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Experimental cross sections for L-shell x-ray production and ionization by protons

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HIGHLIGHTS

- An updated database is presented, increasing by 94% the earlier pre-1993 database.
- The update has 40% more data from the pre-1993 period, absent in prior compilations.
- The growth and possible saturation in the number of data is illustrated.
- Ionization cross sections are reconverted to x-ray production cross sections.
- Elements and ion energies are identified where measurements are still necessary.

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ABSTRACT

Tables of compiled cross sections list data for production of individual line and total L x-rays as well as for ionization of L subshells and the total L shell. The present cumulative compilation covers some six decades of measurements on targets from $_{10}$Ne to $_{95}$Am bombarded by protons ranging from 10 keV to 1 GeV. It includes data published in the period 1954–1992 from tables published in this journal, cross sections that were not reported in those tables, and new data from works published after 1992. Existing empirical, semiempirical, and theoretical analyses based on, and relative to, the pre-1993 database are reviewed. The experimental details are summarized for pre-1993 articles that were not referenced in previous compilations and, continuing the practice of these compilations, for each new publication. Covering the period 1954–December 2012, the present tabulation collects (not counting 2519 new data for $L_{\beta 1,3,4}$, $L_{\beta 2,15}$, $L_{\gamma 1}$, $L_{\gamma 2,3}$, and $L_{\gamma 4,4'}$ x ray production) circa 15 500 experimental cross sections and enlarges the database from the previously published tables by 94%.

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Contents

1. Introduction

A comprehensive collection of experimental cross sections that incorporates the past database [1–3] solidifies the ground for testing of inner-shell ionization theories and their utility for quantitative understanding of x-ray production. Reliable inner-shell ionization cross sections by protons and heavier ions provide detailed and better input for track structure calculations [4]. Compiled cross sections obtained with proton bombardment scale as Z_1^2 to cross sections by bare ions of heavier atoms with atomic number Z_1. Such data are utilized in fields ranging from astrophysics for charge-balance calculations and interpretation of x-ray line formation [5] to the Monte Carlo simulation of secondary electrons (delta rays) in lithography [6] and charged-particle dose evaluation and track studies in DNA [7]. Inner-shell ionization contributes to the background in measurements of the e^+e^- pair production cross sections [8]. As could be estimated theoretically (see Fig. 1(c) in Ref. [9]), for radiation dosimetry with 1 MeV to 2.5 MeV proton beams L-shell ionization dominates x-ray production in $_{28}$Ni [10]. An adequate description of inter-atomic Auger processes during charged-particle penetration through solid targets involves L-shell vacancies [11]. Among beam characterization methods [12], inner-shell ionization is exploited with particle-induced x-ray emission (PIXE) analyses [13–17] resting on reliable theoretical predictions that must ultimately be verified by a plethora of measurements over a wide area of target elements and proton energies. This is discussed with the development of PIXE simulations in general-purpose Monte Carlo code Geant4 [18,19]. Experimental K x-ray production in ionization by protons have been tabulated [20,21] in 1989. With a mere 13% increase over a 15-year period as found in Ref. [22], the continued slow growth in publication of K-shell x-ray production cross sections allows that the "reference" ionization cross sections of Paul [21] from nearly a quarter of centuary ago may still be used for analyses of K x-ray cross sections [18,19,23,24].

Although many efforts have been focused to improve on various theories other than the plane wave Born approximation (PWBA) [25], such as the semiclassical approximation [26], binary encounter approximation (BEA) [27], local plasma approximation [28], continuum-distorted wave [29], atomic orbital coupled-state [30] or classical trajectory Monte Carlo theories [31], to describe the ionization process by ion impact, the most widely known and utilized is the ECPSSR theory [23]. It goes beyond the standard PWBA [25] to account for the energy loss and Coulomb deflection of the projectile and for the perturbed stationary state and relativistic nature of the inner-shell electron [23]. Refs. 13 to 21 in Ref. [22] list stand-alone PIXE softwares that employ that theory. To improve its predictions, following the Sarkadi and Mukoyama [32] united-atom approach and its refinements by the group at the University of Naples [33], ECPSSR evolved into the energy loss, Coulomb deflection of the projectile, united and separated atom, relativistic (ECUSAR) theory [34]. While, as it is reviewed in the next section, experimental L-shell cross sections compiled previously [1–3] have often been compared with the results of the ECPSSR theory or its modifications, the presently compiled data are not compared with any theory.

2. Empirical, semiempirical, and theoretical analyses of L-shell cross sections based on pre-1993 databases

As for the K-shell data evaluation, to utilize L-shell cross sections for analytical purposes, the existing databases [1–3] were fitted to empirical [35–37] or, with normalization to the ECPSSR cross sections [23], semiempirical formulae [38–44]. They were in part [43] limited to only the L_α ($L_3 - M_4 + L_3 - M_5$) x-ray line that is the most intense and for which x-ray production cross section has been most frequently measured. Assigning equal weights to these formulae [35–43], Lapicki [45] took their average as an empirical formula for L_α x-ray production cross sections to test the predictions of the ECPSSR theory [23] and its various modifications.

The most comprehensive work hitherto about the status of theories for L-shell ionization by protons was published in Refs. [34,45]. The ECPSSR theory [23] remains the first choice for a wide range of energies while its modifications [34,45] were shown to work better within some energies and Z_2 ranges [19]. Pia et al. [18] analyzed empirical [35,37] and semiempirical [38] fits as well theoretical results of the ECPSSR [23] and ECUSAR [34] for L-subshell ionization against the databases from Refs. [2,3]. Compared with the best overall ECUSAR theory, they found the semiempirical fits of Orlic et al. [38] – considered in an earlier development of Geant4 [46] – could be rejected at 99% level of confidence while the empirical fits of Miyagawa et al. [35] were deemed agreeable at an almost 95% level of confidence. Although empirical fits of Sow et al. [37] and ECPSSR results [23] appeared statistically equivalent to those of ECUSAR [34], Pia et al. [18] found the ECUSAR theory to be the most accurate option for L-shell ionization cross sections (ICS). A validation of K-, L-, and M-shell calculations, implemented in Geant4 for simulation of proton tracks in the 0.05 MeV to 100 MeV range, through their comparison with L-shell measurements taken from a single reference for just one target element over a limited 0.05 MeV to 2.0 MeV range of proton energies with a statement that "the agreement with all