实用X射线谱线图和表

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PREFACE

The X-Ray Fluorescence (XRF) analytical technique is widely applied in many departments as a convenient, flexible and powerful analytical tool. X-ray fluorescence spectrometer can be used as an independent means for composition analysis,as well as combined with Electron Probe Microanalyzer (EPM), Scanning and Transmission Electron Microscopy (SEM and TEM), X-Ray Diffraction(XRD) system, Scanning Proton Microprobe (SPM) or Synchrotron Radiation X-Ray Microprobe (SRXRM) to perform microscopic research on compositions and structures of materials. XRF technique has such advantages as broad analytical range of elements (B→U), widely measurable range of concentration (0.x $\mu g / g \sim 100\%$), simplicity of sample preparation, non-contamination to environment and highly automated operation, and so on.

As a bulk-analysis means, XRF technique can be used for flexible on-site analysis in the field, for automatic process control analysis or monitor in large industrial productions, and for accurate and complicated analysis in research laboratories. On the other hand, as an important microanalysis means, it can perform non-destructive microanalysis and elemental space-distribution analysis in many fundamental research fields. Therefore, XRF technique has wide applications and good prospects.

The X-ray spectrum line tables are indispensable to the above-mentioned applications and research works.In order to meet the practical requirements from wide applications of XRF analytical technique, a set of concise and practical X-ray spectrum line atlas has been designed,which comprises two kinds of spectrum charts and nine kinds of spectrum digital tables. It is a try to represent the X-ray Energy or Two-theta charts in line segments. Compared with traditional digital tables, this expression form of X-ray spectrun is more clear, visual and convenient for analytical applications. It not only enables analysts to work out analytical schemes for a given task promptly,but also is very beneficial for beginners to know spectrum lines well and to raise the ability of selecting excition-sources, analyzed lines, background positions and searching possible interference-lines, and so on.

The book contains over 1400 emission lines and absorption edges with more than 1% relative intensity, a number of weak spectral lines of target elements for some commercial X-ray tubes, nondiagram(or statellite) lines for some light elements, two-theta data for ten commonly used crystals TAP, RAP, KAP, ADP, PET, InSb, Ge, LiF(200), LiF(220) and LiF(420) as well. In resent years a variety of multilayer film crystals special for analyzing light elements have been developed, for which the $2d$ value of each crystal is not completely identical even for a same type of crystal,therefore, the 2θ value of each multilayer crystal in respect to various diffraction spectral lines should be calculated according to Bragg's equation when using the real $2d$ values.

In addition, the importance of absorption edge data is stressed here and data of

absorption edges are expressed with various eye-catching ways in spectrum charts and tables. It is considered that absorption edge data not only would be used when selecting excitation sources,understanding generation of spectral lines and determining background sites,but also would be of special meaning when evaluating or correcting interelemental absorption and enhancement effects.

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APPENDIX

BRIEF ILLUSTRATION

This book includes two sets of spectrum charts and nine kinds of data tables based on different uses.

1. X-ray energy chart is designed for energy-dispersion analysis, in which spectral lines are arranged in energy increasing order from the left to the right (horizontal), and lines of various spectrum series are separately arranged in order of K-, L-, and M-series from the botton to the top (vertical),for various spectral lines in a same spectrum series (here mainly for L series) they are grouped according to correspending transitions (KL_{III}, KL_{II}, KL_{I}). Principal analytical lines (Kα or Lα) of elements are presented by bold line segments and the others by fine lines. γ-rays emitted from radioisotope sources and spectrum lines of some radioelements are preseted by lines with an arrow mark so as to distinguish them from others.

Absorption edges are not emission lines,but they are important data concerning generation, measurement and correction of spectrum lines.For the sake of emphasizing importance of the data of absorption edges in XRF analysis and making their positions more obvious in charts, the edges are all presented by colour line segments. Thus, some physical conceptions such as relations between spectral lines, interelement absorption and enhancement effects,as well as generations of spectrum lines become more clear, moreover, monotonous digital-type spectrum tables turn into colourful, visual and eye-catching pictures.

