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PHOTON CROSS SECTION COMPILATION ACTIVITY IN THE U. S. IN THE RANGE 1 keV TO 100 GeV

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Résumé. — Nous exposons brièvement les mesures de sections efficaces photoniques (coefficient d'atténuation) disponibles dans le domaine d'énergie de 10 eV à 100 GeV et pour les éléments de $Z = 1$ à 100, les résultats de ces mesures, extraits de la littérature de 1909 à 1970, sont réunis au « Centre d'information sur les coefficients d'absorption des rayons X » du NSRDS (National Standard Reference Data Center) au NBS. Ces données ainsi que des valeurs théoriques récemment disponibles pour la photoabsorption, les sections efficaces de diffusion et de production de paires sont l'objet d'un programme permanent d'évolution et de compilation au NBS, au L. R. L. (Lawrence Radiation Laboratory, Livermore) et ailleurs. Nous décrivons le travail de compilation du NBS. (10 keV-100 GeV, 23 éléments) et du LRL-NBS (1 keV-1 MeV, 87 éléments) et les comparaisons qu'il permet. Nous discutons les incertitudes provenant de l'interpolation en Z et la structure finie des discontinuités d'absorption.

Abstract. — A brief survey will be presented of photon cross section (attenuation coefficient) measurements available over the range of photon energies 10 eV to 100 GeV and elements $Z = 1$ to 100. The results of these measurements, extracted from the 1909-1970 literature, are on file at the NSRDS (National Standard Reference Data Center) « X-Ray Attenuation Coefficient Information Center » at the NBS. These data, plus newly-available theoretical values for photoabsorption, scattering and pair-production cross sections, are the subject of continuing evaluation and compilation programs at the NBS, LRL (Lawrence Radiation Laboratory, Livermore) and elsewhere. Present compilation efforts by NBS (10 keV-100 GeV, 23 elements) and by LRL-NBS (1 keV-1 MeV, 87 elements) will be described and compared with input information. Compilation uncertainties from Z -interpolation and absorption-edge fine-structure will be discussed.

I. Introduction. — The first X-ray attenuation coefficient measurements, following the 1895 work of Röntgen, appear to be those of Barkla and Sadler in 1909, using characteristic fluorescence radiation. Vigorous measurement programs are still in progress, using newly-developed sources and detectors, higher sample purities, and newly available elements.

At the same time, compilation activity in this area has been perhaps even more vigorous than measurement activity as a result of increasing need for realistic X-ray cross section data by the medical, engineering, and scientific communities. The purpose of this talk is to review the general status of (1) the available measured data and (2) some current compilations representing these data for purposes of practical application.

II. General features of the total photon cross section.

— The general energy-dependence of the photon total cross section or attenuation coefficient between the vacuum ultra-violet region and the GeV regions

is shown in figure 1 for copper. The circles are the measured total cross section values taken from 78 independent literature sources and the underlying curves are the predominant contributing cross sections. Coherent scattering and the photonuclear effect

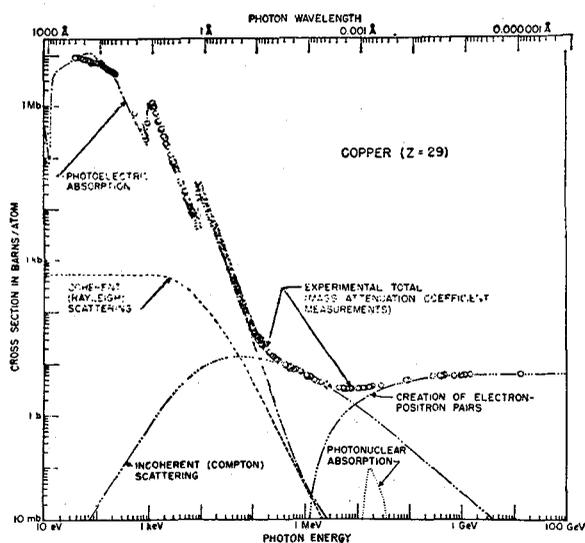


FIG. 1.

