Graphical Representation of Stereochemical Configuration (IUPAC Recommendations 2006)

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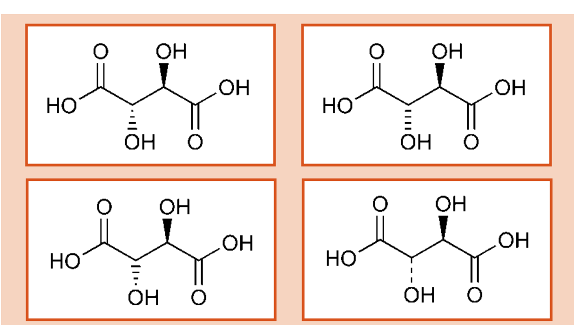
Stereochemical configuration is determined by the relationship of atoms in three-dimensional space, yet it is still most commonly represented in two-dimensional media such as printed publications or computer screens. This article provides recommendations for the display of three-dimensional stereochemical information in two-dimensional diagrams in ways that avoid ambiguity and are likely to be understood correctly by all viewers. Examples are provided for all types of stereochemical configuration, with explanations of which styles are preferred and which should be avoided. The principal recommendations of the article include:

- Know your audience: Diagrams intended for a wide audience should be drawn as simply as possible.
- Avoid ambiguous drawing styles.
- Avoid the use of perspective diagrams and class-specific drawing styles (Fischer projections, Haworth projections, etc.) when structures are to be interpreted by computers.
- Use solid wedges to indicate bonds that project above the plane of the paper and hashed wedges to indicate bonds that project below the plane of the paper; in both cases, the bonds must be oriented with the narrow end at the stereogenic center.
- Avoid connecting stereogenic centers with a stereobond.

www.iupac.org/publications/pac/2006/7810/7810x1897.html



Want to find out why these diagrams are either preferred, acceptable, or simply not acceptable? Read the recommendations to find out.

Atomic Weights of the Elements 2005 (IUPAC Technical Report)

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The latest evaluation of atomic weight determinations and other cognate data has warranted 16 changes for the standard atomic weights of the elements, A_r(E), from those published previously in the 2001 Table of Atomic Weights. The revised standard atomic weights are as follows: A_r(Al) = 26.981 5386(8), A_r(Bi) = 208.980 40(1), A_r(Cs) = 132.905 4519(2), A_r(Co) = 58.933 195(5), A_r(Au) = 196.966 569(4), A_r(La) = 138.905 47(7), A_r(Mn) = 54.938 045(5), A_r(Nd) = 144.242(3), A_r(P) = 30.973 762(2), A_r(Pt) = 195.084(9), A_r(Sm) = 150.36(2), A_r(Sc) = 44.955 912(6), A_r(Na) = 22.989 769 28(2), A_r(Ta) = 180.947 88(2), A_r(Tb) = 158.925 35(2), A_r(Th) = 232.038 06(2).

A recommendation is made that δ^{13}C values of all carbon-bearing materials be measured and expressed relative to Vienna Pee Dee Belemnite (VPDB) on a scale normalized by assigning consensus values of -46.6 ‰ to L-SVEC lithium carbonate and +1.95 ‰ to NBS 19 calcium carbonate.

www.iupac.org/publications/pac/2006/7811/7811x2051.html

Terminology of Polymers Containing Ionizable or Ionic Groups and of Polymers Containing Ions (IUPAC Recommendations 2006)

M. Hess, R.G. Jones, J. Kahovec, T. Kitayama, P. Kratochvíl, P. Kubisa, W. Mormann, R.F T. Stepto, D. Tabak, J. Vohlídal, and E.S. Wilks
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This document defines the terms most commonly encountered in the field of polymers containing ionizable or ionic groups and polymers containing ions. The scope of the document has been limited to organic polymers. Inorganic materials, such as certain phosphates and silicates, which also may be considered ionic polymers, are excluded from the present document. The terms selected are those that are widely used in the field of polymers containing ionizable or ionic groups and polymers containing ions. Only those terms that could be defined without ambiguity are considered. The terms are listed in alphabetical order, and cross-references to definitions given in other documents are provided.

www.iupac.org/publications/pac/2006/7811/7811x2067.html

Cytokine Profiles in Human Exposure to Metals (IUPAC Technical Report)

Reinhild Klein, Michael Schwenk, and Douglas M. Templeton
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Cytokine production is altered in most, if not all, disease states. In disorders arising from human exposure to noxious substances, there is an extensive literature on the involvement of cytokines. Consequently, measurements of cytokines have been performed and their use propagated as a diagnostic procedure in a number of relevant disorders. In recent years, several methods and test kits have become available for cytokine measurement, including for studying allergic disorders where cytokines have been shown to play an important role. However, cytokine profiles in biological fluids are rather unstable, and are influenced by various exogenous and endogenous factors. Moreover, it has recently become evident that analysis of single cytokines in the blood has little diagnostic relevance.

