

Non-LTE coronal Au plasma simulation in the configuration average approximation

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Abstract

We present the non-LTE calculation for a highly ionized Au plasma using our atomic package YAC to compare experiment recently done at the Livermore electron beam ion trap EBIT-II. The configuration average model explicitly includes all possible opened M-shell configurations from a given configuration group. The needed collisional and radiative rates connecting the included configuration are calculated in the configuration average approximation for population kinetics. Parallel iterative solvers in PETSC are used for the solution of the rate equation.



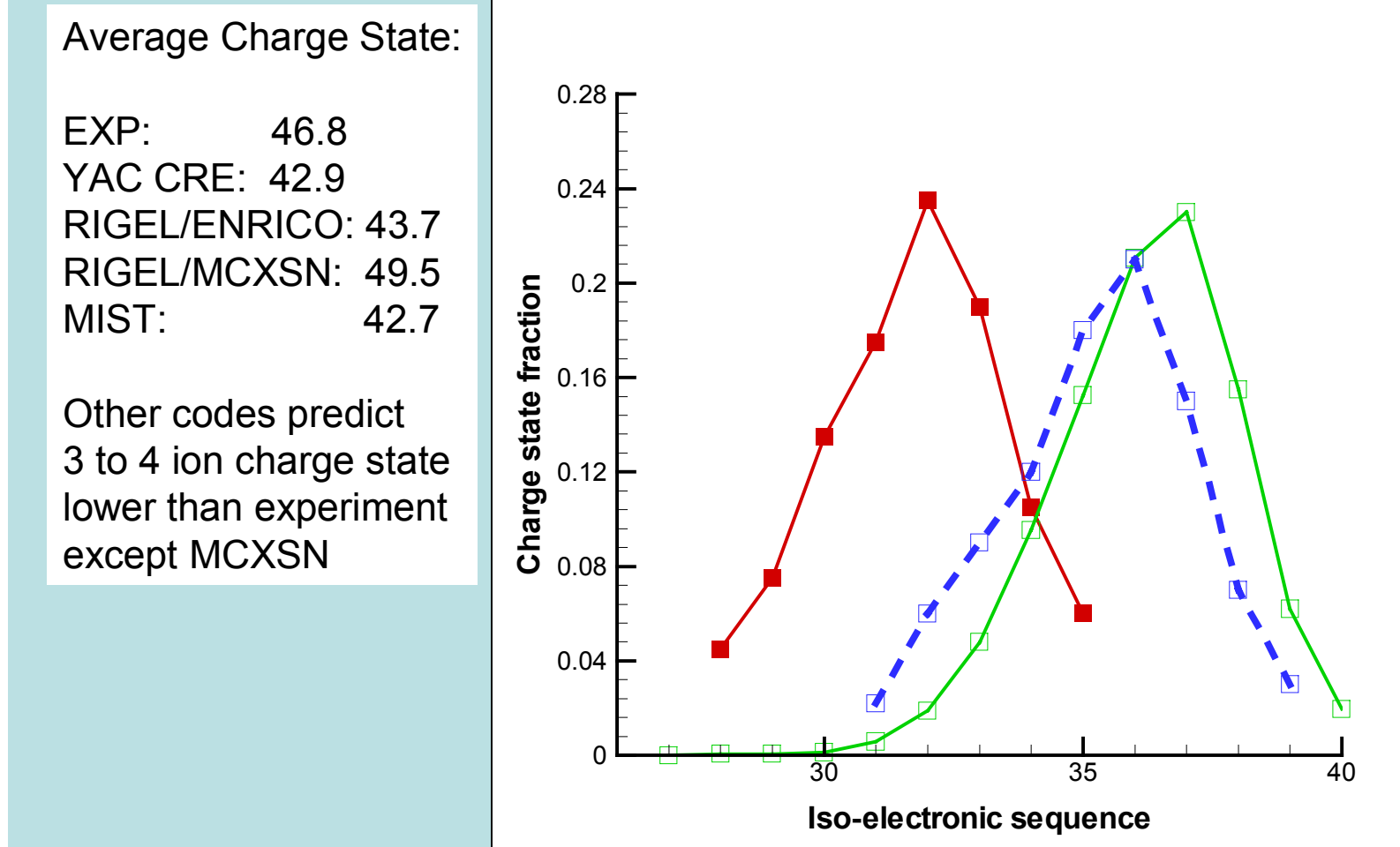
Example of Macro Configuration Input

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<elesys elenum="33">
<cfg group="1*2 2*8 3*18 4*5" />
