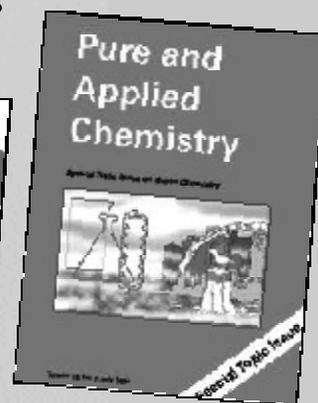
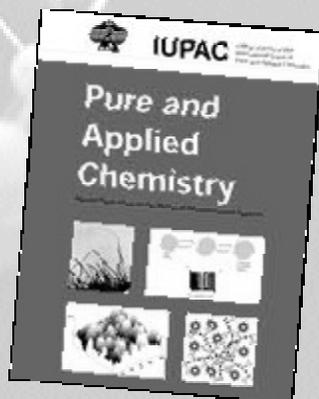


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Highlights from *Pure and Applied Chemistry*

Presenting recently published IUPAC technical reports and recommendations

Guidelines for the Representation of Pulse Sequences for Solution-State Nuclear Magnetic Resonance Spectrometry (IUPAC Recommendations 2001)

by A.N. Davies, J. Lambert, R. J. Lancashire, P. Lampen, W. Conover, M. Frey, M. Grzonka, E. Williams, and D. Meinhart
Pure and Applied Chemistry, Vol. 73, No. 11, pp. 1749–1764 (2001).

In drawing up the specifications for a standard for multidimensional nuclear magnetic resonance spectroscopy (NMR) it became clear that the spectroscopic data content

needed to be qualified by experimental condition information especially pertaining to the pulse sequences used to obtain the free induced decays or spectra. Failure to include this information not only severely inhibits the ability of subsequent data handling packages to work with the experimental data, but also makes interpretation of the final results virtually impossible.

This paper has been produced in collaboration with the NMR spectrometer manufacturers in an attempt to reach agreement on a definitive list of the most frequently used pulse sequence programs. The list includes entries where common agreement has been reached as to the acronym to name the experiment and the key instrument independent parameters needed to report concisely. It is not intended to restrict in any way the freedom of manufacturers or users to develop new and novel experimental pulse sequences,

but should aid reporting of experimental data where the more common sequences are in use.



[www.iupac.org/publications/pac/
2001/7311/7311x1749.html](http://www.iupac.org/publications/pac/2001/7311/7311x1749.html)

JCAMP-DX. A Standard Format for the Exchange of Ion Mobility Spectrometry Data (IUPAC Recommendations 2001)

by J. I. Baumbach, A. N. Davies, P. Lampen, and H. Schmidt
Pure and Applied Chemistry, Vol. 73, No. 11, pp. 1765–1782 (2001).

The relatively young field of ion mobility spectrometry has now advanced to the stage where the need to reliably exchange the spectroscopic data obtained worldwide by this technique has become extremely urgent. An internationally recognized electronic data exchange format is essential to assist in the validation of the various new spectrometer designs and to assist in intercomparisons between different laboratories' reference data collections.

To make the data exchange between users and system administration possible, it is important to define a file format specially suited to the requirements of ion mobility spectrometry. The format should be computer readable and flexible enough for extensive comments to be included. In this document, we define a data exchange format, agreed on by a working group of the International Society for Ion Mobility Spectrometry at Hilton Head Island, USA (1998), and Buxton, UK (1999).

This definition of the format is based on the IUPAC JCAMP-DX protocols, which were developed for the exchange of infrared spectra and extended to chemical structures, nuclear magnetic resonance data, and mass spectra. This standard of the Joint Committee on Atomic and Molecular Physical Data is of a flexible design. IUPAC has taken over the support and development of these standards and recently introduced an extension to cover year 2000 compatible date strings and good laboratory practice. The aim of this paper is to adapt JCAMP-DX to the special requirements of ion mobility spectra.



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2001/7311/7311x1765.html](http://www.iupac.org/publications/pac/2001/7311/7311x1765.html)

Molality-Based Primary Standards of Electrolytic Conductivity (IUPAC Technical Report)

by K. W. Pratt, W.F. Koch, Y. C. Wu, and P. A. Berezansky
Pure and Applied Chemistry, Vol. 73, No. 11, pp. 1783–1793 (2001).

New values of electrolytic conductivity were determined for aqueous KCl solutions with molalities of 0.01, 0.1, and

1.0 mol/kg in the temperature range 0 to 50 °C, at 5 K intervals. Expanded uncertainties, $2u_c$, were also calculated in accordance with the presently accepted protocol for the treatment of uncertainty. The new conductivity values are recommended as primary standards of electrolytic conductivity based on molality. They replace the previous values, based on the nonstandard demal scale, which were determined only at 0, 18, and 25 °C. The accuracy of the technique used was evaluated by repeating the determination of the previously recommended demal-based IUPAC standards of electrolytic conductivity and through comparison with other absolute measurements.



[www.iupac.org/publications/pac/
2001/7311/7311x1783.html](http://www.iupac.org/publications/pac/2001/7311/7311x1783.html)

NMR Nomenclature. Nuclear Spin Properties and Conventions for Chemical Shifts (IUPAC Recommendations 2001)

by R. K. Harris, E. D. Becker, S. Cabral de Menezes, R. Goodfellow, and P. Granger
Pure and Applied Chemistry, Vol. 73, No. 11, pp. 1795–1818 (2001).

A unified scale is recommended for reporting the NMR chemical shifts of all nuclei relative to the ^1H resonance of tetramethylsilane (TMS). The unified scale is designed to provide a precise ratio, X , of the resonance frequency of a given nuclide to that of the primary reference, the ^1H resonance of TMS in dilute solution (volume fraction, $j < 1\%$) in chloroform. Referencing procedures are discussed, including matters of practical application of the unified scale. Special attention is paid to recommended reference samples, and values of X for secondary references on the unified scale are listed, many of which are the results of new measurements.

Some earlier recommendations relating to the reporting of chemical shifts are endorsed. The chemical shift, δ , is redefined to avoid previous ambiguities but to leave practical usage unchanged. Relations between the unified scale and recently published recommendations for referencing in aqueous solutions (for specific use in biochemical work) are discussed, as well as the special effects of working in the solid state with magic-angle spinning. In all, nine new recommendations relating to chemical shifts are made.

Standardized nuclear spin data are also presented in tabular form for the stable (and some unstable) isotopes of all elements with nonzero quantum numbers. The information given includes quantum numbers, isotopic abundances, magnetic moments, magnetogyric ratios and receptivities, together with quadrupole moments and line-width factors where appropriate.



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