§10. Massive Configuration Interaction in High-Charge Ions

More, R.M., Murakami, I.

Configuration interaction (CI), which occurs when states from two atomic configurations have nearly the same energy and are mixed by the electron-electron interaction, has a strong effect on electron-ion collision cross-sections and on emission line spectra.

On the basis of elementary chemistry one can predict unusual configuration interaction for certain ions. From the periodic table, we know that in neutral atoms the one-electron shells are filled in the order 1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d,... However, energy-levels in most high-charge ions follow the hydrogen-like sequence. For example, nickel-like ions important for x-ray laser experiments have a closed shell ($3d^{10}$) ground-state configuration, unlike neutral nickel.

These well-known facts imply there must be special ions for which one-electron levels are nearly equal. The inversion of 5p, 4f levels for neutral Gd means that for some Gd ion, $E_{5p} \sim E_{4f}$. This in turn implies that several configurations have nearly-equal energies. For example, $E_{5p} \sim E_{4f}$ implies

$$E[4f^7] \sim E[4f^6 5p^1] \sim E[4f^5 5p^2] \sim \ldots \quad (1)$$

With term splitting, each of these configurations gives rise to many levels. In this circumstance, many levels from many configurations interact to give an unusually complex atomic structure.

Figure 1 shows calculations including several configurations for gadolinium ions (Z = 64) performed with the HULLAC code.[1-2] As the ion charge varies from Q = 9 to Q = 12, the configurations overlap strongly. CI increases the width of the $4f^6$ configuration by about 15%. For Gd^{10+} the calculations include almost 3000 levels; however inclusion of all the relevant configurations would require inclusion of many more levels. In this ion there are overlapping configurations with thousands of interacting levels, a situation which can be described as "massive configuration-interaction".

We have performed non-relativistic Thomas-Fermi calculations for all 4,186 ions in order to identify ions for which the one-electron energy-levels coincide (Fig. 2). Fig. 2 gives a first guide to the location of "massive CI" ions, but more accurate calculations are needed.

Ions with massive configuration interaction are interesting because these ions have many levels with low excitation energy. Probably these ions have resonance lines in the visible range

Ions with massive configuration interaction define a natural boundary between low-charge and high-charge ions.

REFERENCES:

1.) Bar-Shalom, A., and Klapisch, M., Computer Physics Communications **50**, 375 (1988).

2.) Bar-Shalom, A., Klapisch, M., and Oreg, J., Computer Physics Communications **p**, 21 (1996).

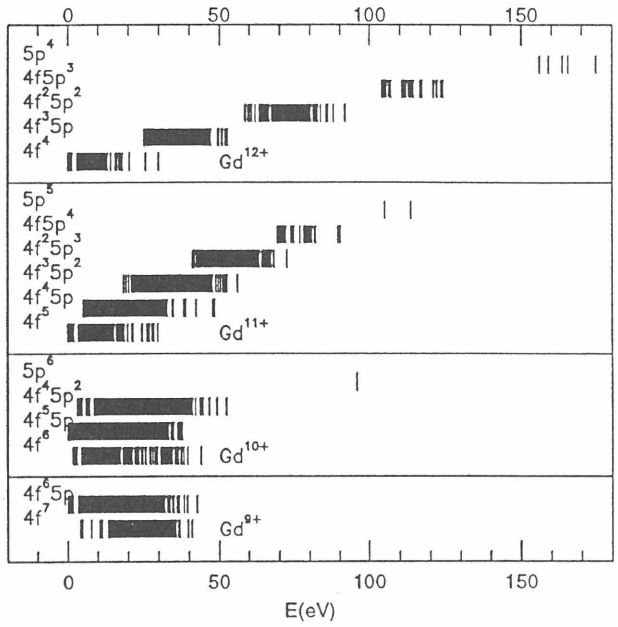

Figure 1. HULLAC calculations for low-lying energy levels of ions of Gd. The abscissa is the excitation energy E in electron volts. The figure shows the approximate equality of 4f and 5p levels for the ions with Q = 9-10.

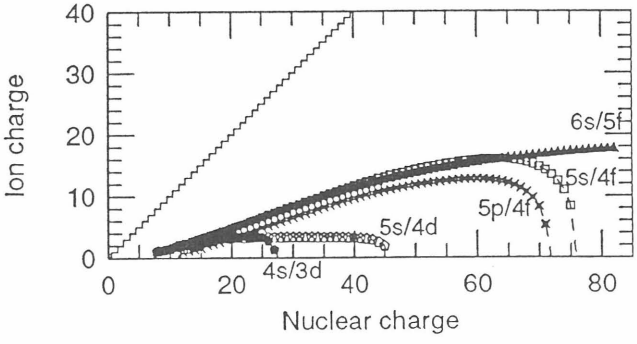

Figure 2. Statistical model calculations for all ions have been analyzed to approximately locate the ions for which the indicated one-electron levels are equal.