(Hyper)activating the chemistry journal.

Henry Rzepa[1]

[1]Affiliation not available

April 17, 2023

the WINNOWER

CHEMISTRY

(Hyper)activating the chemistry journal.

HENRY RZEPA

CORRESPONDENCE:
h.rzepa@imperial.ac.uk

DATE RECEIVED:
December 03, 2015

DOI:
10.15200/winn.144913.32187

ARCHIVED:
December 03, 2015

CITATION:
Henry Rzepa, (Hyper)activating the chemistry journal., *The Winnower* 2:e144913.32187 , 2015 , DOI: 10.15200/winn.144913.32187

0000-0002-8635-8390

The science journal is generally acknowledged as first appearing around 1665 with the Philosophical Transactions of the Royal Society in London and (simultaneously) the French Academy of Sciences in Paris. By the turn of the millennium, around 10,000 science and medical journals were estimated to exist. By then, the Web had been around for a decade, and most journals had responded to this new medium by re-inventing themselves for it. For most part, they adopted a format which emulated paper (Acrobat), with a few embellishments (such as making the text fully searchable) and then used the Web to deliver this new reformulation of the journal. Otherwise, Robert Hooke would have easily recognized the medium he helped found in the 17th century.

In 1994, a small group of us thought that one could, and indeed should go further than emulated paper. We argued [1] that journals should be **activated** by delivering not merely the logic of a scientific argument, but also the data on which it might have been based. Of course, we encountered the usual problem; doing this might cost publishers more in production resources, and in the absence of a market prepared to pay the extra, the business model did not make sense (to the publishers). Well, 15 years later, and most publishers are indeed now thinking about how their journals can be enhanced. A number of interesting projects (the RSC's Project Prospect is one which strives to *bring science alive*) have emerged. Another is the topic of this blog; the activation of the journal with molecular coordinates and data using the Jmol applet.

Initially (~2005), this project met with resistance from publishers, and the issue really amounted to what the definitive version of a scientific article should be. Should that definitive version be printable? That model, after all had served the community well for more than 300 years! And journals from the very beginning are still as readable now as when first published. In other words, print lasts! But print is pretty limiting after all. For a start, it is limited to 2D static representations. Molecules, by and large, do their magic in a dynamic three dimensions (4D in an Einsteinian sense). But print is also expensive; not merely to produce, but to transport paper around the world.

From the turn of the millennium, a number of publishers, amongst them the American Chemical Society, started to evolve the scientific article such that the pre-eminent version would now be considered to be the HTML form (perhaps as a prelude to phasing out print entirely? See an interesting commentary by a journal editor) and perhaps a digital Acrobat form which would be deemed to loose some of its functionality once printed (again see here for how Acrobat can be used to enhance things). Again however, a chicken-and-egg scenario resulted. To enhance the articles with extra functionality (such as data), they would need to find authors prepared to put the extra work into preparing the material. In fact, most authors already do that, but they call it *supporting information*. This is often highly data rich, covering materials such as spectra, coordinates and other information nowadays

provided to researchers for analysis. Unfortunately, what has been missing is the education of authors to provide this information in a proper digital form which can be easily re-used by others, and on a Web page, converted automatically to nice interactive models. Most spectra which form part of the supporting information are in fact still scanned versions of printed spectra!

Enter computational chemists. Nowadays, they live in a world that truly does not need printing! Almost all of their data is already suitably digital. So perhaps it is no surprise to find that when enhanced journal articles started appearing around 2005, many were produced by this group of chemists. By now perhaps you are wondering what such an article might look like. Well, the remainder of this blog will be devoted to listing some examples. You will also notice that they come exclusively from our own publications. Perhaps someone will find the time to collect a far more representative set to better illustrate the diversity of this form, and how it is evolving. Meanwhile, you might wish to take a look at the following.

Part 1: The early days: 1994 onwards

These examples all relied on a browser plugin called Chime, which is no longer with us! Hence the pages designed to invoke it no longer display properly. But the data associated with the articles is still there!