2. The two-theta charts are specially used for wavelength-dispersion analysis.Six most commonly used analyzing crystals, i.e. LiF(220), LiF(200), Ge, PET,InSb and TAP are included in the charts. The horizontal scale of the chart is 2θ in degree. The compiling form for first-order diffraction lines is as same as that for the energy chart, however, for higher order diffraction lines they are separately arranged above or under first-order lines, e.g. higher-order lines of K-series are under first-order lines of K-series, but higher-order lines of L-series are above first-order lines of L-series. Higher-order lines are marked by multi-segment lines with two-segments, three-segments, four-segments and five-segments, which stand for 2nd, 3rd, 4th and 5th order line respectively. Consequently, a clear-cut pattern is formed: in which analytical lines are located in the center as a main body and other spectra lines and absorption edges are dispersed around it. The pattern, however, makes absorption and enhancement relation between analyzed elements and other matrix-elements, as well as relative position between analytical lines and interference lines more clear and visual.

3. The purpose of table 3 is to provide basic wavelength and energy data of characteristic lines and absorption edges of elements. Energy values are computed as

$$E(\text{keV}) = 12.398541 \;/\; \lambda$$

where the wavelength unit is 10^{-10}m [1] and the energy unit keV. The subscript "a.e."

means absorption edge, for example, K a.e., L_{III} a.e., M_V a.e., represent absorption edges for K, L_{III}, M_V series respectively.

L-lines of Np and Pu emitted from some radioisotope sources such as ^{241}Am and ^{244}Cm are also listed in the table, but other lines of both elements are omitted.

4. Table 4 shows wavelengths and energies of essential spectral lines arranged in the order of increasing energy and it is mainly used for energy-dispersion analysis. Meanings of various symbols in the table are as follows:

Z —— atomic number,
EL —— element symbol,
LINE —— spectral line name,
I —— relative intensity.

The wavelength of Kα is calculated from the following equation:

$$\lambda_{K\alpha} = (2\lambda_{K\alpha 1} + \lambda_{K\alpha 2}) / 3$$

Relative intensity data is taken from literatures[2]. In order to facilitate looking for, the marks " * * " (Kα) and " * " ($L\alpha_1$) are given before principle analytical lines of elements in the table.

5. Table 5 is a two-theta table of principle lines arranged in the order of decreasing $n\lambda$, concerning with ten crystals. Since each crystal is used in a certain range of wavelengths, ten crystals will be present in the table one after another, however there are three crystals to be chosen for every spectral line. The table is important for wavelength-dispersive XRF analysis. 2θ values can be given by

$$2\theta = 2 \cdot \sin^{-1} (n\lambda / 2d)$$

The meanings of various symbols in the table are as same as in table 4. Data relevant to the ten crystals employed in the book will be shown in the following table.

Informations for ten analyzing crystals used in the book

Crystal Designation	Crystal Name	Miller Index (*hkl*)	$2d$ (10^{-10}m)
KAP	Potassium hydrogen phthalate	100	26.632
RAP	Rubidium hydrogen phthalate	100	26.121
TAP	Thallium hydrogen phthalate	100	25.75
ADP(101)	Ammonium dihydrogen phosphate	101	10.642
PET	Pentaerythritol	002	8.742
InSb	Indium antimonide	111	7.4806
Ge(111)	Germanium	111	6.532
LiF(200)	Lithium fluoride	200	4.0267
LiF(220)	Lithium fluoride	220	2.848
LiF(420)	Lithium fluoride	420	1.8

6. Table 6 and 7 are compiled for finding out 2θ of essential analytical lines of various elements rapidly. As a result, it is much more easy to use both tables than to use table 4 to

find out 2θ.

7. Emission lines of X-Ray tube target-elements are important fundamental data for both qualitative and quantitative analysis. In table 8, target-element lines are listed for certain X-ray tubes commonly used, such as Sc, Cr, Mo, Rh, Ag, W, Pt and Au. The Roman numerals in 2θ column, Ⅰ, Ⅱ, Ⅲ, individuelly show the order number of diffractions.

8. In XRF analysis, especially in quantitative analysis, Compton-scattering lines of excitation source radiations are often used as the basis of matrix correction and background calculation. Table 9 and 10 provide the wavelenth, energy and relevant 2θ of Compton-scattering lines of essential emitted lines for some commonly employed X-ray tubes and radioisotope sources respectively.The wavelenth of Compton-scattering line, λ', can be calculated from

$$\lambda' = \lambda_0 + 0.0243(1-\cos\varphi)$$

in which λ_0 is the wavelenth of incident X-ray, φ is scattering angle, here $\varphi = \varphi_1$(incident angle) + φ_2(take off angle). R and C in the tables mean Reyleigh(coherent) and Compton(incoherent) scatter respectively, and values in paratheses after the letter C show scattering angles ($\varphi = \varphi_1 + \varphi_2$).

