of work that has been carried out previously. How many literature references appear on average in a CPS paper? About 40 papers were selected for examination, by taking about 60 of the most viewed and the most recent papers and excluding duplicate authors, "unreadable" papers where the PDF is no longer available, two very short papers, and a novel periodic table submission. In these 40 papers, the highest numbers of references were 642, 171, and 207; the minimum nine, four, and one. The rest had 16 or more references. Clearly, most authors are not neglecting the prior art and a literature survey.

One could also ask the converse question. Has anyone cited a CPS paper? This question is proving difficult to answer. A search using the google[64] search engine produced many University and author Web pages but no journal articles. One example was found on Elsevier's ScienceDirect.[65] There were no hits in ISI's Web of Science.[66] There are probably two reasons for these inconclusive results: it is still rather early to expect citations to CPS papers to appear (indeed, up until May, this author had only found the CPS server itself mentioned about twice in the main printed information science journals) and where such citations do appear they may well be syntactically incorrect (we searched for "CPS: physchem" etc.). One factor that is very significant is that major learned organizations are scanning CPS for new research of consequence. Evidence of this is seen in news items in *Nature*[67] and in ACS' *Modern Drug Discovery*.[68]

Print Publication. Some 90% of arXiv papers go on to be published in journals or conference proceedings. A good measure of the quality of papers which have appeared on CPS might be the number that go on to be published in traditional journals and the impact factors of those journals. It has proved impossible to do an accurate study of those CPS papers that go on to be traditionally published because of the missing links. This is most unfortunate because an author survey (detailed below) has shown that a very high proportion of preprints does indeed go on to be published.

Supplementary Files. While having little bearing on traditional impact factors, the value added to CPS by "live" supporting information might be seen as a quality issue. Unfortunately, as Rzepa[1] has stated: "*The supplemental files when present...seem rarely to enhance the article in the sense of presenting readily reusable and semantically rich data and information*". ChemWeb maintains that about one paper in 10 has supplementary files, but this author has found that most of these supplementary files are word processor files, or spreadsheets, or PowerPoint. Other common file extensions are .jpg, .gif, .eps, and .avi.

1. Why did you choose the CPS?
2. Did you consider submitting the paper to a peer-reviewed electronic journal (for example, the *Internet Journal of Chemistry*)?
3. Did you receive any comments from readers OFFLINE (that is, readers who contacted you personally rather than contributing to the open discussions on CPS)?
4. Did you find the online discussion useful?
5. Did you find the offline comments useful?
6. Was your paper published in a "traditional" source after it appeared on CPS?
7. If so, which journal or book published the paper?
8. Was your paper rejected, for any reason, by any journal, before or after the preprint appeared on CPS? If so, which journal and why?
9. Would you use the CPS in future?

Figure 5. Questions in straw poll.

AUTHOR SURVEY

Basis of Survey. The e-mail address of each corresponding author is freely available on the CPS. It would therefore have been possible to bombard all 251 of them with questions. Ethical constraints, however, discourage this, since both readers and authors of CPS have to join ChemWeb as members and agree to adhere to strict privacy conditions. A "straw poll" thus seemed a better approach than a survey of all authors. As it happened, this proved to be the sort of survey where the same answers were repeated over and over again.

The number of authors contacted by e-mail was 55. Authors from the medicinal chemistry papers, the 20 most visited papers, papers from major universities, papers from Brazil, and a few others at random were chosen, eliminating duplicates and eliminating the author of the most dubious papers. At least five of the e-mail addresses turned out to be invalid, but coauthors were tried in two cases. Of the 22 replies, only 21 were analyzed, since one respondent felt that it was too early to draw conclusions. Some authors had published multiple preprints: the 21 authors were responsible for about 55 papers. Thus the survey covered nearly 10% of CPS authors and about 12% of the preprints. The survey questions are given in Figure 5.

Results of Survey. Most respondents gave multiple reasons for using CPS. The most common answer (cited nine times) was that the research would be broadly disseminated and widely read. Seven authors said that speed of publication influenced them; five wanted to try CPS out or thought that it would be exciting or "fun". Two mentioned convenience and two, easy access. Other (singular) answers were that a traditional journal was unsuitable for the nature of the preprint, that the author wanted to reach a different community from the one he usually informed, that CPS was backed by Elsevier (seen as commendable), and (a response

