4. PRODUCTION AND PROPERTIES OF RADIATIONS

Table 4.2.2.6. Wavelength conversion factors

Numbers in parentheses are standard uncertainties in the least-significant figures.

| | Cu Kα ₁ | Mo <i>K</i> α ₁ | W $K\alpha_1$ |
|--------|--------------------|----------------------------|----------------|
| λ(Å) | 1.54059292(45) | 0.70931713(41) | 0.20901313(18) |
| λ (Å*) | 1.540562(3) | 0.709300(1) | 0.2090100 |
| 1 kxu | 1.537400 | 0.707831 | |
| Å*/Å | 1.0000201(20) | 1.0000242(22) | 1.00001498(86) |
| kxu/Å | 1.00207683(29) | 1.00209955(58) | |

are recent measurements by Kraft, Stümpel, Becker & Kuetgens (1996), and the numbers in normal type are from the Bearden database or a reference that appeared after the Bearden database corrected to an optically based scale. Figure 4.2.2.2 shows relative deviations between the theoretical and experimental values for most of the tabulated data. The error bars shown in the figure are the experimental uncertainties.

4.2.2.13. Availability of a more complete X-ray wavelength table

This article and the accompanying X-ray wavelength tables are an up-dated version of the contribution to the *International Tables for Crystallography*, Volume C, 2nd edition that was published in 1999. This article has been subject to more critical review and analysis and the data are consistent with the most recent adjustment of the fundamental physical constants (Mohr & Taylor, 2000). We believe that these data represent a significant improvement in consistency, coverage and accuracy over previously available resources. The results presented here are a subset of a larger effort that includes all K- and L-series lines connecting the n=1 to n=4 shells. The more complete table has been submitted for archival publication and will be made available on the NIST Physical Reference Data web site. Electronic publishing of this resource will provide a convenient

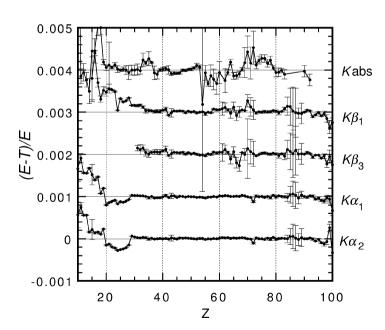


Fig. 4.2.2.1. Relative deviations between theoretical and experimental results for K-series spectra. The topmost data set concerns the K-edge location, while the other data sets, beginning at the bottom, refer to the $K\alpha_2$, $K\alpha_1$, $K\beta_3$ and $K\beta_1$, respectively. The ordinate scales have been displaced for clarity by the indicated multiples of 0.001.

data resource to the scientific community that can be more easily up-dated and expanded.

4.2.2.14. Connection with scales used in previous literature

In order to compare historical data for X-ray spectra with the results in the present tabulation, certain conversion factors are needed. As discussed in the introduction, the principal units found in the literature are the xu and the Å* unit. There is the additional complication that there were several different definitions in use at various times and at the same time in different laboratories. For the convenience of the reader, we summarize in Table 4.2.2.6 the main conversion factors needed. The numerical values for the wavelengths in Å can be converted to energies in electron volts by using the conversion factor 12 398.41857 (49) eV Å (Mohr & Taylor, 2000).

Our current efforts owe their inception to the encouragement of the late A. J. C. Wilson, who persistently communicated the need for an updated wavelength resource for the crystallographic community. The larger effort evolved at NIST with the support of the Standard Reference Data Program as established with the help of the late Jean Gallagher, and sustained by the program's current Director, John Rumble. Early phases of the preparation of this material benefited from the efforts of John Schweppe. Cedric Powell supplied valuable advice in the area of electron binding energies. We are particularly grateful to the Editor, E. Prince, for his help and patience in the development of these wavelength tables. Richard Deslattes died between the first publication of this article and this revision. This work would not have been possible without his dedication to this project over more than a decade. The earlier wavelength table of the late J. A. Bearden, under whom one of the present authors (RDD) studied, was a significant influence on this project.

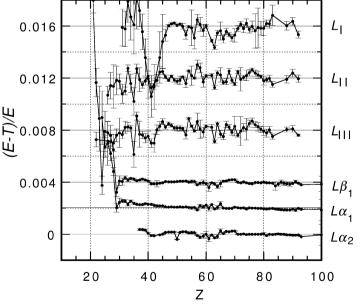


Fig. 4.2.2.2. Comparison of L-series data with experiment for the indicated range of Z. Indicated data, beginning at the bottom, refer to the $L\alpha_2$, $L\alpha_1$, and $L\beta_1$ emission lines and the $L_{\rm III}$, $L_{\rm II}$, and $L_{\rm I}$ absorption edges. For clarity, the plots have been displaced vertically by multiples of 0.002 for the emission lines and 0.004 for the absorption edges.