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LETTER TO THE EDITOR

Kr–Kr correlation diagram and its use in heavy-ion collisions†

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Abstract. A realistic self-consistent charge correlation diagram calculation of the Kr^{2+}–Kr^{2+} system has been performed. We get excellent agreement for the $4(3/2)_u$ level with an experimentally observed MO level at large distances. Possible reasons for discrepancies between experiment and theory at small distances are discussed.

In a recent paper Gordeev *et al* (1981) and earlier Afrosimov *et al* (1977) discussed the possible experimental evidence that they may have observed, in Auger electron spectroscopy, a specific MO level during heavy-ion Kr–Kr collisions. They extracted the binding energy as a function of internuclear distance R and interpreted this to be the $4p_\pi$ quasimolecular level. This conclusion is based on the two calculations known to date (Eichler *et al* 1976, Nikulin *et al* 1978). Both calculations yield the $4p_\pi$ MO level to be the most probable candidate for the level observed in the experiment, although the comparison between experimental results and calculations is very poor. Both calculations are approximate non-self-consistent non-relativistic calculations which are not too realistic because the $4p_\pi$ level in the Kr–Kr quasimolecule is an outer level already strongly affected by the electron–electron interaction and the specific occupation of the outer molecular states.

We cannot comment on the validity of the experimental analysis but from the theoretical point of view it is very important to have a realistic correlation diagram for this system. We therefore performed a full self-consistent charge relativistic Dirac–Fock–Slater calculation for the Kr^{2+}–Kr^{2+} colliding system. The method is described by Rosén *et al* (1976). The resulting correlation diagram for the levels of interest in this discussion is shown in figure 1.

In the experiment initial holes are in the 4p level of the Kr projectile. Using the relativistic molecular notation these are the levels $11(1/2)_g$, $12(1/2)_g$, $11(1/2)_u$, $12(1/2)_u$ as well as $5(3/2)_g$ and $5(3/2)_u$. All four 1/2 levels connect adiabatically to levels of the united system with main quantum numbers of five and above. If the holes are transferred across four crossings (which is a realistic assumption) the holes in the $12(1/2)_g$ level reach the $8(1/2)_g$ level below 0.1 au and the $12(1/2)_u$ holes come into the $8(1/2)_u$ level below 0.2 au. The diabatic connection of these levels is shown in figure 1. The binding energy of all these levels is not much more than 200 eV for all internuclear distances above 0.2 au. This immediately shows that none of the 1/2 levels can be the reason for the observed quasimolecular level above 0.2 au. The $5(3/2)_g$ level can easily

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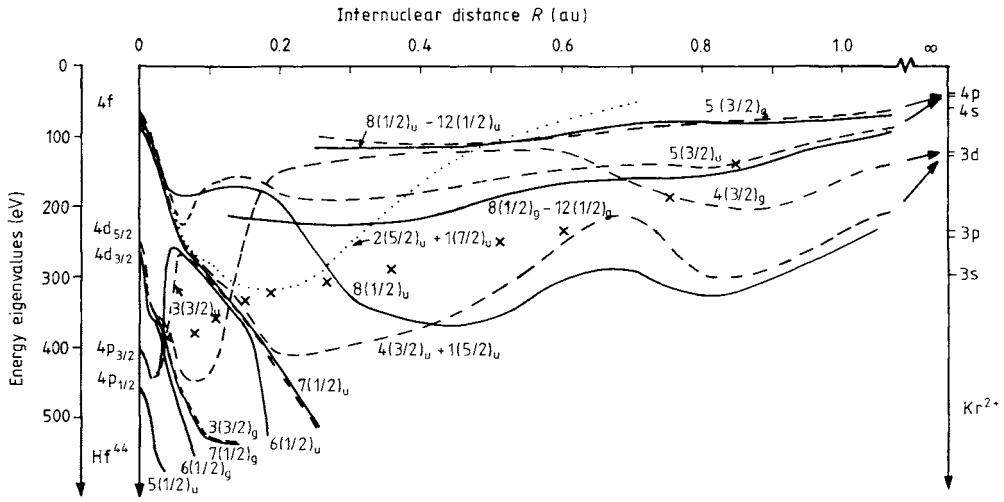

Figure 1. Kr^{2+}–Kr^{2+} correlation diagram calculated with a self-consistent charge relativistic Dirac–Fock–Slater code. Only the levels of interest between 100 and 400 eV binding energy are drawn. ———, (1/2) levels; – – –, (3/2) levels; · · · · ·, (5/2) level. The crosses are the experimental points of Gordeev *et al* (1981).

couple to the $4(3/2)_g$ level near 0.5 au. However again the binding energy of both levels is much too small for the interesting internuclear distances above 0.2 au. The $5(3/2)_u$ level on the other hand has one broad avoided crossing with the $4(3/2)_u$ level between 0.7 and 0.8 au. In this level holes can be transferred down to 400 eV binding energy above $R = 0.2$ au.

The experimental points of Gordeev *et al* (1981) are also included in figure 1. The three outermost points above 0.6 au lie on the $5(3/2)_u$ level and its diabatic connection into the $4(3/2)_u$ level. The experimental points below 0.5 au are parallel to the $4(3/2)_u$ level but systematically too high. Below 0.2 au the situation becomes very complex. At least three levels which carry holes come into play. The $4(3/2)_u$ level which decreases again in binding, the $4(3/2)_g$ level which dramatically gains binding energy below 0.2 au and the $2(5/2)_u$ and $1(7/2)_u$ levels which are completely empty from the beginning of the collision. This demonstrates that the extraction of experimental values below 0.2 au is *not* possible anymore, at least not in the simple way it has been done by Gordeev *et al* (1981).

As a summary we can say that at large distances the agreement between experiment and theory is now very good. It is obvious that the $4(3/2)_u$ level is observed in the experiment. For distances 0.2 to 0.5 au it is not yet clear why the experimental points are about 80 to 90 eV above the theoretical values. The reason for this discrepancy may be that the Auger transitions into the outer empty levels with binding energies around 200 eV sum up to a steeper decrease of the observed electron spectrum thus simulating a smaller binding energy. It has to be borne in mind that only the low-energy part of the electron spectrum is used in the extraction of the experimental points. The observed decrease of the experimental points below 0.2 au may be the result of the strong increase of the binding of the $4(3/2)_g$ level. However, again the increase in the experiment is not as dramatic as in theory because of the possible influence of the three other levels which carry holes near 300 eV binding energy.

Due to these possible contributions from various other levels at small internuclear distances the experiment is not very specific for the observation of one level only. Therefore further, more specific, experiments should be performed.

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