resulting ESR spectra can provide rate coefficients of each elementary process and the activation energy ($E_a$) of the reactions based on temperature dependent measurements. Figure 1 shows a typical 3D image of the TR ESR spectrum of radical polymerizations of tert-butyl methacrylate (a) with a scheme of observed radical addition reaction (b) as an example. Slice at constant time provides a spectrum with hyperfine splitting (Fig. 1(c)) and detailed structure can be determined from the spectrum. Time profiles of the each spectroscopic line (Fig. 1(d)) are strongly correlated with reaction kinetics. When the same polymerization was observed by SS ESR, the ESR spectrum of propagating radicals can be detected, as shown in Figure 2. Initiation and propagating processes of the same polymerization system were observed by TR and SS ESR spectroscopies.

Moreover, single pulse experiments provide access to chain-length-dependent termination, to transfer, and even to propagation rate coefficients. The method is also applicable to reversible addition fragmentation transfer (RAFT) and atom-transfer radical polymerization (ATRP) kinetics. The multitude of powerful ESR techniques enables the quantitative detection of specific radicals over the entire course of a polymerization reaction. Application of these methods requires the accurate knowledge of the ESR spectra and associated hyperfine coupling constants (hfcs). Since values of hyperfine splitting constants were determined very precisely from the spectrum, it was reasonably well simulated as the corresponding propagating radical. Absolute values of the hyperfine splitting constants are proportional to the spin densities of each element and the spin density is strongly correlated with electron density. The precisely determined hfcs data will provide significant information on theoretical calculations of properties of radicals. No hfcs on polymerization-related radicals have been tabulated since Rånby and Rabek’s book on ESR Spectroscopy in Polymer Research (Springer, 1977).

A critically evaluated update of the available data and of recommended experimental methods is urgently required, in particular as novel monomers and polymerization techniques have been introduced. Experimentalists, methodologists, and theoreticians will cooperate within the project to establish a database of reliable ESR spectra for use in academia and industry.

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www.iupac.org/project/2015-034-1-400

Which Elements Belong in Group 3 of the Periodic Table?

The question of precisely which elements should be placed in group 3 of the periodic table has been debated from time to time, with apparently no resolution up to this point. [1] This question has also received a recent impetus from several science news reports following an article in Nature in which the measurement of the ionization energy of the element lawrencium was reported for the first time. [2,3]

We believe that this question is of considerable importance for chemists and physicists, as well as students of the subjects. Students and instructors are typically puzzled by the fact that published periodic tables show variation in the way that group 3 of the periodic table is displayed. An IUPAC task group has now been formed in order to make a recommendation regarding the membership of group 3 of the periodic table.

Various forms of evidence have been put forward in support of each version of group 3, appealing to chemical as well as physical properties, spectral characteristics of the elements, and criteria concerning the electronic configurations of their atoms. The task group will aim to evaluate all this evidence in order to reach a conclusion that encompasses these different approaches. [4]

It is proposed that IUPAC should make an official recommendation in favor of the composition of group 3 of the periodic table as consisting either of

(1) the elements Sc, Y, Lu and Lr, or
(2) the elements Sc, Y, La and Ac.

It should be stated categorically that the task group does not intend to recommend the use of a 32-column periodic table or an 18-column. This choice is a matter of convention, rather than a scientific one, and should be left to individual authors and educators. As Jeffery
Leigh has asserted recently, IUPAC has not traditionally taken a view as to the correctness of one or the other periodic table and there is no such thing as an officially approved IUPAC periodic table. [5] We will only concern ourselves with the constitution of group 3. Once this is established, one is free to represent the periodic table in an 18 or 32 column format. The conclusions of the task force will form the basis for a report to appear in Pure and Applied Chemistry.

The task group welcomes comments on this project.

**References**


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