(*) Supported primarily by the NBS office of Standard Reference Data. Support was also received from the Defense Atomic Support Agency.

never dominate, but can contribute as much as 5 or 10 % to the total cross section. The photonuclear effect is important in shielding and irradiation technology, and information on this effect is indexed and available from the Photonuclear Data Center at the National Bureau of Standards [See Fuller *et al.*, 1970].

For lower- Z elements the range dominated by incoherent (Compton) scattering widens in both directions, and narrows for higher- Z elements. For copper, shown here, the lowest energy data, extending down to 37 eV, were obtained by Haensel *et al.* [1967-1968] using synchrotron light from the DESY machine at Hamburg. Here and for other elements the DESY data indicate that the McGuire [1968] theoretical results for all elements $Z = 2$ to 54 will be useful for extending compilations below 1 keV.

The highest-energy point, at 13.5 GeV, was obtained by Fidecaro *et al.* [1962] and indicates that available theoretical estimates of extreme high-energy pair production cross sections can be used for compilation purposes, as they are in the current NBS tabulation [Hubbell, 1969]. In the region 3-50 MeV, complete « *ab initio* » calculations of pair production (nuclear field) cross sections are not available, so empirical adjustment of the incomplete theory must be made in this region for compilation purposes.

III. Compilation method. — For purposes of compilation it is convenient to assume that all but one contributing cross section are theoretically « *known* », subtract these from the total measured cross section, and fit the remaining « *unknown* » to simple empirical functions of appropriate form. These fitted values evaluated for a fixed energy mesh and interpolated across Z , with the subtracted theoretical values added back in, provide the compilation.

In the LRL-NBS 1 keV-1 MeV compilation [McMaster *et al.*, 1969] the « *unknown* » was taken to be the photoelectric effect cross section for fitting purposes. However, highly realistic (5-10 % or better) theoretical photoeffect results have become available in extensive numerical form from the work of Rakavy and Ron [1967], Schmickley and Pratt [1967] and others. In the fitting procedure theoretical photoeffect data-points were weighted into the fit along with experimentally-deduced data-points from the above subtraction process and the few explicit photoeffect measurements. In the highest-energy regions where the photoeffect becomes less than 5 % of the total cross section, such theoretical values were used to the exclusion of experimental data. The fitting function was a first, second or third degree polynomial of the log of the photoeffect cross section versus the log of the photon energy.

IV. Measurement coverage. — In figure 2 the coverage of measurements for additional elements is given, at least according to what is now in the NBS data file. This chart represents the information in

~ 260 independent literature-sources which contain total cross section values in absolute units, either graphical or numerical. These values have been extracted numerically into the NBS data file for compilation or other purposes.