<cfg group="1*2 2*8 3*18 4*4 (5,6,7,8,9)*1" />
<cfg group="1*2 2*8 3*18 4*3 5*2" />
<cfg group="1*2 2*8 3*18 4*3 5*1 (6,7,8,9)*1" />
<cfg group="1*2 2*8 3*18 4*2 5*3" />
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<cfg group="1*2 2*8 3*17 4*5 (5,6,7,8,9)*1" />
<cfg group="1*2 2*8 3*17 4*4 5*2" />
</elesys>
```

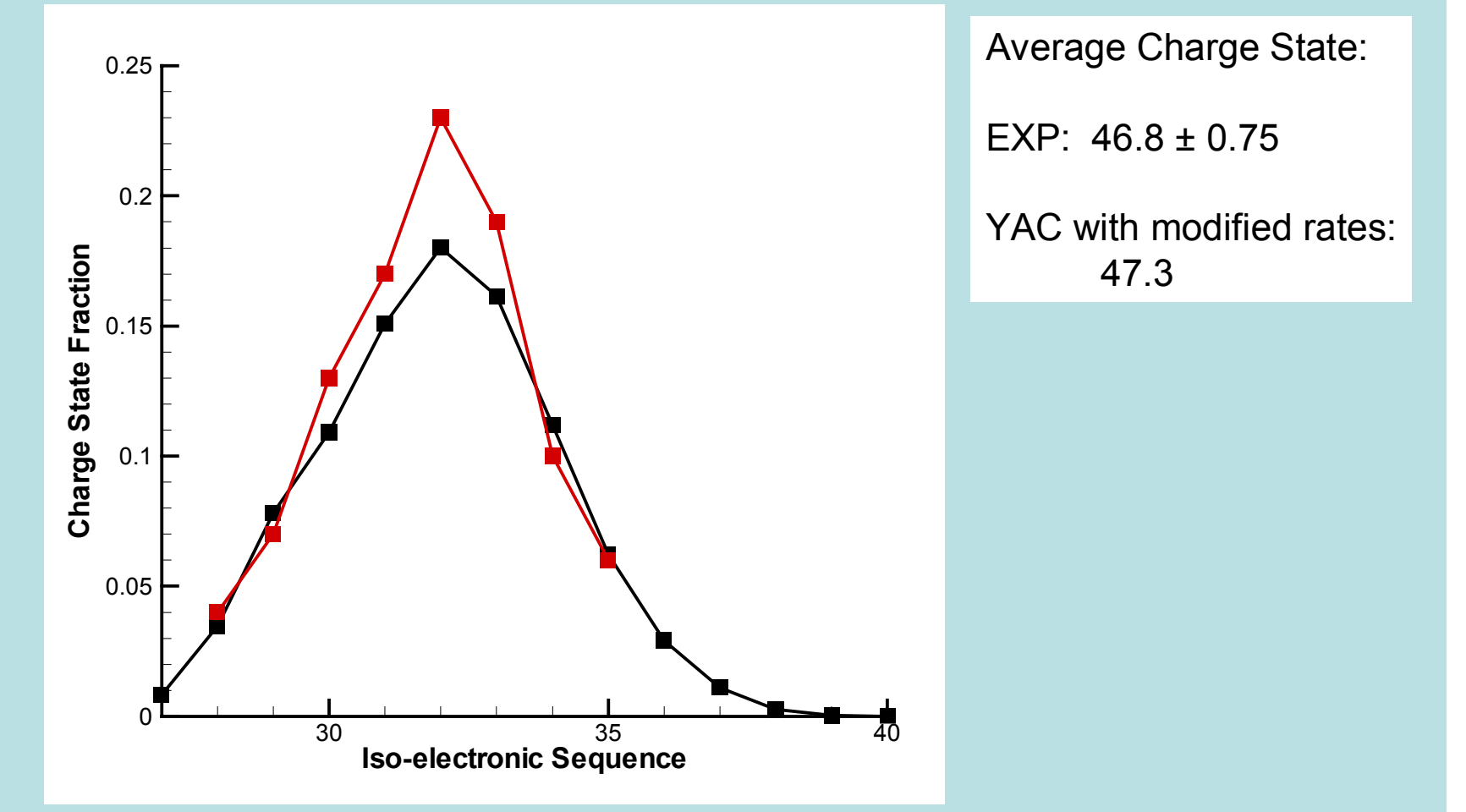
[4*5 means 5 electrons distributed among n=4]



Compare Charge State Distribution With Exp.



