INTERPRETATION OF QUASIMOLECULAR L X-RAYS IN HEAVY-ION COLLISIONS*

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Using a relativistic selfconsistent correlation diagram a first interpretation of the shape and position of L MO X-rays is given within a quasi-adiabatic model.

During the past few years the observation of non-characteristic molecular (MO) X-rays in heavy ion-atom collisions became a field of increasing interest [1–4]. These X-rays are interpreted as radiative transitions between the time dependent quasi-molecular orbitals built up during the close approach of the two nuclei.

The experimentally observed spectrum so far is an integration over all relative distances and impact parameters. Of particular interest is the M and L non-characteristic radiation. The observed spectra show a pronounced shoulder (or peak) behaviour thus reflecting a great amount of specific information about the collision process [2–4]. The K MO X-rays on the contrary are all exponentially decreasing continua [3, 4].

In a recent paper [5] we gave a detailed interpretation of the structure and threshold behaviour of the M MO X-rays observed in systems like I–Au. Also the threshold behaviour of the L X-rays of Au has been explained. The interpretation was based on a molecular correlation diagram calculated with a recently developed relativistic Dirac-Slater molecular program [6]. This type of calculation is the most realistic one, because: first the large influence of the electron-electron interaction is fully taken into account, second the relativistic effects (mainly spin-orbit splitting) are large and third, due to selfconsistent effects, the level

behaviour for intermediate distances is very different as compared with all other approximations [7].

We report in the present work the first interpretation of a L MO X-ray structure exemplified for the Xe–Ag system. Such a calculation is a consistency check for the method of interpretation given in ref. [5] because the main contributions of the M and L MO's are explained through different transitions and at different radial distances in the correlation diagrams. The same argument holds true for the connection to specific characteristic X-ray lines. Fig. 1 shows the correlation diagram for the Xe–Ag system taking 58 electrons into account. The transitions relevant for the description of the L MO spectrum in this case are those into the 3σ to 6σ levels as well as the 1π level (see fig. 1).

Taking this correlation diagram we have extracted all possible transitions within a broad energetic window where the non-characteristic radiation occurs. The spectrum was calculated by an analytical integration over all impact parameters and a numerical integration over the internuclear distance R as described in the earlier paper [5]. A collision broadening proportional to the slope of the transition energy as a function of R within a Gaussian line shape and a cubic dependence of the transition probabilities on the transition energy were assumed. Of course, the calculation of the occupation numbers as function of R and impact parameter can clearly be performed only by time dependent relativis-
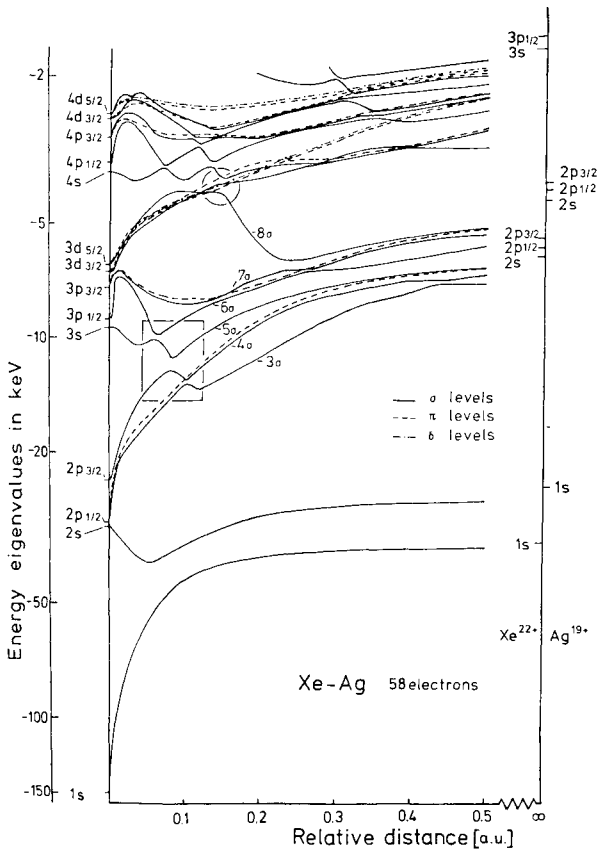
Fig. 1. Selfconsistent relativistic correlation diagram of the system Xe−Ag including 58 electrons. The relevant levels for the MO X-rays are the $3\sigma-6\sigma$ and 1π levels. Through the encircled crossing the characteristic Ag L X-rays at low impact energies are fed. The crossings within the square distribute the holes into the L sublevels of Xe.

Fig. 2. Experimental X-ray spectrum for 17 MeV I on Sn compared with the unnormalized theoretical MO spectrum of Xe on Ag.

tic Hartree-Fock calculation which are not available up to now. We therefore assumed here that much more holes will be generated by Coulomb ionization during the first half of the collision process in the $n = 3$ levels of the projectile and the target atoms than in the $n = 2$ levels. A large percentage of the holes in the $n = 3$ levels will be transferred through strong coupling at very small distances into the $n = 2$ levels of the system. The pronounced well separated crossings among the 3σ to 6σ states (shown in the square in fig. 1) allow the use of Landau-Zener type calculations for the occupation numbers as a good approximation. The resulting hole distribution was used in the calculation of the spectrum given in fig. 2. We get an overall
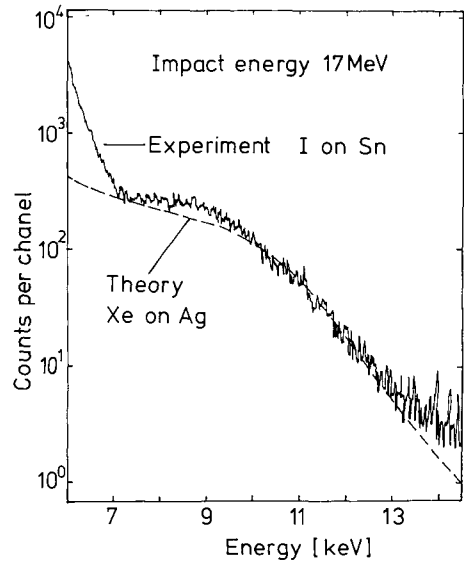
good agreement for the L MO X-rays with the available experimental data.

The quality of the calculation of the hole distribution can be checked in the experiment where the relative L X-rays intensities ratio $(L_1 + L_2)/L_3$ from the M shell of the projectile was measured [8]. Our value yields a ratio of about 0.5 whereas the experiment gives 0.4.

For the impact energies lower than needed to reach the crossings at and below 0.03 au, in the vicinity of the united atom 3d levels (equivalent to approximately 6 MeV projectile energy), a transfer of holes into $n = 2$ levels of the separated atoms should not take place and the L MO X-rays will not be observed anymore. Only the contribution of direct Coulomb ionization of the $n = 2$ levels in the projectile and target may still yield a small contribution to the MO X-rays. On the other hand, due to the strange behaviour of the 8σ level a transfer of holes into the $n = 2$ states of the separated system is still possible down to less than 2 MeV projectile energy where the two nuclei just reach the encircled crossing at 0.16 au. All holes transferred at this crossing will produce characteristic L lines in the lighter atom. The experimental proof of this last prediction will be hard because the projectile energy is already so small that only few electrons will be removed

by direct Coulomb ionization even in the higher levels.

As a conclusion we may say that even by using the integral experimental information of the MO radiation we do learn quite a lot about the complicated system formed during the collision. More details in non-characteristic spectra are expected to be seen in refined coincidence experiments which are under way.

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