Provisional Recommendations

IUPAC seeks your comments

In this section we publish synopses of IUPAC's latest provisional recommendations on nomenclature and symbols. All comments on these recommendations are welcome and will be taken into consideration. The final revised versions are published in *Pure and Applied Chemistry* and synopses of these are published in *Chemistry International* as recent reports.

If you would like to comment on the provisional recommendations please write to your nearest national/regional centre requesting a copy of the full report. Copies are not available from the IUPAC Secretariat. The most recent list of the national/regional centres appeared in *Chemistry International* 1995, **17**, 141.

Names for Inorganic Radicals

Radicals are important in a variety of catalytic processes and in the atmospheric gas and liquid phases; furthermore a substantial number of inorganic radicals have been observed in interstellar gas clouds.

In biology, the interest in radicals increased after the discoveries that superoxide and nitrogen monoxide are formed *in vivo*; these radicals play an important role in cell–cell signalling, the immune response and disease.

Rules have been developed to name inorganic radicals in a systematic manner.

It was found that for inorganic radicals coordination nomenclature yielded unique names that are descriptive of composition and structure (where known).

The strategy to name a radical is to select a central atom and name all other atoms (or groups of atoms) as ligands, or, if the name ends in '-yl' and the Ewens–Bassett number. As an example, CO_2- is named 'dioxidocarbonate-yl(1-)'.

These rules are intended to replace those found in Section I-8.4 of *Nomenclature of Inorganic Chemistry, Recommendations 1990*, Blackwell Scientific Publications, Oxford, 1990 (the 'Red Book').

Comments on these recommendations are welcome and should be sent by 30 November 1997 to: Prof W.H. Koppenol, Laboratorium für Anorganische Chemie, Eidgenössiche Techniche Hochschule, Universitätstrasse 6, CH-8092 Zürich, Switzerland. Tel.: +41 1 632 2875; Fax: +41 1 632 1090; E-mail: koppenol@inorg.chem.ethz.ch

Recommendations for the presentation of NMR structures of proteins and nucleic acids

During the past several years the determination of NMR solution structures of small proteins has found widespread application, and the NMR method is being used increasingly for structural studies of nucleic acids and their complexes with proteins, drugs and other molecules. In the course of this development, a certain con-

sensus has developed on the presentation of NMR solution structures. This has been helped indirectly by guidelines established for depositing primary experimental data and resulting structures in databanks such as the Protein Data Bank, BioMagResBank, Nucleic Acid Database, and by conventions used for abstracting services, for example, *Macromolecular Structures*, Current Biology, London, UK, 1991ff. In consideration of making good future use of the experience accumulated during the past few years, the present Task Group has been convened as an IUPAC/IUBMB/IUPAB Inter-Union venture, which was also supported by ICSU and CODATA. The group has gone through formal examinations of the reporting conventions of biomolecular NMR used in the past. The present recommendations also build upon earlier rules for biochemical nomenclature and for the presentation of proton and non-proton NMR data. Consultation with a large fraction of the leading research groups in the field of NMR structure determination with biological macromolecules indicates that these guidelines will be widely accepted by the community.

Comments on these recommendations are welcome and should be sent by 30 November 1997 to: Prof. Kurt Wüthrich, Institut für Molekularbiologie und Biophysik, ETH-Hönggerberg HPM, CH-8093 Zürich, Switzerland. Tel.: +41 1 633 24 73; Fax: +41 1 633 11 51; E-mail: wuethrich@mol.biol.ethz.ch

Comments

The work of IUPAC has featured recently on the 'Editor's Page' of both *Chemistry in Britain*, published by the Royal Society of Chemistry, UK, and *Chemical & Engineering News*, published by the American Chemical Society. The two articles are reproduced below.

An editor's lot is not always a happy one…

***…*observes Richard Stevenson, Editor of *Chemistry in Britain* and Chairman of the Association of British Science Writers.**

'What's in a name? That which we call a rose, by any other name would smell as sweet.' And certainly brimstone smells as pungent whether it is called sulphur or sulfur—but try telling that to some chemists. A number of eagle-eyed readers noted that last month's *Chemistry in Britain* carried the cover line 'Chemistry of sulfur'. Innocent enough in all conscience, but a hanging offence according to one correspondent, who wrote: 'I look to the Royal Society of Chemistry to uphold standards in our subject and feel that you have failed to do this'.

Yet when IUPAC (in 1990) and the RSC (in 1992) adopted 'sulfur' as the correct spelling for element 16, *Chemistry in Britain* hung back—only to be told off by other correspondents, one of whom wrote: 'We try to persuade students that they must abandon old habits and move with the times...our efforts are not aided when they open their *Chemistry in Britain*'.

Readers who are interested enough can look up the correspondence we published at the time (*Chem. Br.*, April 1992, p. 324; July 1992, p. 604), but suffice it to say that I promulgated the doctrine that *Chemistry in Britain,* being aimed at a wider audience than the RSC's primary and secondary journals, would continue to use the familiar 'sulphur', at least until general usage began to reflect the change.

However, last year I was persuaded by the *Chemistry in Britain* Editorial Board to relax this ruling, so that dyed-in-the-wool sulfur chemists could spell their element that way if they so wished. This is not the only case where *Chemistry in Britain* allows two forms of nomenclature to run in parallel. For example, the nomenclature rules adopted by the Association of Science Education mandate the use of 'ethene' and 'ethyne', which would be unrecognisable to their industrial colleagues used to making and selling ethylene and acetylene. Even IUPAC accepts these two trivial names. Being pragmatic, *Chemistry in Britain* accepts whichever an author prefers, though leaning towards the spellings familiar to our predominantly industrial readership.

