Open Letter to the XAFS Community

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Maintaining and improving the quality of published XAFS data: a view from the UK XAFS user group

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Proposals are made to enhance the perceived and actual quality of published XAFS data.

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1. Introduction

Despite the very significant recent advances in the theoretical basis and subsequent analysis of X-ray absorption fine structure (XAFS) spectra, there are still the lingering comments amongst one's colleagues that XAFS is a 'sporting technique' and that it is possible to obtain the 'answer you want'. Whilst the 'Standards and Criteria Guidelines' (Lytle *et al.* 1989, Bunker *et al.* 1991, Koningsberger 1993) have been in place for a number of years, and no doubt authors have been following them scrupulously(?!), the implementation and enforcement of them by journals and editors seems to be more patchy. One notable exception to this is *The Royal Society of Chemistry*, which has included a modified set of 'The Guidelines' in the instructions for authors since 1996 and has sent this out to referees since 1995 with each paper that contains XAFS data for review for publication in *Dalton Transactions, Faraday Transactions, Journal of Materials Chemistry* and *Chem Comm.*

We believe that it is up to the XAFS community itself to set in place mechanisms to maintain and improve both the perceived and actual quality of published XAFS data. To this end, recent meetings of the UK XAFS User Group have formulated several ideas which we believe if widely adopted will result in a substantial improvement in the quality of published work.

2. Recommendations

The recommendations of the UK XRS User Group are.

i. All papers should be written conforming to the 'Standards and Criteria Guidelines'.
ii. The use of Fourier filtered data for anything but initial atom-type identification should be discouraged, and raw, unsmoothed, data should always be presented to allow for an accurate assessment of signal to noise and general data quality.
iii. Journal editors should be encouraged to send a copy of the 'Guidelines' (or modified version) to referees/reviewers for papers that contain XAFS data.
iv. Journal editors should consider the use of specialist XAFS referees/reviewers for papers that contain a substantial degree of XAFS data which are central to the paper. A list of such people should be drawn up and circulated to editors.
v. Often only representative spectra are published, and other data are given in a table or discussed in the text. Therefore, we believe that authors should be required to submit additional material (as $\chi(k)^n$ and FT plots) for referee/reviewer use, of all the XAFS data presented and discussed in the text or tables. This is especially important for 'Communications', where space for published figures is usually at a premium. This practice is not uncommon, and it should be noted that *The Journal of Organic Chemistry* requires the submission of all spectral data (NMR. mass. spec.) when reporting new compounds.
vi. Access to analysis programs should be subject to acceptance of an agreement to follow a set of 'Quality Guidelines'.

3. Conclusions

Whilst many of these recommendations are not new and have been suggested before, we believe that it is time to approach editorial boards in a concerted fashion in order to spread the good practice already set in place by *The Royal Society of Chemistry.* The publication of the latest version of the 'Guidelines' on the Web and on mirror sites should also be encouraged.

Discussions were also held as to the advantage of requiring authors to deposit their XAFS data as is required for crystallographic data. Whilst it was felt that there might be some advantage for fellow practitioners to have access to other worker's data, there seemed to be no obvious benefit to the improvement in the quality of the published data. There is also the question of what data is to be deposited, as in the crystallographic case it is not the original data that is deposited, but a processed set. It should also be noted that at The Daresbury SRS all the original, raw data is archived by the facility computing staff, so that any XAFS data recorded can be accessed by the original investigators in a matter of minutes for analysis by the latest software.

References

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Note from the Main Editors of the *Journal of Synchrotron Radiation*: The *Journal of Synchrotron Radiation* has, from its launch in 1994, insisted on rigorous standards for XAFS data presentation as well as encouraging primary XAFS data deposition.

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