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A PROPOSAL FOR IMPROVED IRON PROJECT CALCULATIONS FOR COLLISION STRENGTHS

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Perhaps it bears reminding that in spite of about 1.5 decades of effort we still do not have definitive high-accuracy collision strengths for some of the key ions of astrophysical interest. Not only are the heavy ions of iron group elements not quite within the reach of ongoing calculations, some unexpected problems are encountered even for apparently simply atomic systems. Among the former are old chestnuts like Fe II and Ni II, for which the available results are largely non-relativistic; fine structure is incorporated by algebraic transformation (although limited Breit-Pauli R-matrix calculations have been done). In the latter category are "simple" ions like O II which, as recent calculations show, turn out to be problematic in unexpected ways.

There are two essential and coupled problems: (i) target ion wavefunctions and (ii) relativistic fine structure. Construction of target eigenfunctions using both SUPERSTRUCTURE and CIV3 is not straightforward if $\sim$1% accuracy is desired (the O II target turns out to be very complicated, especially when including the excited even partity levels). Needless to say, the problems are vastly exacerbated in the case of low ionization stages of Fe and Ni, especially when fine structure is considered. The R-matrix II (PRMAT) codes are a huge improvement regarding high-accuracy targets, and enable systematic inclusion of interacting configurations according to one-electron, two-electron excitations. However, thus far R-matrix II calculations have been in LS coupling and carried out only for a few ions. I will discuss some recent results to illustrate the nature of these problems. The talk by Werner Eissner describes the "full" inclusion of Breit-interaction terms in the standard R-matrix codes that should provide a partial solution to the accuracy problem.

We are now beginning to acquire observational data from the new 8m class telescopes with high-resolution spectrographs for many ions. The astronomy needs will increase vastly as nearly a dozen such telescopes come on-line, almost all with unprecedented spectroscopic capabilities. However, to realize even a fraction of the potential afforded by new ground and space observatories, and to make spectroscopy front-and-center of their scientific investigations, high-accuracy collisional and radiative parameters for heavy atomic systems need to be re-visited by the Iron Project group.