Industry, of course, can be slow to move: an academic acquaintance tells the story of visiting—not all that many years ago—a petrochemical plant and asking what the labels 'OV' and 'MA' meant on two of the site's pipelines. 'Oil of vitriol and muriatic acid', he was told. A former colleague—who as a subeditor had been a punctilious user of the education world's 'ethene' and 'ethyne'—joined that same petrochemical company as a press officer. A few weeks into the job she telephoned me on the QT to ask what 'muriatic acid' was, because she didn't want to appear stupid. Humphry Davy identified and named chlorine as far back as 1810, yet the fertiliser industry does still sometimes refer to 'muriates'

not chlorides.

One argument for rigid nomenclature is that searches on computers with massive memories but very little intelligence will not pick up references to sulfur if you key in sulphur. Yet I recently saw a scientific paper on 'diatom–diatom interactions' and had to read a lot further before I could be sure the authors meant reactions between H_2 molecules and not relations between little silica-walled algae in ponds. What is a dumb computer to make of that?

The 'ultras' of chemical nomenclature will not have it, of course. Off with decadent Sulphur's head! Etymologically correct Citizen Sulfur is to take over the kingdom. My pragmatism in allowing dual standards will see me reviled by both sides, while my comrades in the ranks of scientific editors (for whom House Style Rules OK!) will have me cashiered and my red pen broken before my eyes.

I am still waiting for my US colleagues to face up to IUPAC's ruling that 'aluminum' and 'cesium' are wrong.

Reprinted from Chemistry in Britain *(May 1997) with the permission of its Editor.*

The antiscience cancer

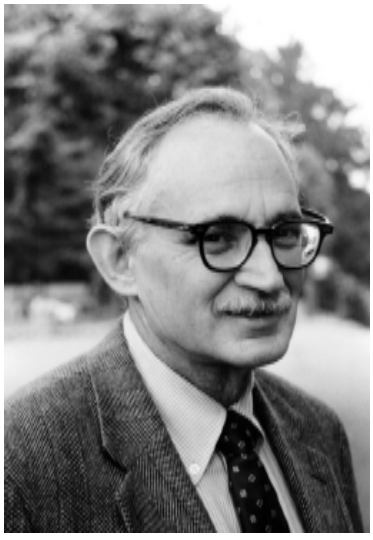
A guest editorial by Allen J. Bard, Norman Hackerman-Welch Regents Chair in Chemistry at the University of Texas, Austin, Editor of the *Journal of the American Chemical Society* and President of IUPAC during 1991–1993.

In February, NBC televised a movie called 'Terminal' about a physician who had discovered the cure for a particular form of cancer. Rather than revel in his discovery, he sought out wealthy patients who were in the hospital for other ailments, surreptitiously infected them with this form of cancer (which he apparently could induce to appear in days like a bad cold) and then came to their rescue with his cure. These patients were so grateful that they showered him with funds to support his research. Even more scurrilous than this far-fetched story, however, were the postmortem comments shown with the credits. These claimed that scientists were competing for the monetary rewards that will come with the discovery of a cure for cancer and that 'so far they have only discovered how to cause cancer'.

The antiscience flavor of this movie is only one example of the attack on science in the US from all sides. From the left, the postmodernists declare that science does not really deal with facts and that accepted models only represent the opinion of the scientific establishment. Those with a particular social agenda rewrite the history of science and create scenarios that have little connection with reality and actual science. For example, the notorious 'Baseline Essay on Science' adopted by the Portland, Ore., Public Schools seeks to promote multiculturalism by proposing fantastic contributions of ancient inhabitants of Africa (*Phi Delta Kappan*, November 1993, p. 266). These include knowledge about the moons of Jupiter, acquired in pre-telescope days through parapsychological powers. This essay also proposes that melamin can convert light to knowledge and also absorb the wave energy of magnetism. On the right, creationists want to teach religious concepts as science. On other fronts, a large fraction of the populace believes in ghosts, angels, ESP, astrology, and magic crystals.

Scientists usually respond to such attacks and anti-intellectualism from a defensive posture. We try to explain the fallacies in the arguments and hope that better education will undo the attackers. This approach has not worked very well in the past, and it will be a disaster to wait the length of time it would take to produce an educated populace to deal with these immediate problems. Seventy years after the Scopes trial and the widespread teaching of evolution, school districts still are under attack by fundamentalists, and a law punishing teachers of evolution came close to passing in late March in the Tennessee legislature.

It is time for scientific societies to take the offensive and attack the pseudoscience and misinformation eating away at our profession. For example, they could establish offices and member networks to respond quickly to antiscience attacks and to aid groups fighting creationism and pseudoscience in their school districts. If the TV movie had the equivalent racial or sexual overtones, NBC would have been inundated with letters and protests, supported by a number of organizations. Yet we sit by and passively watch and hope that people will recognize the fantasy in the presentation.



Prof. Allen J. Bard

Scientists also should confront the sociologists and philosophers at their institutions who are attacking the foundations of science. Presumably, tenure decisions and promotions at universities are based on scholarship, and academic scientists must take an interest in the academic decisions in other departments on campus. This is not a question of academic freedom, but rather one of competency. We should expose political correctness and fundamentalism that lead to misinformation about science.

We also should clean our own house and speak out when scientists overplay their findings or promise more than they can deliver. We must be totally honest when discussing the impact of our work in real world situations and in differentiating unsupported opinion from conclusions drawn from sound research. Shoddy work and bad science should be exposed. However, if the mainstream scientific organizations, like ACS, the American Association for the Advancement of Science, the National Academy of Sciences, the Council on Chemical Research, and the International Union on Pure and Applied Chemistry just sit back and watch, the future of science, at least in the US, is bleak indeed.

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