9. Table 10 is used for energy dispersion and nondispersion analyses, in which data and informations are quoted from literatures[3,4].

10. In XRF analysis, escape peaks of working materials in detectors are usually one of the important interference sources. Escape peak data of NeKα, KrKα are included in table 11, while these of SiKα and ArKα are also provided for multichannel instrument users. The energy of escape peaks is calculated as

$$E_e = E - E_{D-X}$$

where E is the full energy of incident X-ray photons and E_{D-X} is the characteristic X-ray energy of detector working materials.

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PART I

X-RAY SPECTRAL LINE CHARTS

SYMBOLS AND LEGEND

Unit of the scale : keV for energy chart

degree (2θ) for 2θ charts

N : order of diffraction (I, II, III, IV, V, VI)

L : name of X-ray spectrum line

K X-ray absorption edge of elements

L_{III} X-ray absorption edge of elements

L_{II} X-ray absorption edge of elements

L_I, M_V or M_{IV} X-ray absorption edge of elements

X-ray emission or 1st order diffracted line of elements

2st order diffracted line

3st order diffracted line

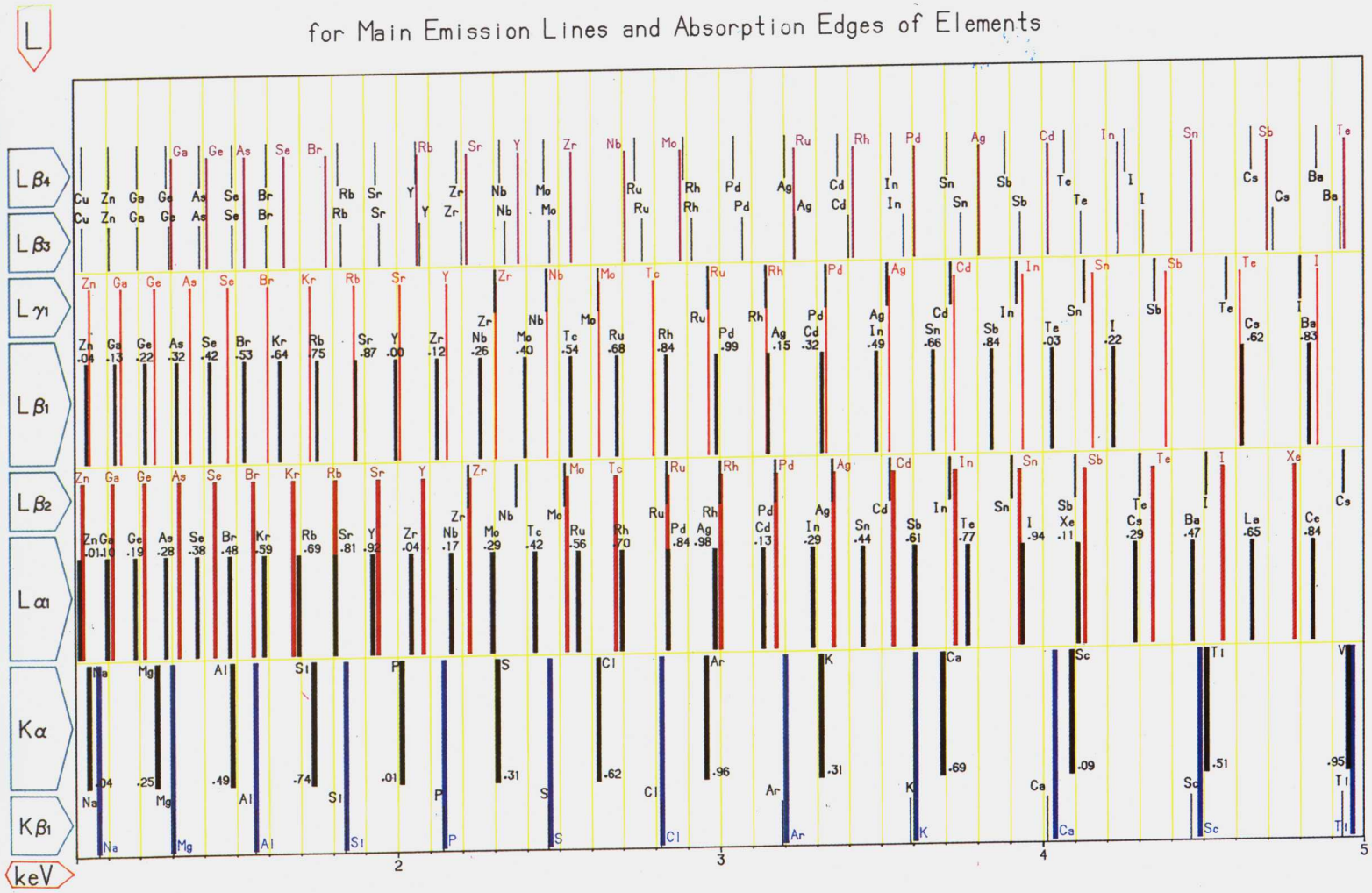
4st order diffracted line

5st order diffracted line

γ-ray from radioisotope source

1. THE X-RAY ENERGY CHARTS

for Main Emission Lines and Absorption Edges of Elements



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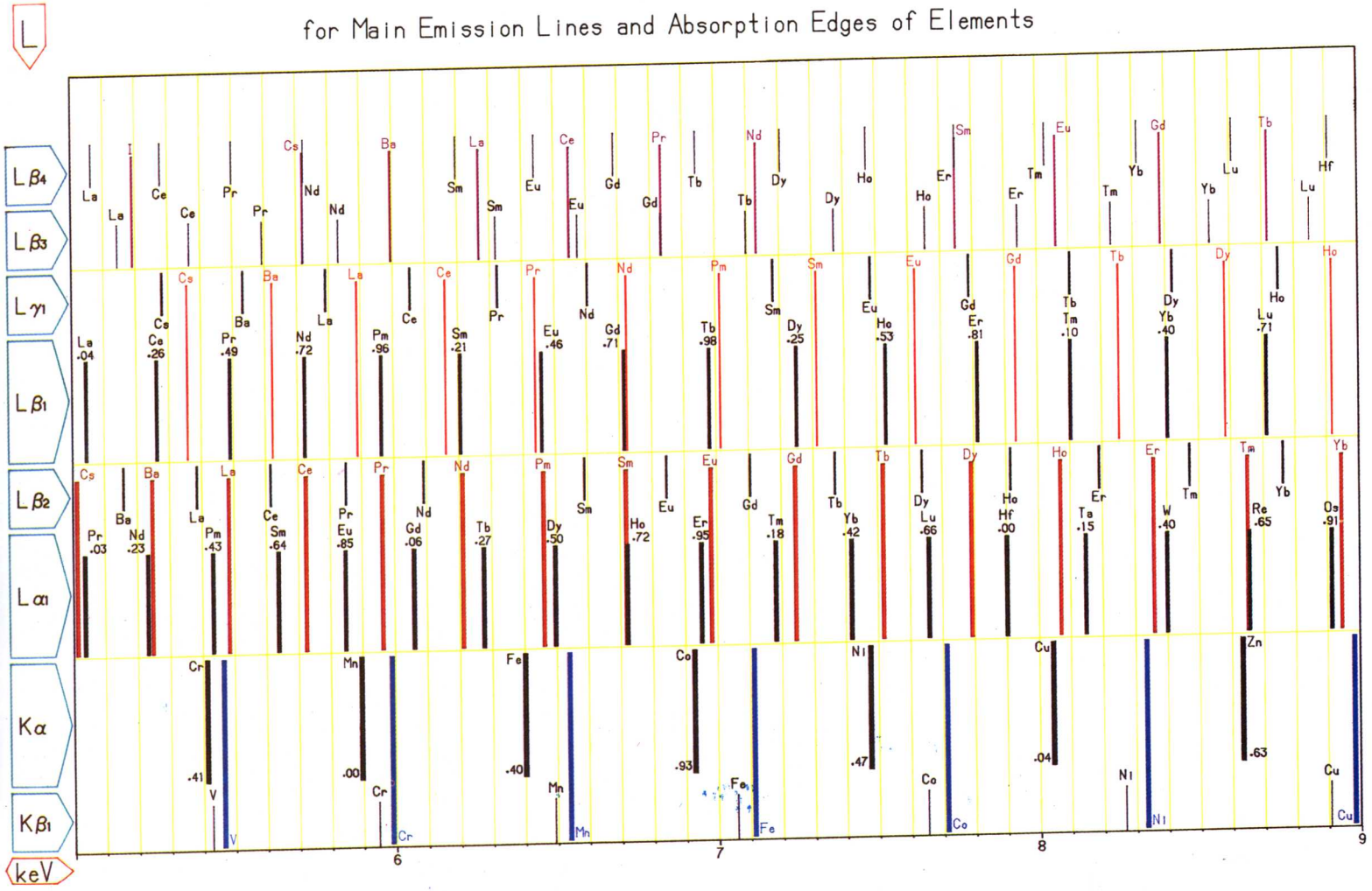
for Main Emission Lines and Absorption Edges of Elements



