current, and rather different, approach can be compared. Although a detailed comparison of the historical databases may be of some interest, the result would have only very small influence on the outcome presented here. To specify this framework, we begin with a brief description of the procedures used in establishing this reference database.

Bearden and his collaborators remeasured a group of five X-ray lines (Bearden, Henins, Marzolf, Sauder & Thomsen, 1964), with the remaining entries in the wavelength table coming from a critically reviewed, and re-scaled, subset of earlier measurements (Bearden, 1967). Line locations were given in Å* units, a scale defined by setting the wavelength of W $K\alpha_1 = 0.2090100$Å*. It was Bearden's intention that, for all but the most demanding applications, one could simply assign Å*/Å $= 1$, with an uncertainty arising from the fundamental physical constants, particularly N_A and hc/e, combined with uncertainties arising from the measurement technology (Bearden, 1965). Not long after the publication of the final compilation (Bearden, 1967), it became clear that the fundamental constants used in defining Å* needed significant revision (Cohen & Taylor, 1973), and that there were some inconsistencies in the metrology (Kessler, Deslattes & Henins, 1979).

4.2.2.2. *Known problems*

Aside from the particular issues noted above, all previous wavelength tables had certain limitations arising from the procedures used in their generation. In particular, except for a small group of five $K\alpha$ spectra (Bearden, Thomsen *et al.*, 1964), the Bearden tables relied entirely on data previously reported in the literature. Both of the other tabulations also proceeded using only reported experimental values (Cauchois & Hulubei, 1947; Cauchois & Senemaud, 1978). In the Bearden compilation process, available data for each emission line were weighted according to claimed uncertainties, modified in certain cases by Bearden's detailed knowledge of the measurement practices of the major sources of experimental wavelength values. The complete documentation of this remarkable undertaking is, unfortunately, not widely accessible. Our evident need to understand the origin of the 'recommended' values has been greatly aided by the availability of a copy of the full documentation (Bearden, Thomsen *et al.*, 1964).

The actual experimental data array from which the previous tables emerged is not complete, even for the prominent ('diagram') lines. In the cases where experimental data were not available [as can be seen only in the source documentation (Bearden, Thomsen *et al.*, 1964)], the gaps were filled by interpolated values based on measurements available from nearby elements, plotted on a modified Moseley diagram in which the Z^2 term dependence is taken into account (Burr, 1996). In the end, such a smooth scaling with respect to nuclear charge suppresses the effects of the atomic shell structure, a practice that must be avoided in order to obtain the significant improvement in the database that we hope to provide. Also obscured in smooth Z scaling are detectable contributions arising from the fact that nuclear sizes do not change smoothly as a function of the nuclear charge, Z.

4.2.2.3. *Alternative strategies*

There are several possible approaches to generating an improved, 'all-Z' table of X-ray wavelengths. These range from the option of conducting a massive measurement campaign to populate more fully the currently available tabular array to a large computational endeavor that might purport to carry out multiconfiguration, relativistic wavefunction calculations for the entire Periodic Table. It seems evident to us that there is little interest in, and even less support for, mounting the large effort needed to realize an improved tabulation of X-ray wavelengths by purely experimental means, while the possibility of proceeding in an entirely theoretical mode is not consistent with the evident need that at least some wavelengths be reported with uncertainties that approach the limit of what can be obtained from the naturally occurring X-ray lines. The actual location of any useful feature of a line is influenced not only by the physical and chemical environment of the emitting atom but also by inevitable multi-electron excitation processes that perturb the entire spectral profile. Calculation of such complexities currently lies beyond the limits of practicality, eliminating the option of proceeding without strong coupling to experimental profile locations, at least for crystallographically important X-ray lines. Similar considerations apply *a fortiori* to those lines needed as reference wavelengths for exotic atom measurements, such as those leading to masses of elementary particles and tests of basic theory [see *e.g.* Beyer, Indelicato, Finlayson, Liesen & Deslattes (1991)].

In constructing the accompanying tables, we have chosen a new procedure that differs from those described above, and accordingly requires some detailed commentary. We begin with the presently available network of well documented experimental measurements, originally established to provide a test bed for the theoretical methods developing at that time (Deslattes & Kessler, 1985). This modest network was the first compilation to make use of the, then newly available, connection between the X-ray region and the base unit of the International System of measurement (the SI) based on optical interferometric measurement of a lattice period as revealed by X-ray interferometry. Details of the generation of this network and its subsequent expansion will be given below. Using this network as a test set gave clearer suggestions as to specific limitations of the theoretical modelling than had been evident from using other, less selective, experimental reference compilations available at that time. Extensive theoretical developments before and, especially, after the appearance of this new experimental reference set have shown a steady convergence toward these critically evaluated data. Following this evolution further, our long-term plan is to use these new theoretical calculations to provide a more structured and accurate interpolation procedure for estimating the spectra of elements lying between those for which we have accurate measurements, or spectra well connected to a directly established reference wavelength. The present table provides experimental and theoretical values for some of the more prominent K and L series lines and is a subset of a larger effort for all K and L series lines connecting the $n = 1$ to $n = 4$ shells. The more complete table will be published elsewhere and be made available on the the NIST Physical Reference Data web site. In addition, experimental values for the K and L edges are provided. Although the reference data are inadequate in both low and high ranges of Z, the general consistency of theory and experiment through the region $20 < Z < 90$ for the strong K-series and L-series lines suggests that, in the absence of good reference measurements, the uncorrected theoretical values should be considered for applications not requiring the highest accuracy.

4.2.2.4. *The X-ray wavelength scales, old and new*

Historically, from the first realizations of refined spectroscopy in the X-ray region (*ca* 1915–1925) up to the period 1975–1985, the best measured X-ray wavelengths had to be expressed in some local unit, most often designated as the xu (x unit) or kxu

references