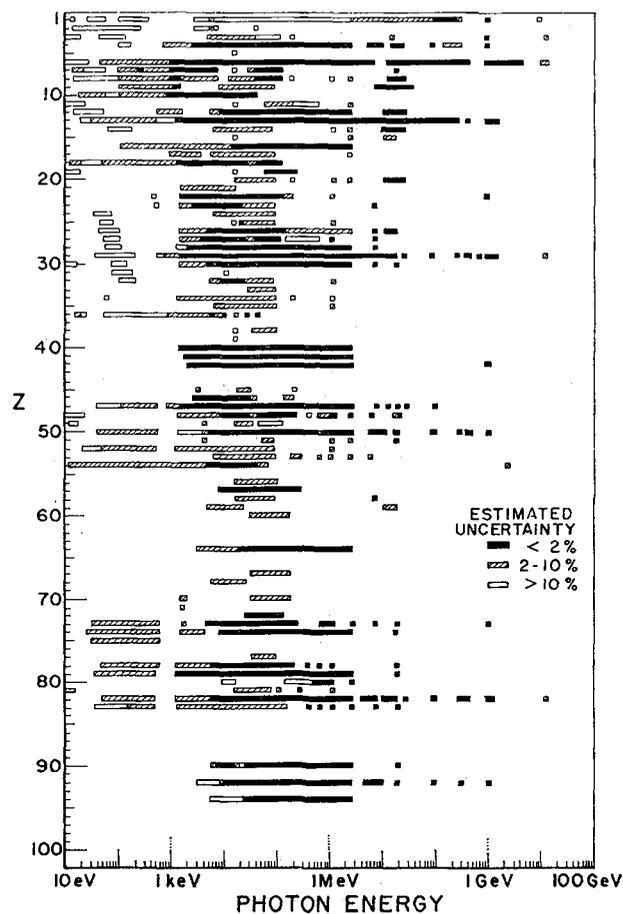


FIG. 2.

Ranges of uncertainty of the cross-section values, either as quoted by the authors or based on compiler experience, are indicated. The blank areas, and the unshaded boxes indicating greater than 10 % uncertainty, point out areas where further measurements would be useful. Boron ($Z = 5$), for example, has only a single worse-than-10 % measurement at 17.5 keV, and cesium ($Z = 55$) as yet has no data in the NBS file. Hydrogen, although « *well-known* » theoretically, is a particularly bad case experimentally because of large effects of trace-amount high- Z impurities on the measurements.

V. Present U. S. compilations : comparison with experiment. — These uncertainties lead to differences between independent compilations, as is shown in figure 3 for hydrogen. The solid curve is the LRL-NBS 1 keV-1 MeV compilation [McMaster *et al.*, 1969], which relies almost exclusively on theory for this element. The upper dashed curve is the Kaman Nuclear 0.1 keV-1 MeV compilation [Veigele *et al.*,

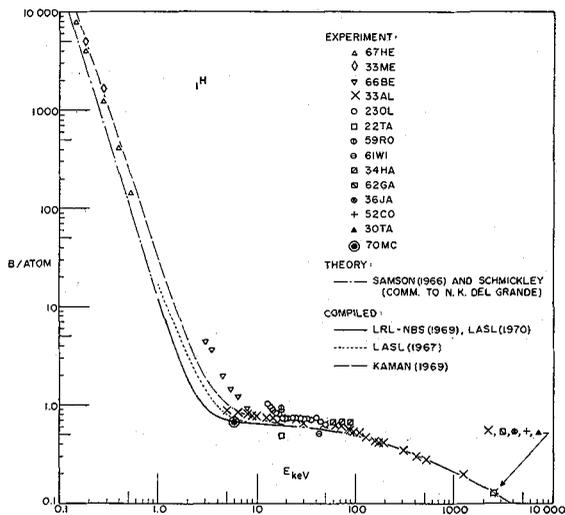


FIG. 3.

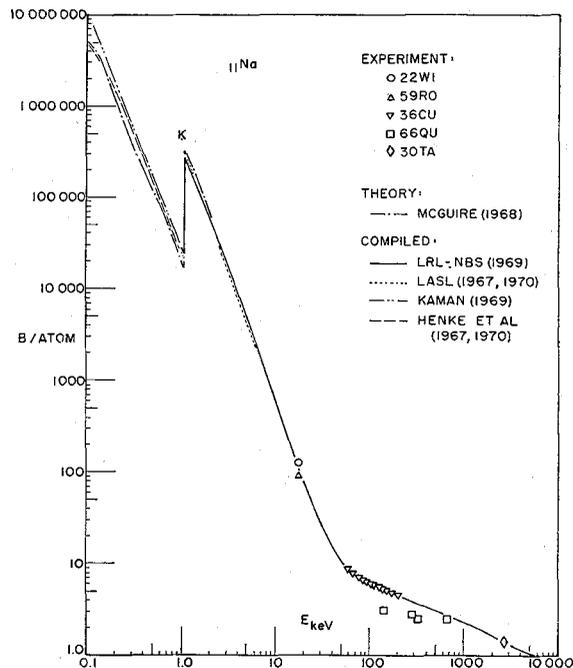


FIG. 4.