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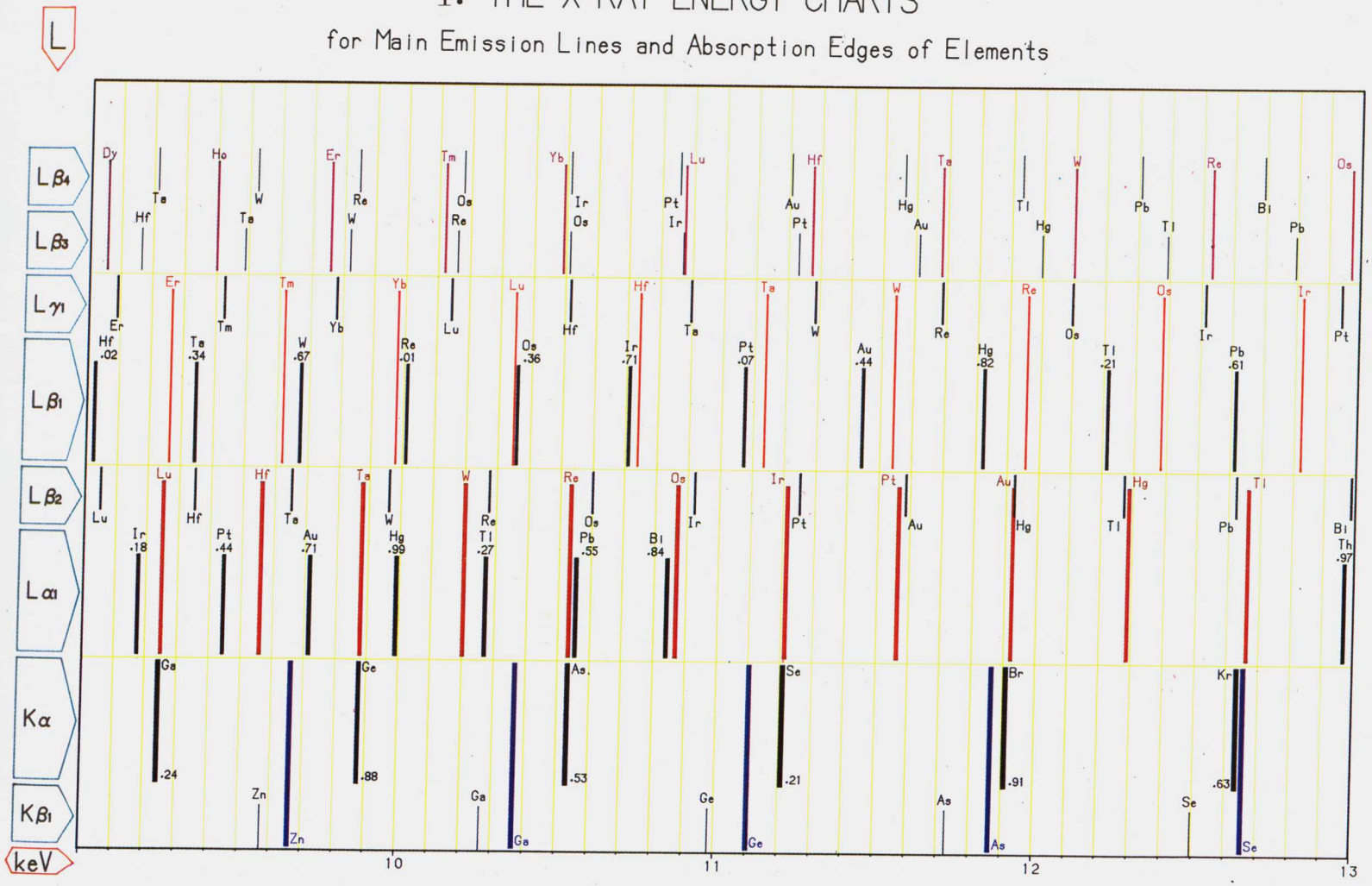