Charge State Distribution With Modified Rates

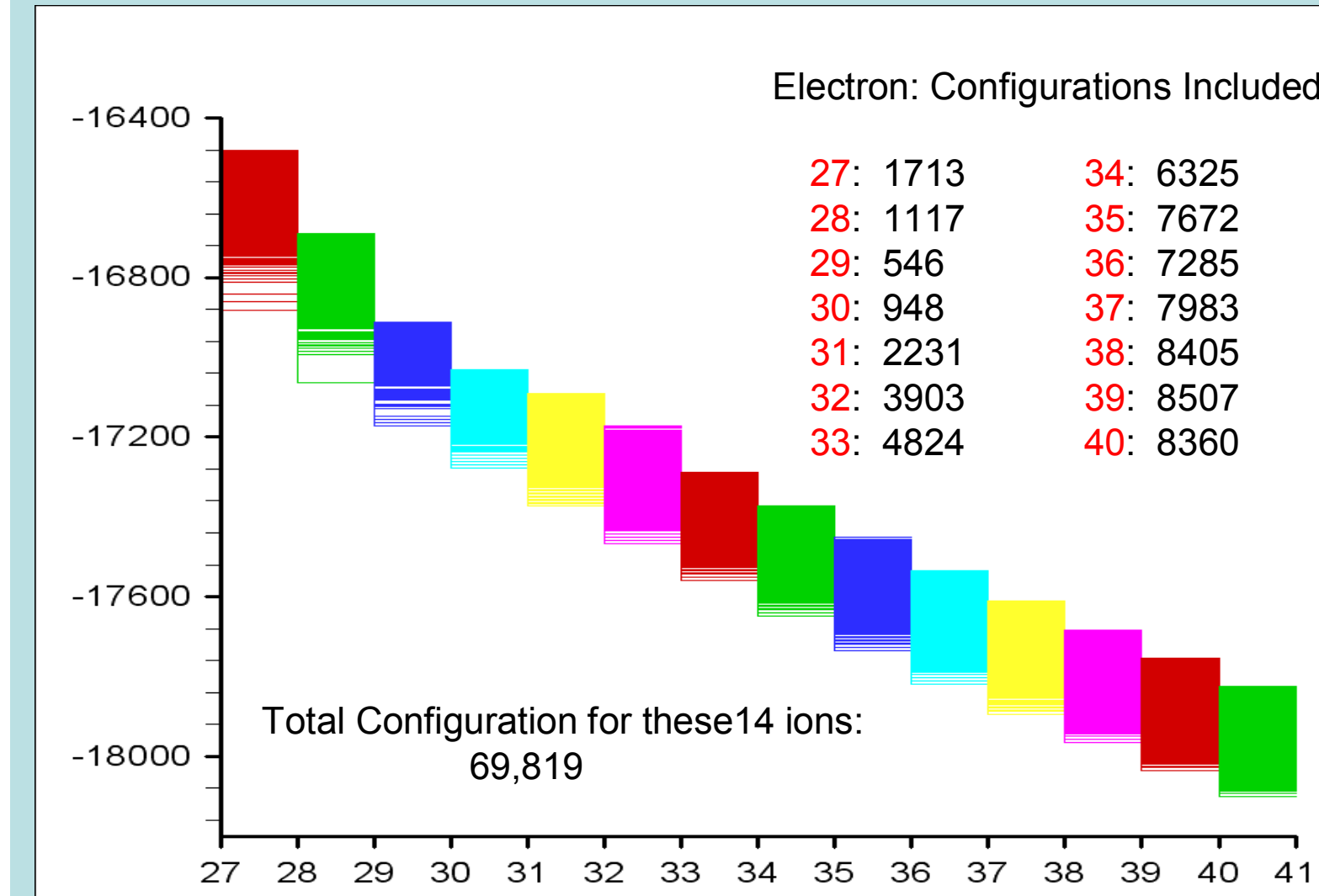


Overview

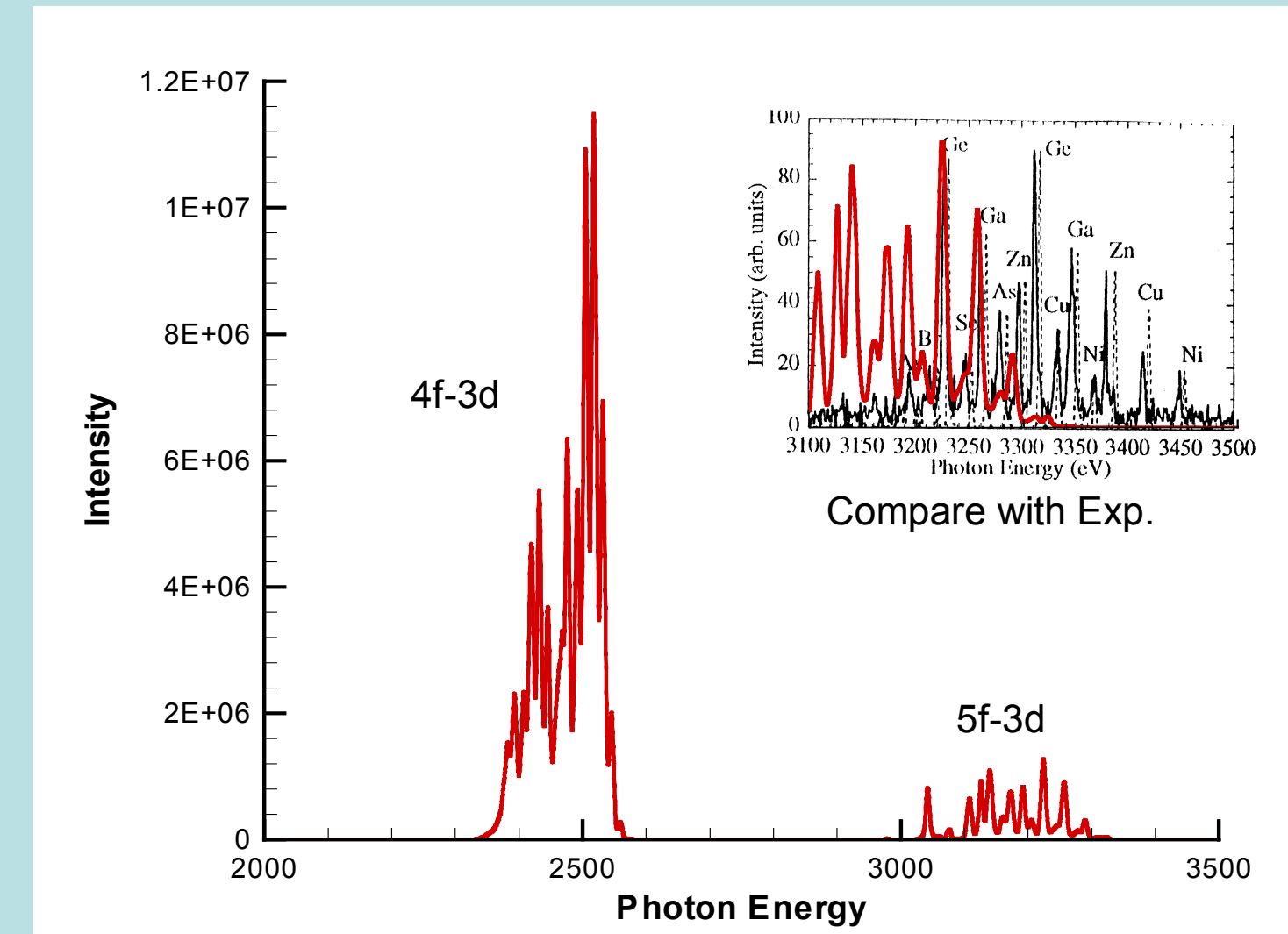
- I. Introduction of YAC code package
- II. Simulation of Non-LTE Au emission spectrum
 - 1) Configuration definition
 - 2) Comparison with other calculations
 - 3) Application to spectrum analysis
 - 4) Graphical user interface
- III. Summary and Future work



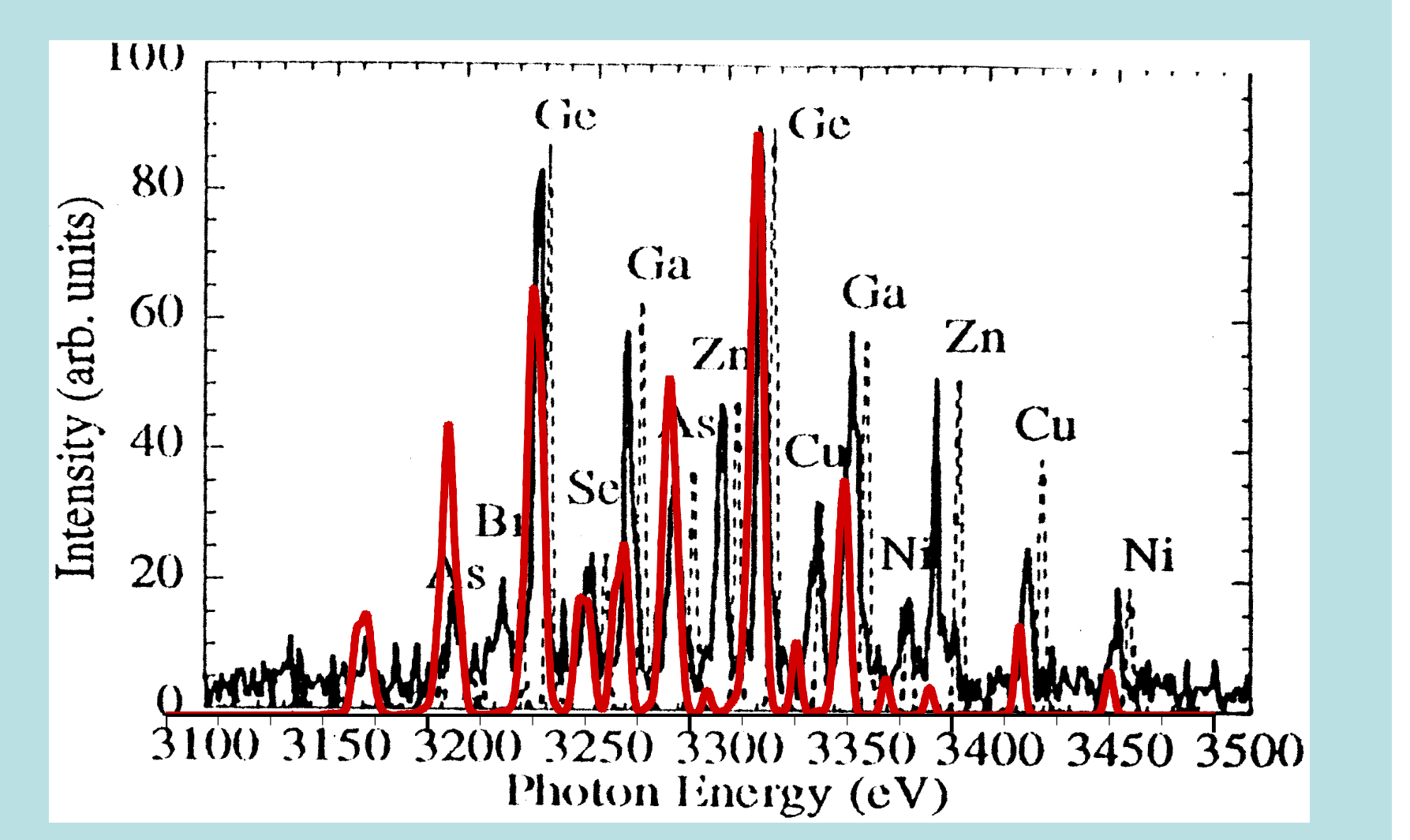