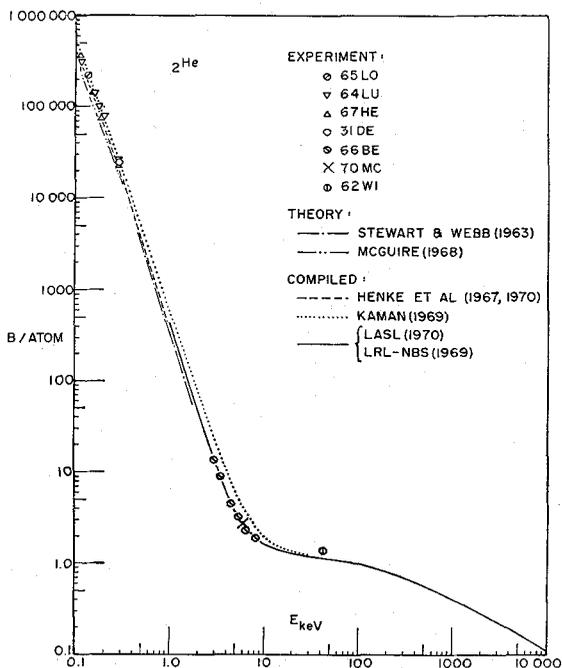


FIG. 3 a.

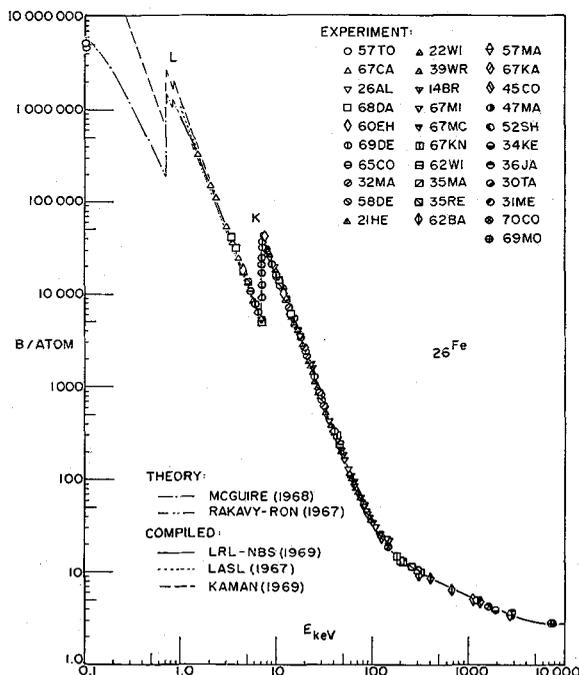


FIG. 5.

1969] which has avoided the use of theory. The intermediate dotted curve is the LASL 1 keV-100 MeV compilation [Storm and Israel, 1967] which in the latest revision [Storm and Israel, 1970] is identical with LRL-NBS in this region.

The only data-point between 100 eV and 100 keV in agreement with theory is that of McCrary *et al.* [1970] at 6 keV. Further high-precision measurements, particularly at around 1 keV, would lessen the divergence of subsequent compilations.

Figure 4 for sodium mainly shows that recency is not necessarily an index of accuracy. Also the need for cross-Z interpolation or theoretical guidance is shown here for the sodium K-edge region.

In figure 5 for iron we see that both theory and experiment are adequate above 1.5 keV, but further

measurements in this vicinity of 1 keV and just below would be useful for extending compilations below the L-edges.