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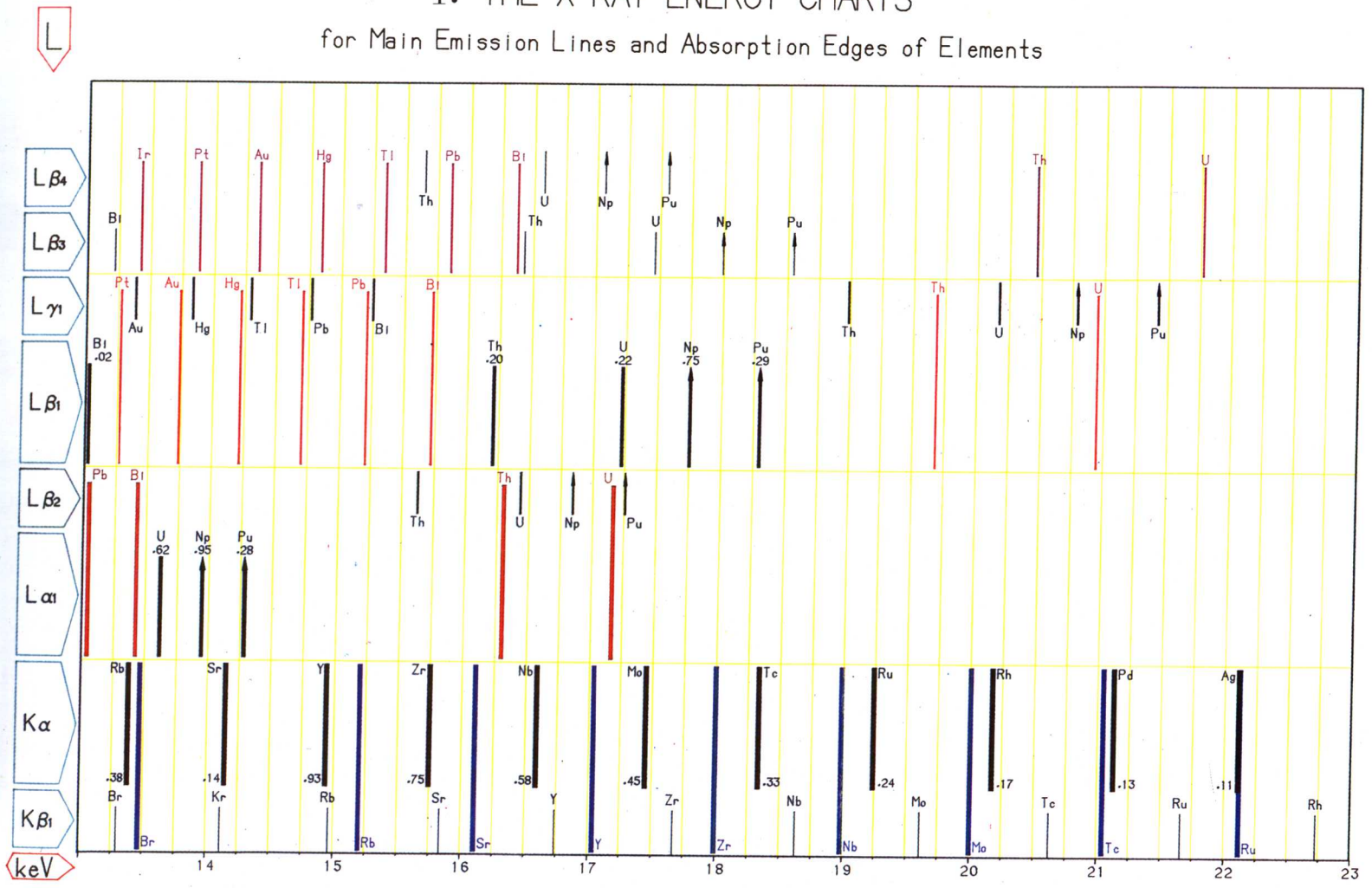

