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X-RAY EMISSION FROM HIGHLY STRIPPED ATOMIC IONS

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X-ray emission from multicharged atomic ions is a process of importance in high temperature plasma studies, solar physics, astrophysics, beam-foil spectroscopy, ion-source diagnostics and in methodical studies of heavy ions inserted in a ring of electrons in a collective heavy ion electron ring accelerator. For modelling the dynamics of highly ionized atomic states, the excitation cross sections, depending on the degree of outer-shell ionization, must be known (with regard to photoionization cf.[1]). X-ray emission contains information on the vacancy configuration both in the energy sites of X-ray lines and in the relative intensities, and it should therefore be a powerful tool in the degree of ionization.

In this paper we give shifts of some lead X-ray lines (K_{α_1}, K_{β_1}, L_{β_1}) and intensity information (total radiative K-shell transition rate Γ_K and K_β/K_α intensity ratio) depending on outer-shell ionization. Furthermore, we discuss the influence of the atomic model employed on these quantities. Comparing these lead data with earlier results (xenon[2], uranium[3]), one can generalize the conclusions derived. The X-ray emission energies were calculated using relativistic atomic models, a DF computer code[4] and a DFS program[5]. The K_{α_1} and K_{β_1} transition energies resulting from different types of calculations are given in the table as an illustra-

Table

Comparison between experimental[6] and calculated K_{α_1} and K_{β_1} transition energies (in eV). The lower theoretical values are corrected for those relativistic effects which are not included in the original computer codes (cf. text)

	exp.[6]	$DF_{adiab.}$	DF_{sudden}	$DFS_{adiab.}$	X_α-TS	$DFS_{bind.en.}$
K_{α_1}	74969.4	75102.3	75397.5	75523.0	75525.0	75462.4
		74934.0	75229.3	74998.9	75001.0	74938.6
K_{β_1}	84936.0	85081.5	85443.3	85516.2	85520.2	85469.5
		84923.1	85284.9	84970.1	84974.1	84923.4

tion of the more general situation. In view of the large nuclear charge involved relativistic effects in the atomic structure (for a survey see ref./7/) are expected to be large, and even higher-order terms ought to be included into consideration before comparing the theoretical values with each other and with experiment. Using the data of paper /8/, the DF values were corrected for the self-energy shifts and for vacuum polarization, and additionally the DFS values for the retardation energy and for the magnetic interaction energy. Due to its less attractive potential, the finite-size nucleus considerably decreases the KX-ray energies (by about 65 eV). An inspection of the corrected values quoted in the table proves that a good quality of adiabatic DF values of X-ray energies is also attainable in adiabatic DFS calculations which can be substituted by the X_α transition state calculations X_α-TS /9/ (exchange parameter α chosen in our calculations was 2/3). One can reduce the computational effort by using the DFS binding energies instead of the energy eigenvalues, since such an approach approximately accounts for the invalidity of Koopmans theorem in a local-potential model.

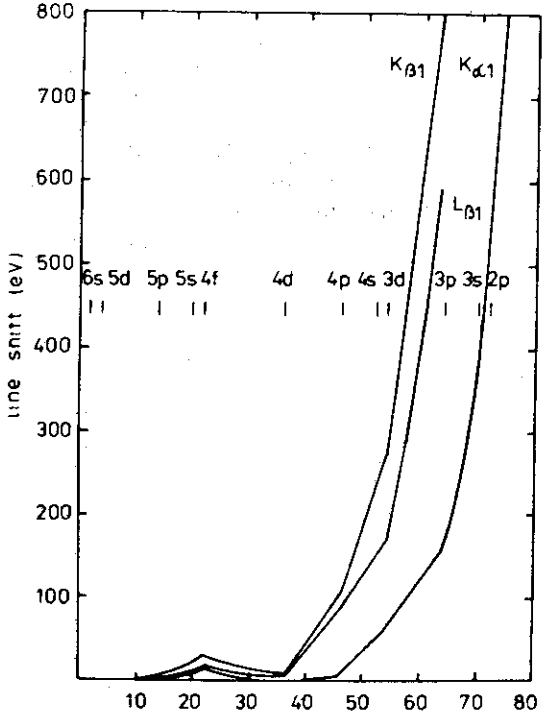

Fig. 1. K_{α_1}, K_{β_1} and L_{β_1} line shifts for lead depending on the degree of outer-shell ionization.