In figure 6 for uranium we have no theoretical results on which to base a compilation extension below 1 keV, since the McGuire [1968] extensive numerical results extend only up to $Z = 54$. Except for the Allen [1926] data, which typically « bend over » at the lowest energies, the available experimental data are consistent with Rakavy-Ron theory to within ~ 10 -

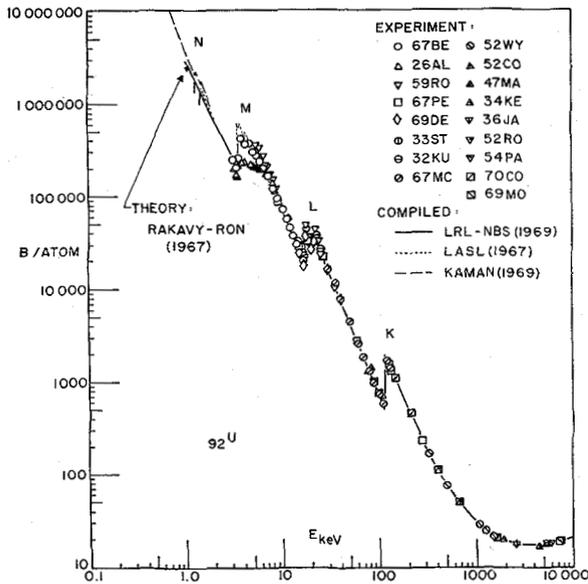


FIG. 6.

15 % from 3 to 10 keV and to within ~ 5 % from 10 to 20 keV. Above 20 keV the various theoretical and experimental data points are generally consistent within ~ 2 %.

VI. Z-Interpolation. — Since reliable cross section measurements for some elements of technical interest are non-existent or over a limited energy range, and coverage by realistic theoretical photoeffect values is incomplete, some form of Z-interpolation is generally necessary for constructing a useful compilation. Smoothness as a function of Z can be safely assumed for each atomic cross section in certain energy regions, but in other regions some structure as a function of Z may be found. In figure 7, Rau and Fano [1968] have suggested that irregularities, if any, would be most likely found in the vicinity of rare gases and

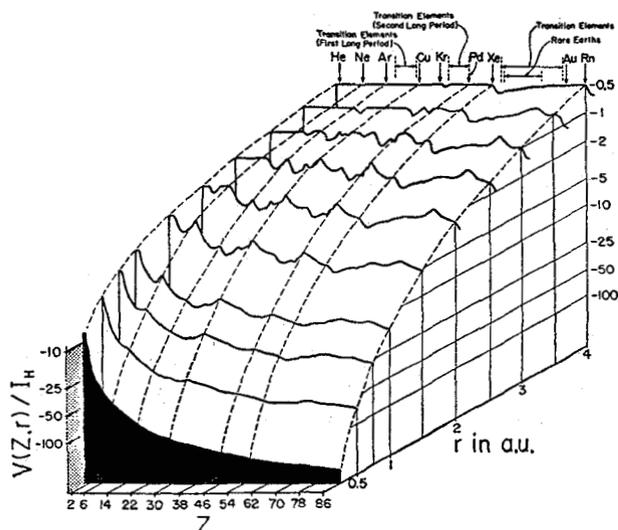


FIG. 7.

noble metals (Cu, Pd, Au) and for energies of about 1-3 keV.

Experimental evidence for these discontinuities is thus far inconclusive, but, as shown in figure 8, Compton scattering total cross sections calculated using Cromer-Mann [1967] incoherent scattering factors predict just such a behavior at 1 keV.

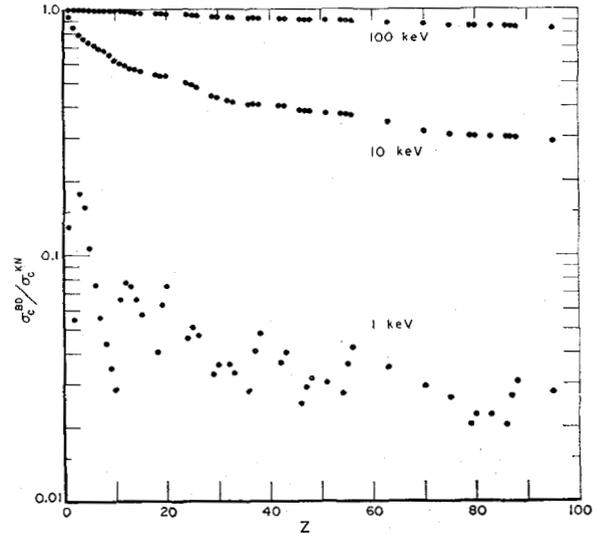


FIG. 8.