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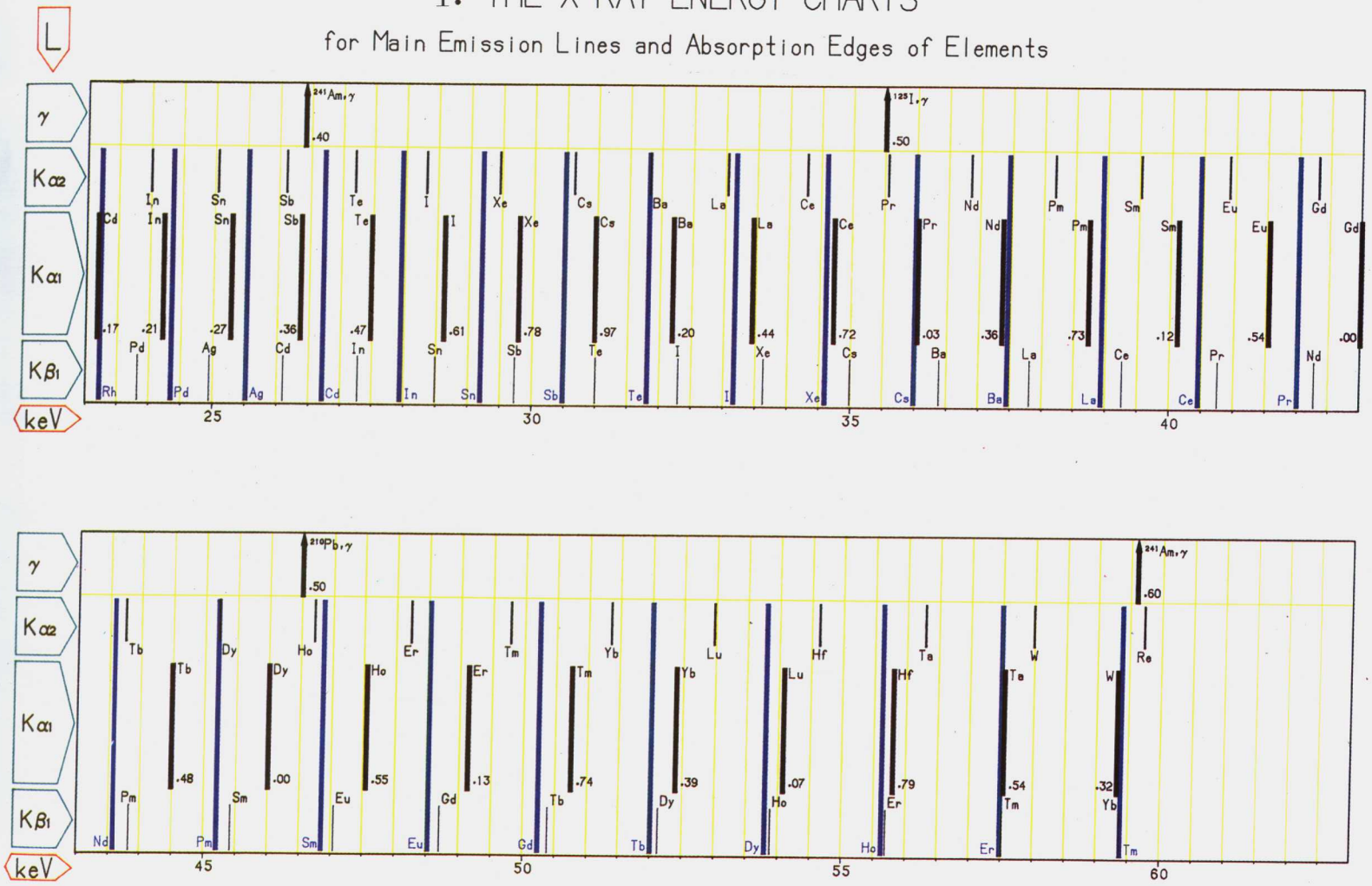
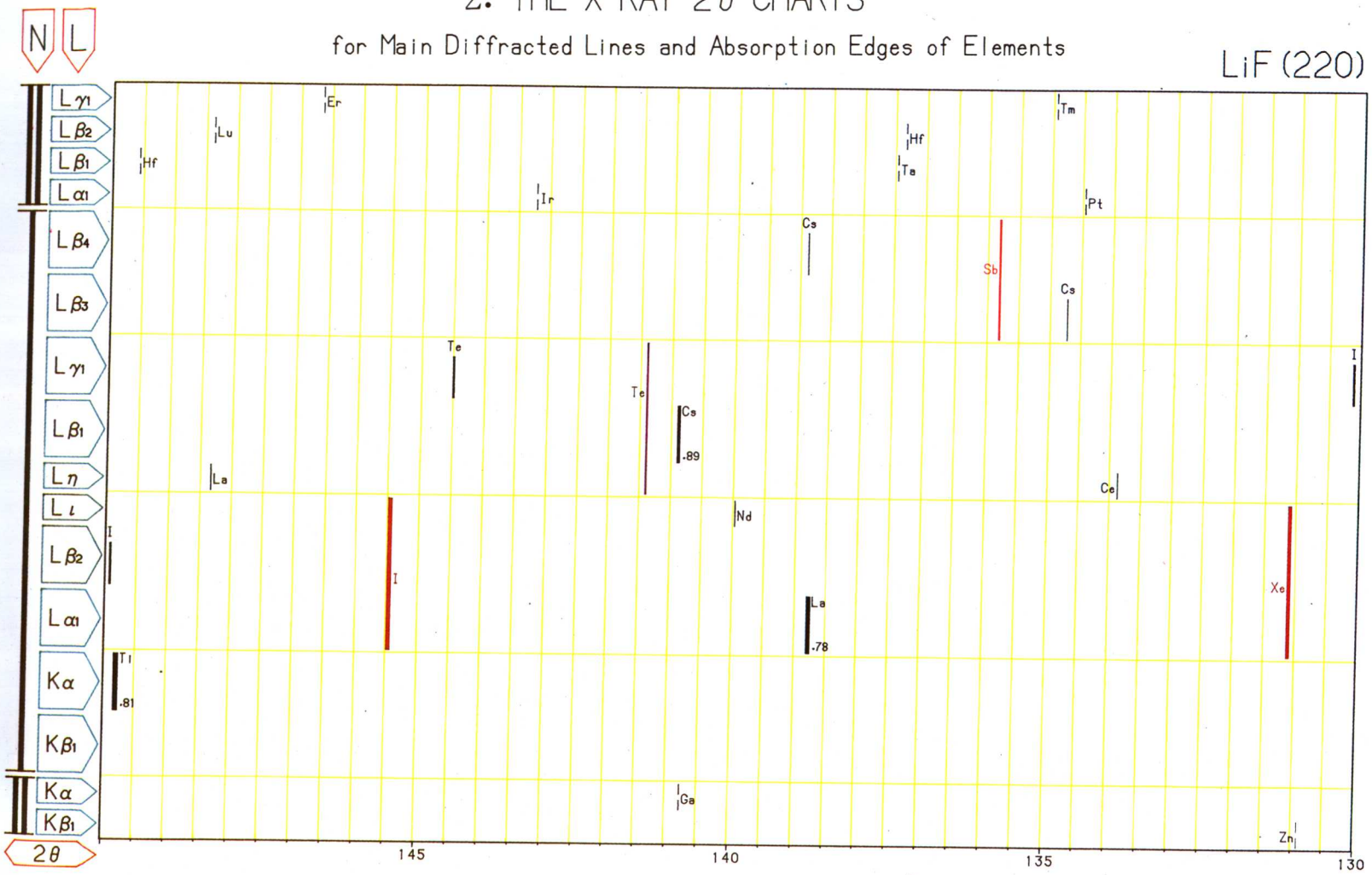


2. THE X-RAY 2θ CHARTS

for Main Diffracted Lines and Absorption Edges of Elements



2. THE X-RAY 2θ CHARTS

for Main Diffracted Lines and Absorption Edges of Elements

LiF (220)