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Editorial X-Ray Wavelength Nomenclature

There has been increasing use of X-ray methods for materials characterization since the early 1950's, and the initial use of the diffraction and emission methods goes back four decades before that time. Along with this increase in the application of X-ray methods there has been a growing problem with the system of X-ray wavelength nomenclature. The current system was proposed by Siegbahn back in the 1920's and since his initial proposal, more lines have been identified, many of which do not fit with the nomenclature system. Over the years, this system has led to an increasing number of inconsistencies within a given line series As an example, in the K series, the $3p \rightarrow 1s$ transitions are labelled $\beta_{1,3}$ rather than $\beta_{1,2}$, because it was originally believed that the line was a singlet, along with the $4p \rightarrow 1s$ transition also believed to be a singlet. Much later, as the resolution of crystal spectrometers improved, it was found that both of these lines were doublets. Because the $4p \rightarrow 1s$ transition was already called β_2 , and because β_3 was already allocated to the $3p \rightarrow 1s(1/2)$, the lines in the newly found doublet were called $K\beta'$ and $K\beta''$.

With the identification of further lines, especially in the longer wavelength series, and with the development of the Auger and other electron spectroscopic techniques, this problem has become intolerable. As an example, a reasonably modern X-ray spectrometer is well able to detect lines from the M series of all elements from the rare earths and on up in the periodic table. At this time, less than one half of these lines have been allocated names within the Siegbahn system!

Commission V.4 of the International Union of Pure and Applied Chemistry has for more than 20 years been addressing the problems of nomenclature, symbols and their usage in the various analytical spectroscopic disciplines.

This group has recently recommended¹ a brand new notation for X-ray spectroscopic wavelengths to be called "IUPAC NOTATION". The proposed system is based on energy level designations and has the advantage of being simple, logical and easy to apply to all types of transition. Moreover, it is consistent with the notations used in electron spectroscopy. As well as being easier to apply, the new system has the added advantage of relying solely on the ASCII character set. With the increasing use of automated typesetting machines for drawing up wavelength tables, there should be no further confusion caused by the inability of the typesetter to print certain characters. The X-ray levels are defined as those states which occur as initial or final states in X-ray transitions. The X-ray level notation follows earlier conventions except for the use of Arabic rather than Roman numerals. As the main rule, transitions between X-ray levels are denoted by the level symbols for the initial and final state separated by a hyphen. The initial state is placed first, irrespective of the energetic ordering. Thus, the $K\alpha_1$ and $K\alpha_2$ will now be known as the K-L3 and K-L2 respectively.

The Editors of *Powder Diffraction* are now seeking permission from IUPAC to reproduce the full report of the new wavelength nomenclature system in a future issue. It is hoped that the new system will soon be ratified, and it should prove a much more practical solution for X-ray line nomenclature.

 Jenkins, R., Manne, R., Robin, J. and Senemaud, C., "Provisional Nomenclature Report from Commission V.4 – Nomenclature, Symbols, Units and their usage in spectrochemical analysis; Part VIII: Nomenclature system for X-ray spectroscopy", IUPAC (1987).

> Ron Jenkins Principal Scientist International Centre for Diffraction Data