Such Compton scattering calculations, as shown in figure 9, however, cannot be taken fully seriously until the question of backward-direction enhancement is resolved. For thallium (Z = 81) at 120 keV the results of Dowe [1965] suggest that this enhancement completely compensates for the forward-direction decrease, leaving a total Compton cross section just equal to that predicted by [the Klein-Nishina formula. No comparable experiments have been done in the neighborhood of 1 keV where the Z-structure effects are predicted.

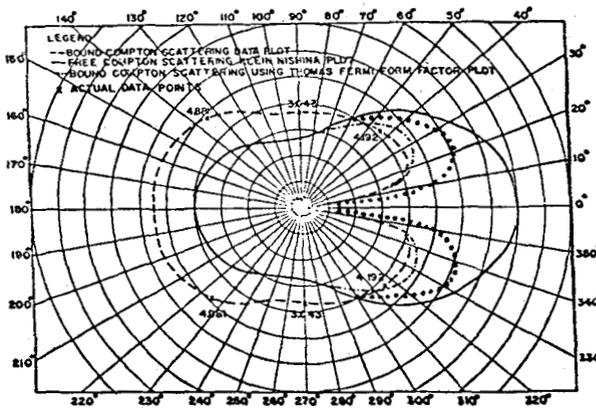


FIG. 9.

For the photoeffect, experimental data have not as yet disclosed any marked anomalies as a function of Z other than at the absorption edges. In McGuire's [1968] theoretical results Z = 2-54 at 10 keV a pro-

nounced structure rising 50 % above a smooth Z-curve was seen in the neighborhood Sr-Zr. However, available Zr experimental data do not depart significantly from a smooth Z-curve.

Pratt [1970] now has made theoretical estimates that such effects are confined to the regions immediately above absorption edges : within 100 eV above a 1 keV edge, 400 eV above a 10 keV edge, and 15 keV above a 100 keV edge. These estimates are based on arguments consistent with the theoretical results of Rau and Fano [1968] and Manson and Cooper [1968].

VII. Absorption edges and fine structure. — The Rakavy and Ron [1967] photoeffect calculations and similar subsequent results by Brysk and Zerby [1968] and others have materially aided in the analysis of data in the absorption edge regions. Figure 10 for

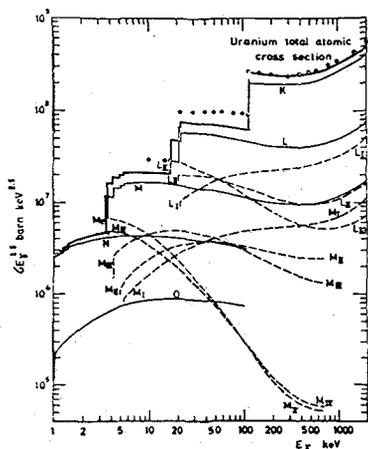


FIG. 10.

uranium clearly shows the subshell magnitudes, including the cross-over of the L_{I} and L_{II} contributions, and similar reversal of the various M subshells. The dots are from an older compilation. Present compilations and experimental data are generally within 2 % of these theoretical values.

Figure 11 for aluminium, also from Rakavy and

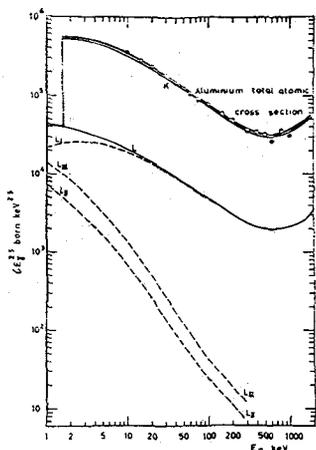


FIG. 11.