1. An early 1994 example of (hyper)activating a journal article can be seen here as the preliminary communication and
2. in 1995 here as the final full article. I am told that this was the article that actually inspired the developers of Chime to enhance (Netscape) with a chemical plugin.
3. This one from 1998 illustrates how articles can decay in functionality when Chime is no longer available.
4. An ab initio and MNDO-d SCF-MO Computational Study of Stereoelectronic Control in Extrusion Reactions of R2I-F Iodine (III) Intermediates, M. A. Carroll, S. Martin-Santamaria, V. W. Pike, H. S. Rzepa and D. A. Widdowson, *Perkin Trans. 2*, 1999, 2707-2714 with the supporting information here.
5. Huckel and Mobius Aromaticity and Trimerous transition state behaviour in the Pericyclic Reactions of [10], [14], [16] and [18] Annulenes. Sonsoles Martên-Santamarêa, Balasundaram Lavan and H. S. Rzepa, *J. Chem. Soc., Perkin Trans 2*, 2000, 1415. with the supporting information here.
6. Peter Murray-Rust, H. S. Rzepa and Michael Wright, “Development of Chemical Markup Language (CML) as a System for Handling Complex Chemical Content”, *New J. Chem.*, 2001, 618-634. DOI: 10.1039/b008780g. This article broke new ground in that the supporting information was something of a misnomer. It was expressed entirely in XML, including all the chemistry data, and used XSLT transforms on the fly to regenerate the article. In that sense, it was actually a superset of the published article. It would be fair to say that this article was rather ahead of its time (although it does seem appropriate to publish it in a new journal!).
7. M. Jakt, L. Johannissen, H. S. Rzepa, D. A. Widdowson and R. Wilhelm, “A Computational Study of the Mechanism of Palladium Insertion into Alkynyl and Aryl Carbon-Fluorine bonds”, *Perkin Trans. 2*, 2002, 576-581 and supporting information.
8. P. Murray-Rust and H. S. Rzepa, chapter in “Handbook of Chemoinformatics. Part 2. Advanced Topics.”, ed. J. Gasteiger and T. Engel, 2003, Vol 1, was not enhanced per se, but did lay out the principles of how it might/should be done.
9. K. P. Tellmann, M. J. Humphries, H. S. Rzepa and V. C. Gibson, “An experimental and computational study of β-H transfer between organocobalt complexes and 1-alkenes”, *Organometallics*, 2004, **23**, 5503-5513. DOI: 10.1021/om049581h and supporting information.

Part 2: 2005.

These four examples all now invoke Jmol, which downloads upon request and hence does not rely on the presence of any browser plugin. The four articles were submited with supporting information in the form of HTML. These were associated with the main article, but were not formal part of that article. In

that sense, they represent an incarnation of the traditional model, with all the data firmly resident in the supporting information.

1. Gibson, Vernon C.; Marshall, Edward L.; Rzepa, H. S. " A computational study on the ring-opening polymerization of lactide initiated by β-diketiminate metal alkoxides: The origin of heterotactic stereocontrol", *J. Am. Chem. Soc.*, **2005**, *127*, 6048-6051. DOI: 10.1021/ja043819b and supporting information.
2. H. S. Rzepa, Mobius aromaticity and delocalization", *Chem. Rev.*, **2005**, *105*, 3697 – 3715. DOI: 10.1021/cr030092l and supporting information.
3. H. S. Rzepa, "Double-twist Mšbius Aromaticity in a 4n+2 Electron Electrocyclic Reaction",**2005**, *Chem Comm*, 5220-5222. DOI: 10.1039/b510508k The supporting information is also available directly.
4. H. S. Rzepa, "A Double-twist Mobius-aromatic conformation of [14]annulene", *Org. Lett.*, **2005**, *7*, 637 – 4639. DOI: 10.1021/ol0518333 and supporting information.

Part 3: 2006 onwards

The supporting information has now been assimilated into the main body of the article proper, and within these confines contribute components such as enhanced figures or tables (i.e. enhanced with **data**)

1. A. P. Dove, V. C. Gibson, E. L. Marshall, H. S. Rzepa, A. J. P. White and D. J. Williams, "Synthetic, Structural, Mechanistic and Computational Studies on Single-Site β-Diketiminate Tin(II) Initiators for the Polymerization of *rac*-Lactide", *J. Am. Chem. Soc.*, **2006**,*128*, 9834-9843. DOI: 10.1021/ja061400a The enhancement can be seen in Figure 11.
2. O. Casher and H. S. Rzepa, "SemanticEye: A Semantic Web Application to Rationalise and Enhance Chemical Electronic Publishing", *J. Chem. Inf. Mod.*, **2006**, *46*, 2396-2411. DOI: 10.1021/ci060139e
3. H S. Rzepa and M. E. Cass, "A Computational Study of the Nondissociative Mechanisms that Interchange Apical and Equatorial Atoms in Square Pyramidal Molecules", I*norg. Chem.*, **2006**, *45*, 3958–3963. DOI 10.1021/ic0519988. Interactive table at 10.1021/ic0519988/ic0519988.html
4. M. E. Cass and H. S. Rzepa, "In Search of The Bailar Twist and Ray-Dutt mechanisms that racemize chiral tris-chelates: A computational study of Sc(III), V(III), Co(III), Zn(II) and Ga(III) complexes of a ligand analog of acetylacetonate", *Inorg. Chem.*, **2007**, *49*, 8024-8031. DOI: 10.1021/ic062473y The enhancement can be seen in Figure 2
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