Configuration Included and Energy Structures



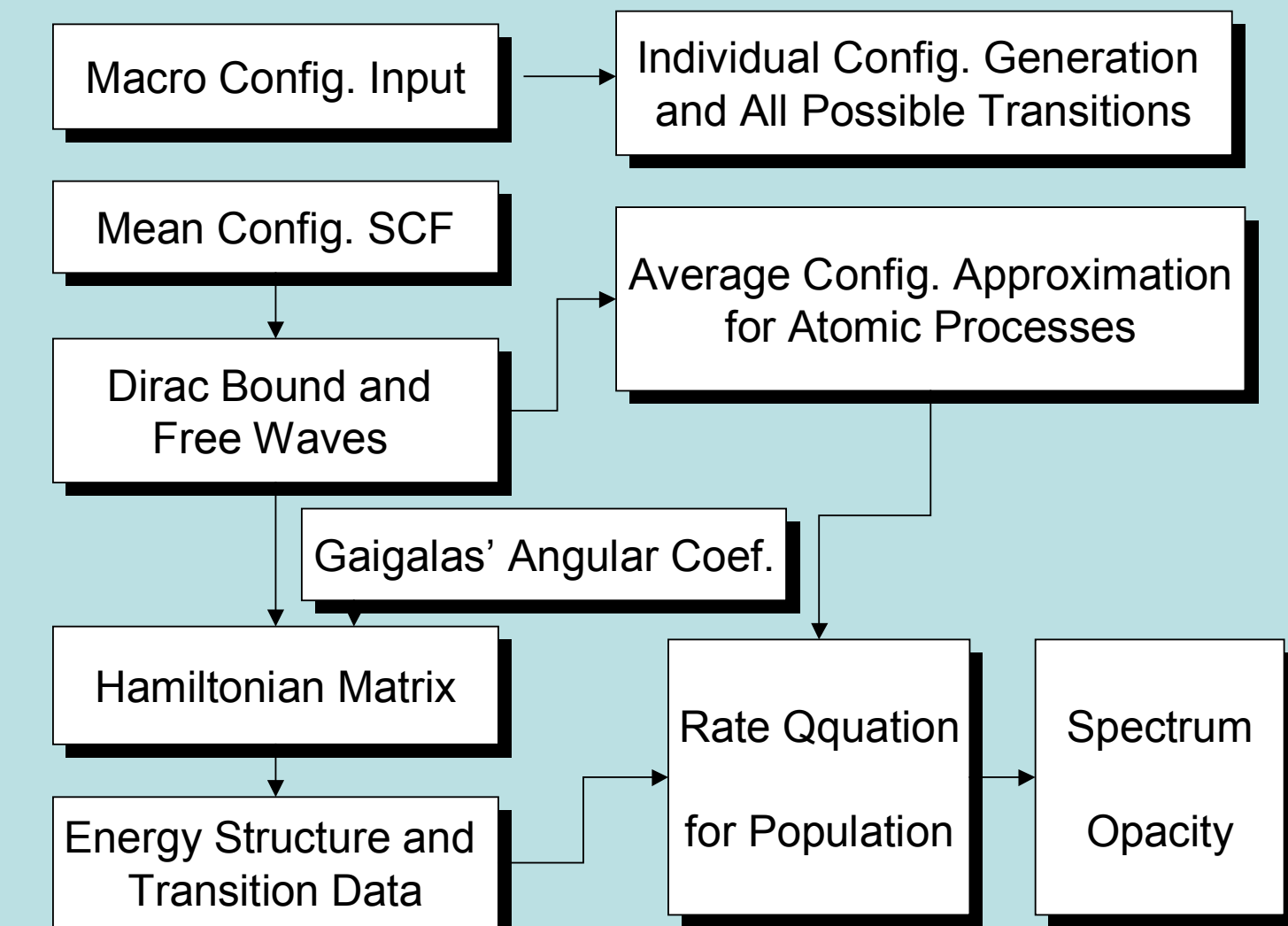
Emission Spectrum for 4f-3d and 5f-3d Transitions



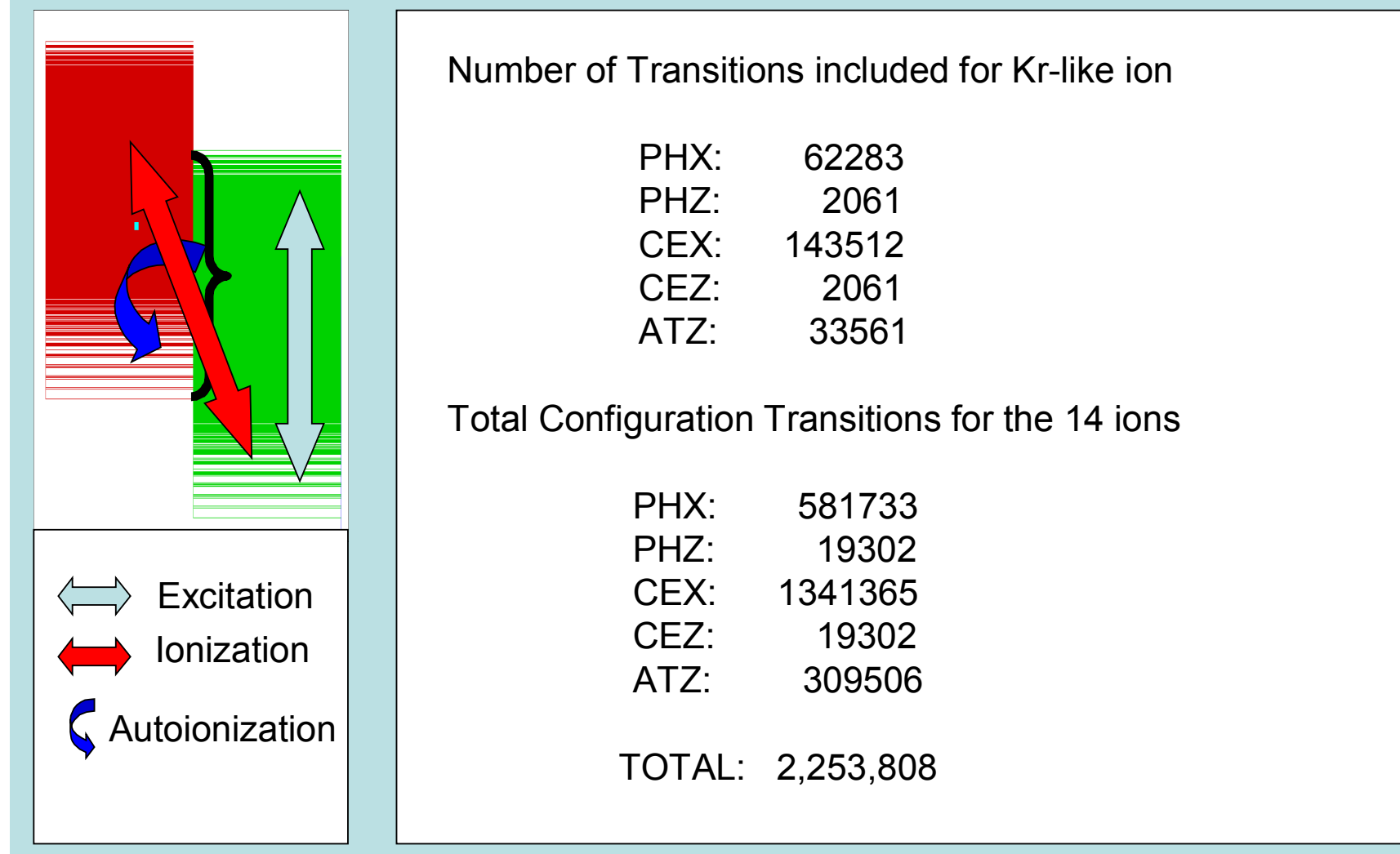
Emission Spectrum With Modified Rates



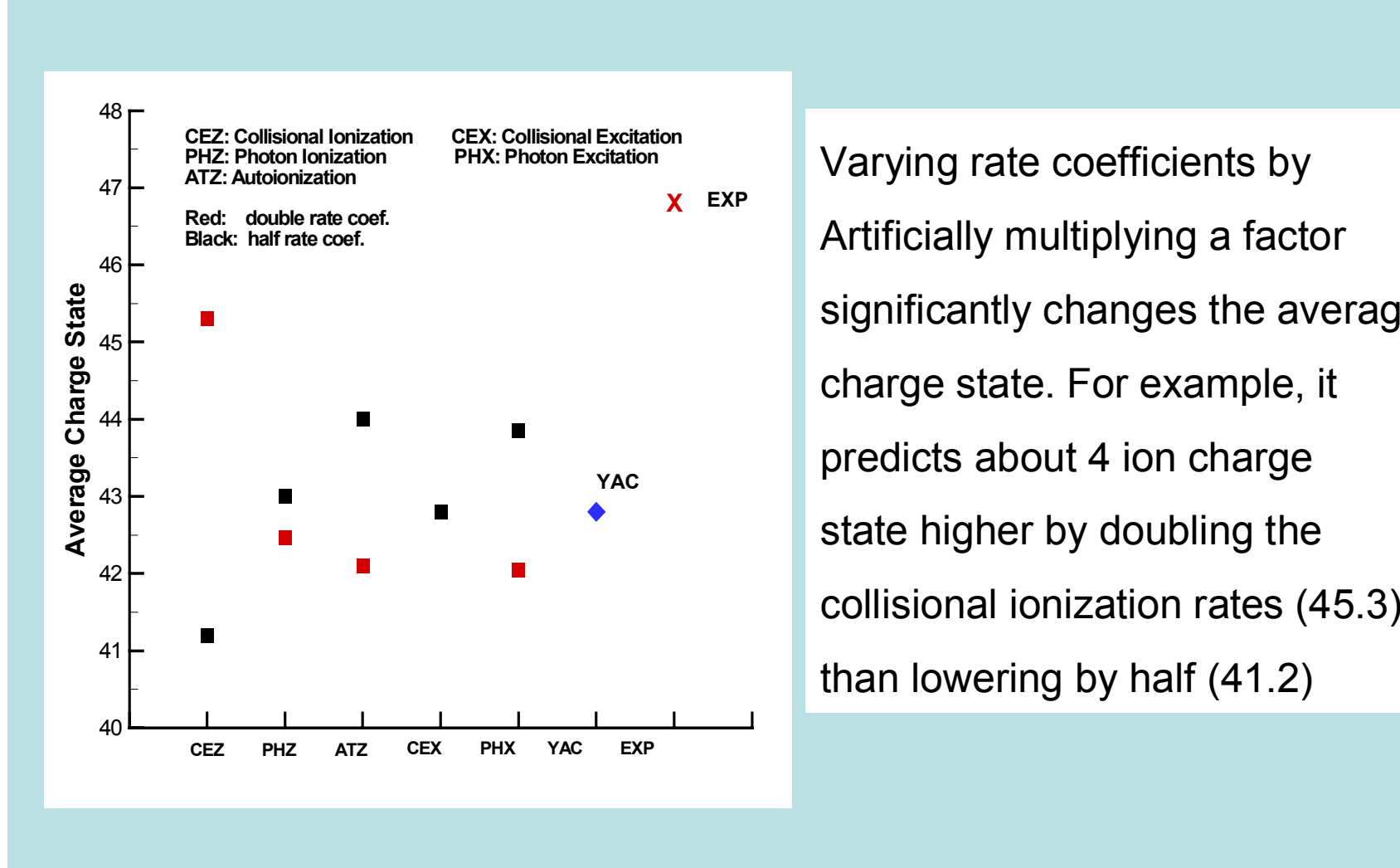
YAC Code Package Structure



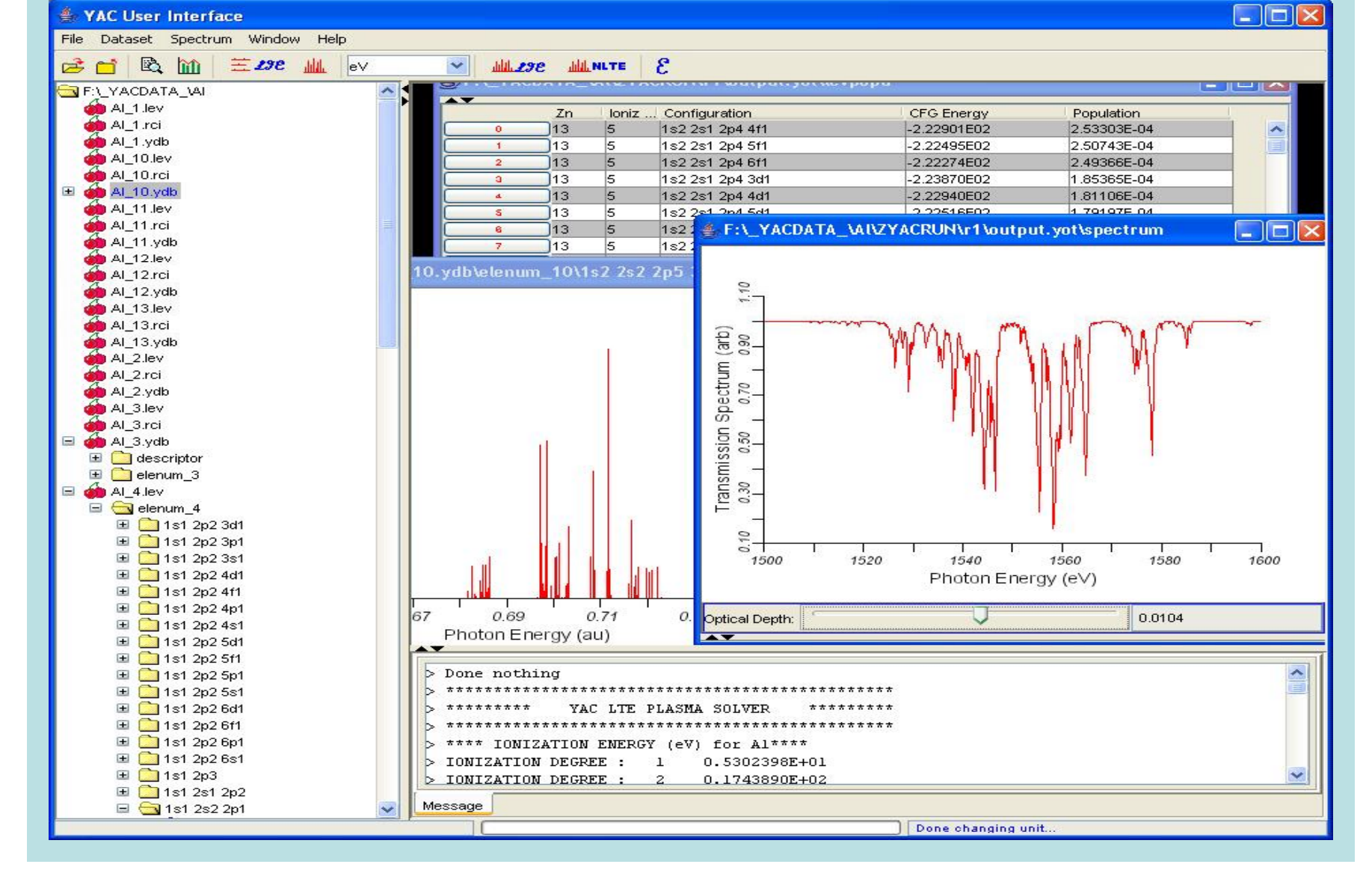
Transitions Between Configurations Auto Defined



Accuracy of Atomic Data is Very Important



A Screen Shot of YAC Graphical User Interface