Ron, again shows the tendency for the L_{III} to dominate near threshold but L_{I} to comprise the bulk of the L -shell cross section at higher energies. Since cross-Z interpolation is best performed on individual subshells, such detailed calculations have been very useful.

If one looks very close to an absorption edge with a high-resolution detector, as in figure 12 for the K-

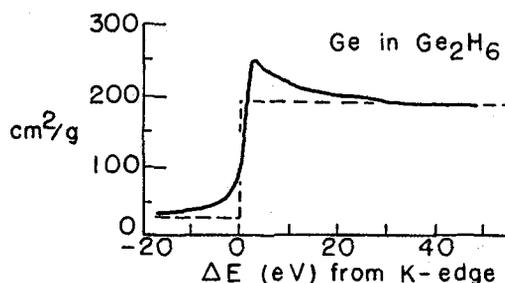


FIG. 12 a.

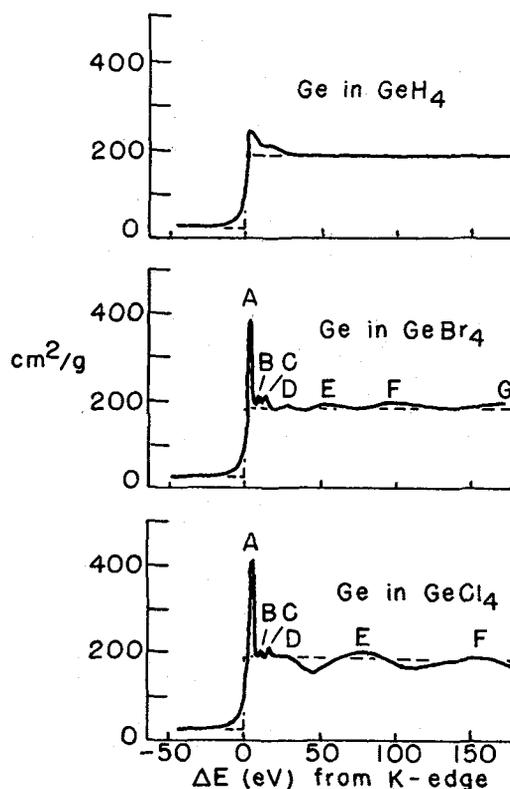


FIG. 12 b.

edge of germanium [Glaser, 1951], one finds fine-structure which casts doubt on the usefulness of the « jump ratio » concept, or indeed the compilation values given for the high-energy side of an absorption edge. Not only does one expect this structure to vary irregularly from Z to Z , but it here clearly depends on the atomic environment, and can also depend on temperature.

Such effects are not confined to solids, but can be also seen in diatomic gases, such as chlorine in figure 13

[Stephenson *et al.*, 1951] and in a monatomic gas argon in figure 14 [Parratt, 1939].

The absorption edges must somehow be taken into account in constructing a compilation. However, they

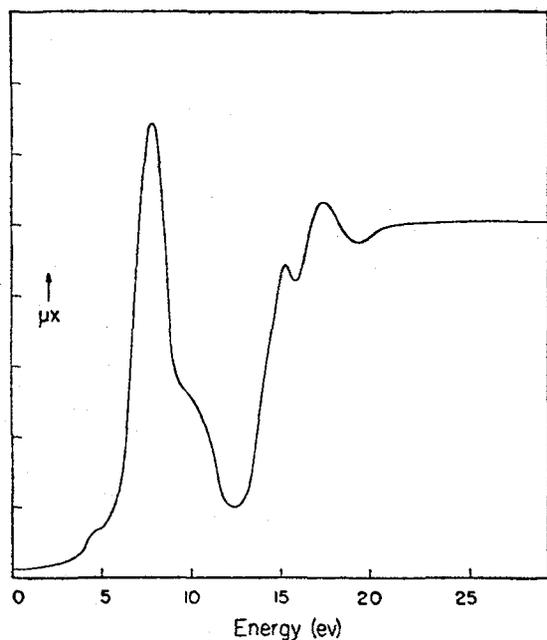


FIG. 13.