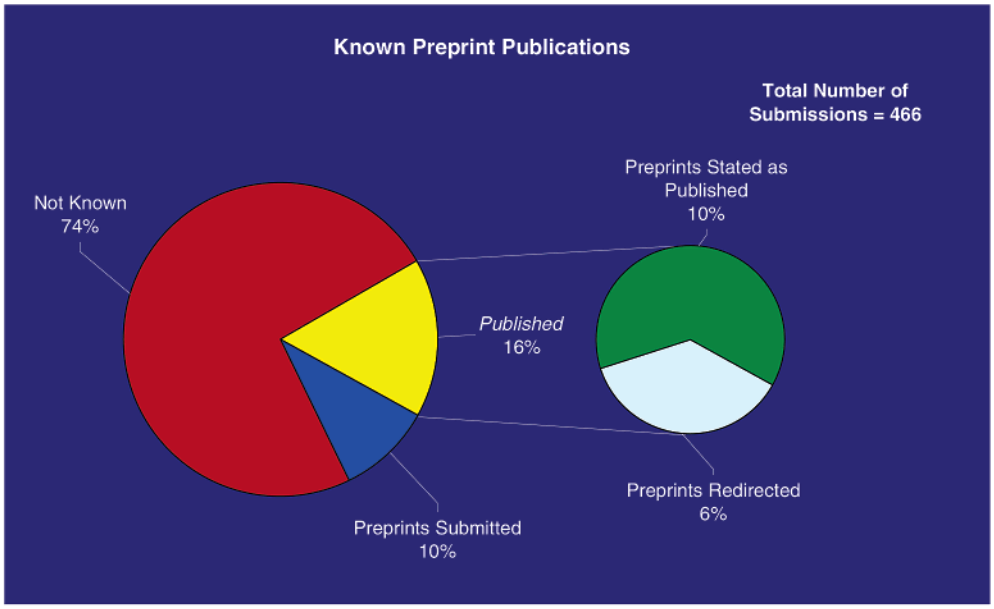


Figure 6. ChemWeb's records of preprints published in print sources.

from a different author) that Elsevier had encouraged the author to post a preprint. Only three respondents had considered publishing in an electronic peer-reviewed journal such as the *Internet Journal of Chemistry*.

Nine authors had received offline comments, eight had not, and four replied "sort of" or "not many". This group of four includes people who mentioned that they were approached for reprints. This last comment might seem odd, but remember that preprints once published might have been unreadable. Most people (13) did not find offline discussion useful; this includes those who received no messages or only messages requesting reprints. Of the remaining eight authors, seven did find offline discussion useful; one was uncertain. These results were similar to those on online discussion: only six people felt it had been useful, while two were undecided. Of the 13 who said that online discussion was not useful, one was highly critical (his comments have been quoted above), but three conceded that the idea was good in principle even though it had not proved useful for their own preprints.

Four papers (out of about 55 in this survey) were admitted to have been rejected by a journal before being posted on CPS. In addition there was one preprint that would not have been suitable for a traditional journal. The question about publication produced some very interesting answers which are best discussed after looking at the data ChemWeb holds about preprints going on to be published (see Figure 6). It is not known what has happened to 74% (345) of the 466 preprints submitted. A total of 76 (16%) have definitely been published. Of these, 48 are known to be published because their authors have stated so in the discussion group, and 28 are known to have been published because access has been redirected (i.e., there is a pointer that should be redirecting the reader to a publisher site, even though that pointer is currently faulty).

The author responses in the survey suggested a much higher level of publication: 15 out of the 21 authors had published one or more of their papers and one paper was of submitted status. More details emerged where the 55 or so preprints of the survey overlapped with the 345 papers in ChemWeb's unknown category (see Figure 6). One author has made a practice of posting *post*prints of articles that have been printed in a reputable journal. One author has published in the ACS journal *Langmuir* and was seemingly as unaware of ACS guidelines as the ACS editor was of the prior publication. As many as eight papers have appeared in RSC journals. Papers have also appeared in *Tetrahedron Letters*, in *Journal of Heterocyclic Chemistry*, in *Advanced Functional Materials*, in conference proceedings, and in various minor journals. All this suggests that authors are not compliant with the CPS concepts of redirection (or with copyright law) and that publication is much wider than CPS records indicate.

When asked whether they would use CPS in future, 14 authors (out of 19 respondents to this question) said "yes", four of them with great enthusiasm. Just one of the 14 qualified his response by saying that he would use CPS only if he were aiming to publish in a journal that will accept "post-preprints". Only one author would definitely not use CPS in future. Other replies were "possibly" (three) and "unlikely" (one). There were lengthy comments from two respondents, one of them a CPS enthusiast who had strong words for the supposedly undesirable qualities of learned journal editors and one a vociferous critic of CPS whose views on discussions are printed above.

VIEWS OF BOARD MEMBERS

Founder members of the advisory board are as follows: Peter Atkins, Oxford University; Steve Bachrach, *Internet Journal of Chemistry*; Ad Bax, National Institutes of Health; Ray Dessy, Virginia Polytechnic Institute; Jonathan Goodman, Cambridge University; Bill Milne, editor of the *Journal of Chemical Information and Computer Sciences*; Paul Schleyer, previously University of Erlangen-Nuremberg, now University of Georgia; Edlyn Simmons, The Procter & Gamble Company; Pieter Steyn, President of IUPAC; and Engelbert Zass, ETH Zürich. Their views were solicited in a general sense: there was no questionnaire. Although their names are publicly available on the CPS Web page, their

anonymity is protected here since only seven out of 10 replied, and multiple quotations from some board members are cited below.