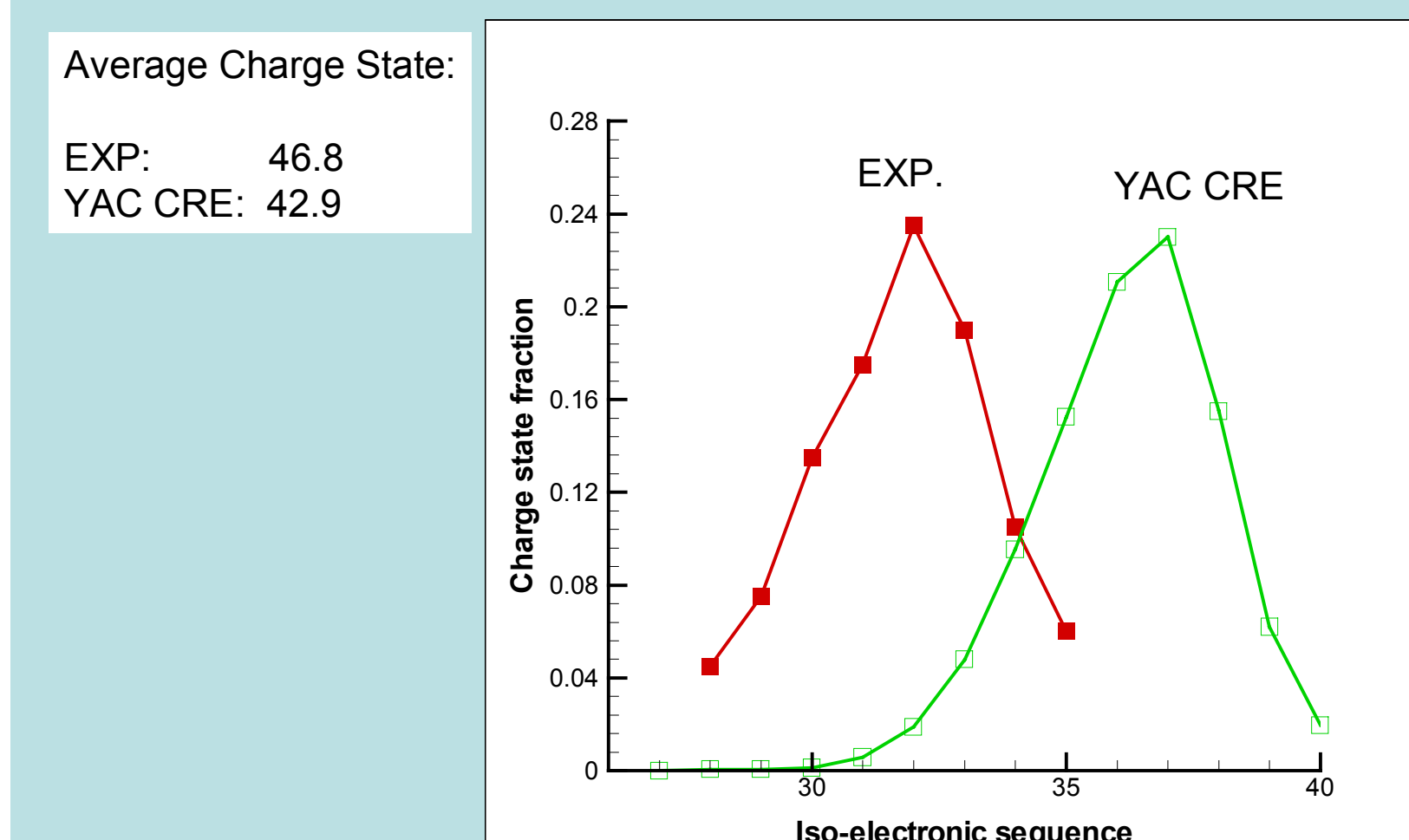


YAC Package for Opacity and Spectrum Analysis

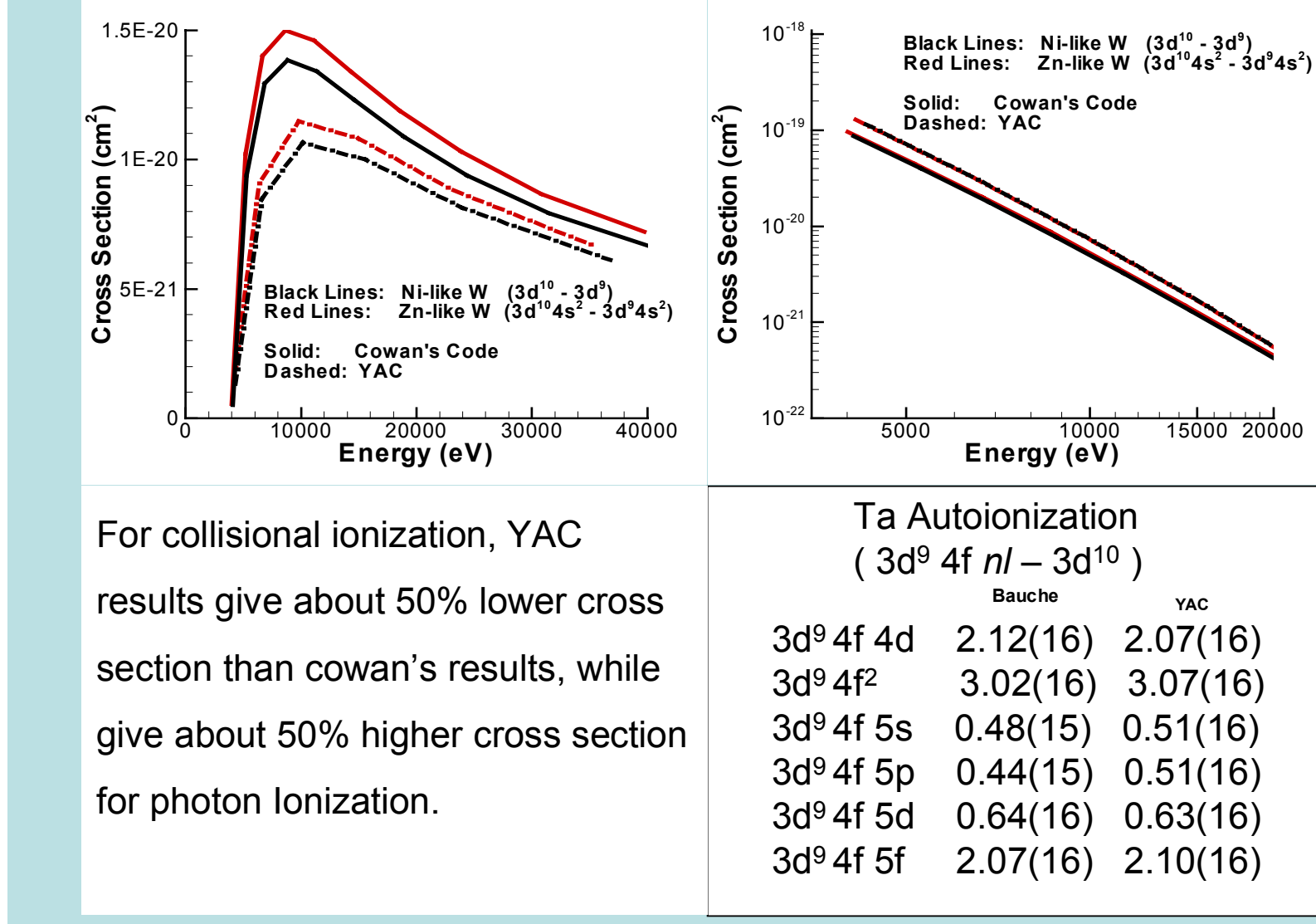
- Detailed configuration accounting (DCA) model for high Z plasmas, which means all configuration-to-configuration transitions are explicitly included as an extreme of the superconfiguration splitting method.
- Configuration average CRE rates computed with a mean configuration potential defined by the initial and final configuration pair
- Transitions between importantly populated configuration are calculated using the detailed term accounting (DTA) method
- CRE rate equation solved by the PETSC package
- HDF5 Data storage format



Compare Charge State Distribution With Exp.



Comparison with Cowan's Code



Summary and Future Work

We have developed an atomic code package for high Z non-LTE spectrum analysis. Detailed configuration accounting model (DCA) is used for construction of the rate equation, in which all related atomic processes are explicitly included. Comparing with recent experiment, there is up to 4 ion stages difference. The ionization balance is very sensitive to the accuracy of the rate coefficients as demonstrated by artificially varying the rate coefficients. Further investigation is needed to resolve the differences between the YAC results with other calculation for the ionization data.