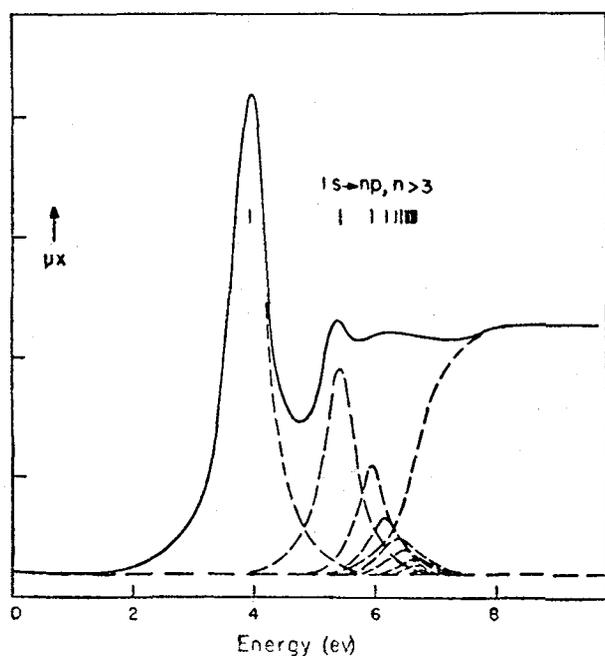


FIG. 14.

clearly do not serve as very stable anchor points. In the LRL-NBS compilation, high-resolution data in the structure region were omitted from the compilation input.

VIII. Asymptotes in time. — Finally, figure 15 provides some idea of the progress in measurements from the time of Röntgen up to the present. These

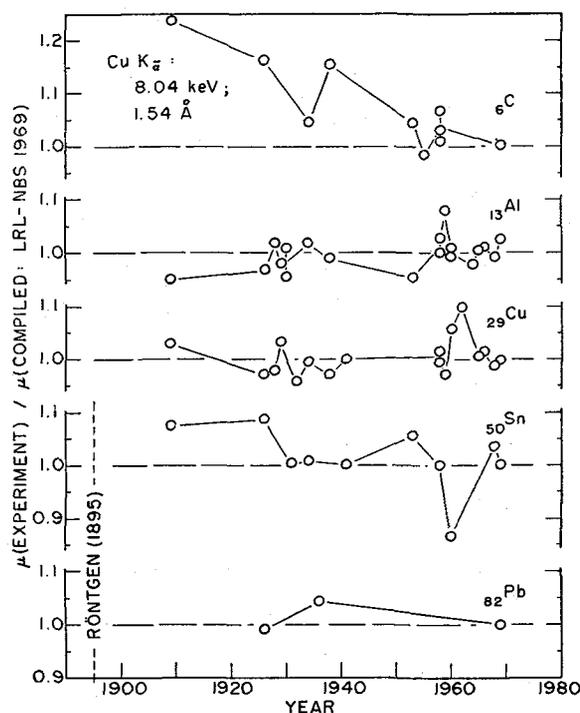


FIG. 15.

ratios are measurements for Cu K_{α} X-rays in the five substances shown, divided by values interpolated from the LRL-NBS compilation to this energy. Although some convergence is suggested, it is again apparent that recency is no guarantee of accuracy. We would like to believe that here, as for other elements and energies, each LRL-NBS compilation value represents a reasonable asymptote to such a progression. There are still regions, as was shown in figure 2, where data are non-existent or insufficient to establish such trends.

IX. Availability. — The recent compilations described or mentioned above are available in report form or on tape as indicated in the references.

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