Six of them visit CPS monthly, one weekly. Five out of the seven have read about five papers in full (one has read and archived 40) and six out of seven have scanned many more papers. There were some guarded reservations about quality but the board members were on the whole pleased with CPS and supportive (as one might have expected if they were chosen as board members). A mixed selection of comments is given below:

"*Quality of submissions is about where I expected − most are not worth reading − but don't take this comment too harshly vis à vis CPS − most articles published in chemistry journals are not worth reading either!*"

"*Some troublesome work has appeared in CPS. But troublesome articles have appeared in print publications.*"

"*When the CPS began accepting papers there were some that seemed to be based on vague ideas of the author without any supporting experimental or computational support; those diminished after the CPS posted some minimum standards for papers.*"

"*Numerical ratings aren't particularly helpful because there aren't enough for most papers to be meaningful.*"

"*Mainly as a result of the ACS interference, the CPS has not developed into as valuable a resource as I had hoped.*"

"*...it is a pity that CPS has not become better established in attracting many more preprints. I presume the attitude of the ACS still poses a major problem.*"

"*I'm pretty satisfied with the number of postings and the range of topics, and particularly with the impression I get that the CPS is providing a venue for publications by chemists from third-world institutions.*"

"*I am most pleased with the flexibility that the Web site has shown both to users' problems and users' abuses. It is a great example of what innovative thought can bring to a developing area.*"

CONCLUSION

This study had a number of limitations. Compared with the scientific literature *in toto*, the number of papers on CPS is insignificantly small. A few papers in CPS are "works in progress" rather than finished papers. For comparative studies of peer review and other issues, there is no traditional journal covering all fields of chemistry that can be used as a CPS equivalent. Some of the issues under evaluation (for example, impact factors) are themselves subject to numerous, known defects. Doing a complete survey of all CPS authors was not possible for ethical reasons. Most important of all, the full text of certain CPS papers is no longer available due to defects in CPS' linking technology.

Bearing in mind all those limitations, is the CPS experiment a success so far? Using the Elsevier criteria (the total number of preprints published, geographic spread, the number of people who access CPS, and the number of articles going on to be published) the experiment seems justified. The total number of preprints published on CPS is not quite as high as ChemWeb might have liked (1000 would have been better than 466), but it is pleasing. The geographic spread (54 countries) is excellent. The number of people who access CPS is high, and the number of visits is steady. Since it is not known what happened to 74% of the preprints, and a complete journal list cannot be produced for the rest, the fourth target may not have been met.

The CPS software appears to be robust, and the site was always accessible during this study. There were some minor problems with Internet Explorer and Adobe Acrobat for which CPS offers "workarounds". This author suggests a number of enhancements. The search engine should be refined: its functionality is almost adequate (were some anomalies to be corrected) while CPS has only 466 articles, but it is not ideal in the long term. It appears to be an engine proprietary to Elsevier Science, and it does not have Boolean keyword, word adjacency/proximity, and tile-bar search strategies such as Dessy[13] suggests for a successful eprint server. Search "hints" and help are not readily available. Similarly, the classification used is adequate while there are only 466 articles, but better subclassification will be needed in future.

The missing literature linking technology needs to be addressed with high priority. The fact that links have been lost to items that were published affects the credibility of the server as a "permanent" archive. In the interim, it would perhaps be worthwhile trying to trace the final fate of 74% of the preprints. The ranking feature should be dropped altogether: it is totally unreliable. No reader knows who voted on a paper, how many votes were counted, or what criteria were used. ChemWeb should also seriously reconsider the other top-20 listings (although "most recent" may well be useful). There are about 20 articles (all of them pre-July 2001) that do CPS serious discredit: they should be deleted (although some authorities would suggest that they should remain on the Web but be inaccessible to the general reader).

This article has covered a small survey of CPS authors. The author embarked on the whole study with a healthy dose of skepticism and gradually warmed to the subject of preprints toward the end. This enthusiasm did not have sufficient effect on the audience for the presentation of the paper orally in Noordwijkerhout. The lack of audience members who would even consider posting a paper on CPS was a disappointment. What might be interesting in the future is a study of people who will *not* publish in CPS.

The branded journal still reigns supreme. It will indeed not be easy to get tenure at Harvard based on publication on CPS, at least not yet. At the other extreme, CPS is most definitely *not* "*The Journal of Not Very Good Science*" as a competing publisher once described it privately. Few chemists read every article in every issue of their favorite journals. Readers *are* finding articles that they want to read in CPS. Like many other publications it has good, average, and bad submissions.

It is a mistake to regard preprints purely as an alternative or competitor to print journals. Scientists want to publish both on eprint servers and in peer-reviewed journals: it is not a case of "either/or" but a case of "both". Publication is not a dichotomous event, rather it is a continuum.[69] Preprints can also be viewed as one part of a global knowledge network, flexible enough to coexist with the traditional publishing system or to help it to evolve into something better.[70] ChemWeb has embarked on a brave experiment. It *is* an experiment. It is a relatively successful experiment so far. The methodology now needs examining and checking

and the parameters may need refining before the next iteration, but the experiment should continue.

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