The X-ray shifts in fig.1 do not increase with outer-shell ionization in a monotonous fashion. For deriving the lower ionization degrees, one must couple X-ray shifts with independent physical information on the ionization stage. The correlations shown in fig.1 were obtained from adiabatic DF calculations and can be reproduced with insignificant deviations by all local calculations (adiabatic, transition-state and those based on binding energies) containing adiabatic features.

The nonmonotonous shift-ionization correlation in fig.1 is connected with the removal of d and f electrons. These electrons reveal a small core penetration but a strong screening of the outer s and p electrons which contract with no d and f electrons. Particularly this net effect of increased core penetration is not correctly reflected in a frozen-orbital treatment, and the resulting deviations from the adiabatic results can lead to discrepancies of 2-3 in the ionization stage derived from the calculated X-ray shifts.

The discussion of the X-ray intensities is based on our own computer code by means of which the radiative-transition matrix elements in the Scofield prescription /10/ are integrated using DF electron wave-functions. In this treatment all multipole orders of the radiation field, the retardation and the effect of the finite-size nucleus are accounted for. Since our attention is focussed on a systematic study of the X-ray intensities depending on outer ionization, separate calculations of the initial and final states have not been carried out so far. The graphical presentation of the radiative transition rates in fig.2 disloses remarked contributions

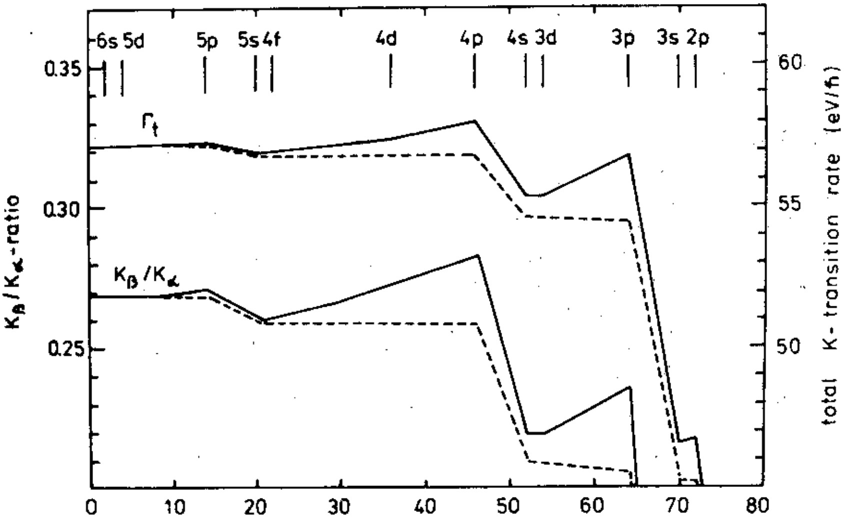

Fig.2. Total K-transition rate Γ_t and K_β/K_α intensity ratio for lead as a function of outer-shell ionization (The dashed lines give the results of a purely statistical scaling /11/; these subshells losing electrons in the course of continuous ionization are indicated above).

stemming from the reorganization of the atom after ionization. These reorganization effects are proved by the deviation of the DF results from the statistical scaling /11/ and occur, to a large extent, in the course of d and f electron ionization since these electrons only slightly contribute to the radiative deexcitation but strongly screen the p electrons which are of greater relevance to K X-ray emission. This adiabatic reorganization manifests itself much remarkably in the individual emission strength than in quantities of a more integral character such as the total K-shell emission rate Γ_K (cf. fig.2). Note that the inclusion of the electron exchange in the consideration of the radiative deexcitation /12/ will emphasize the reorganization effects still more slightly.

In the diagnostics of ionization stages of highly stripped atoms the fluorescence yields are of major importance. Nonradiative deexcitation processes should experience the outer ionizations. Therefore such systematic studies of the influence of outer- shell ionization on the nonradiative deexcitation are being extended.

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