Immunosensitization to metal ions through occupational and environmental exposure has been described in earlier papers from this project.* This paper discusses the possible role of cytokine profiling in demonstrating and understanding this phenomenon. The cytokines are a large family of polypeptides exerting autocrine, paracrine, and/or endocrine effects. They include interleukins (ILs), interferons (IFNs), and growth factors. They may be grouped as pro-inflammatory (e.g., IL-1, IL-6, IL-12, IL-18, TNF-α), anti-inflammatory (e.g., IL-10), or those regulating T-helper (TH) cell function. The latter are subdivided into those associated with TH1 (e.g., IL-2, IL-12, IFN-γ, TNF-β) or TH2 (e.g., IL-4, IL-5, IL-13) cell function. Because different types of immune reactions (e.g., immediate reaction vs. delayed-type hypersensitivity) differentially involve TH1 and TH2 cells, measurement of cytokine production in response to metal ions can potentially give insight into underlying immune mechanisms and responses.

The paper gives examples for species of Ni, Cr, Co, Hg, Cd, and Be; and in less detail for species of Fe, Pt, Pd, and Rh. Antibodies are available commercially that allow for the determination of many cytokines, and such measurements are most usefully performed with body fluids, supernatants from stimulated lymphocyte cultures, or lysates of lymphocytes or other biopsied cells. The predominant methods include enzyme-linked immunosorbent assay (ELISA) and flow cytometric measurement of the cytokine, bioassay of its activity in cell culture, and polymerase chain reaction (PCR) assessment of its mRNA level. In practice, levels of individual cytokines are highly variable between individuals, and reliable reference values are generally lacking. Ratios of cytokines are more informative than absolute concentrations, and biological variability in cytokine production dictates that repeated testing is necessary to confirm trends. Determining cytokine profiles is presently of questionable diagnostic utility in individual cases of metal sensitization, but is providing mechanistic insights in a research context.

*see <www.iupac.org/projects/1999/1999-047-1-700.html>

www.iupac.org/publications/pac/2006/7811/7811x2155.html

Glossary of Terms Relating to Pesticides (IUPAC Recommendations 2006)

Gerald R. Stephenson, Ian G. Ferris, Patrick T. Holland, and Monica Nordberg
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This glossary contains definitions of more than 500 terms frequently used in relation to the chemistry, mode of action, regulation, and use of pesticides. A wide range of disciplines is involved in this field, and the glossary was developed as a step in facilitating communication among researchers, government regulatory authorities, and chemists in associated professional areas. The range of terms relates to pesticide residue analysis, sampling for analysis, good laboratory practice, metabolism, environmental fate, effects on ecosystems, computer simulation models, toxicology, and risk assessment. The number of important, "pesticide-related" terms has more than doubled since 1996, when the first IUPAC glossary of this type was developed, an indication of how this field has become so integrated with many other scientific and regulatory disciplines.

www.iupac.org/publications/pac/2006/7811/7811x2075.html

Education, Outreach, and Codes of Conduct to Further the Norms and Obligations of the Chemical Weapons Convention (IUPAC Technical Report)

Graham S. Pearson and Peter Mahaffy
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The 2002 IUPAC evaluation of scientific and technological advances relevant to the operation of the Chemical Weapons Convention (CWC) included a recommendation that more education and outreach should be directed toward the worldwide scientific and technical community to increase awareness of the CWC and its benefits. In 2004, the president of IUPAC and the director-general of the Organization for the Prohibition of Chemical Weapons (OPCW) agreed on a proposal for a joint project on chemistry education, outreach, and the professional conduct of chemists. This led to a joint IUPAC/OPCW international workshop held in Oxford, UK, from 9–12 July 2005, which attracted 27 participants from 18 different countries. This report sets out the background to the workshop, the scope of the presentations and discussions, the outcomes of the workshop, and the recommended steps to further chemical education, outreach, and codes of conduct in regard to the obligations of the CWC.

Among the key recommendations of the report are the following:

- Chemistry education for secondary and post-secondary students must address the benefits of science and technology using chemicals and the potential for misuse in regard to illicit drugs, chemical and biological weapons, persistent organic pollutants, etc.
- Chemists need to recognize their role in ensuring sustainable development, and that compliance and implementation of international treaties such as the CWC and the BTWC (Biological And Toxin Weapons Convention) contribute to sustainable development.
- OPCW needs to clearly endorse the education and codes initiative, which can be referred to byIUPAC National Adhering Organizations and Associate NAOs in approaching their respective National Authorities and other national ministries.

www.iupac.org/publications/pac/2006/7811/7811x2169.html

Another IUPAC Initiative Relevant to the CWC

Impact of Advances in Science and Technology on the CWC

The objective of a recently initiated IUPAC project is to prepare an assessment of the impact of developments in science and technology on the operation of the Chemical Weapons Convention (CWC) as a contribution to the Second Review Conference of the CWC to be held in spring 2008. IUPAC is in a unique position to tap into a broad spectrum of scientific expertise through its divisions and constituent national chemical societies and science academies. Based on the Bergen experience [project #2001-057-1-020], the project will provide valuable input for the review process of the Member States of the Organisation for the Prohibition of Chemical Weapons.

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www.iupac.org/projects/2006/2006-036-1-020.html