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**Calculation of Atomic Data for Plasma Modeling:
Results from CR Calculation**

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Calculation of Atomic Data for Plasma Modeling: Results from CR calculation

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Collisional radiative model

- With data in place can proceed to study of plasma
- May have interest in radiated power, spectrum, diagnosis of temperature, etc
- All require model of the plasma
- First need is the kinetics – determination of populations of all levels of all ion stages

Rate equations

Time evolution of populations :

$$\begin{aligned} \frac{dN_{i,j}}{dt} = & \sum_k R_{i-1,k \rightarrow i,j}^I N_{i-1,k} - \sum_k R_{i,j \rightarrow i+1,k}^I N_{i,j} + \\ & \sum_k R_{i+1,k \rightarrow i,j}^R N_{i+1,k} - \sum_k R_{i,j \rightarrow i-1,k}^R N_{i,j} \end{aligned}$$

Special cases

- High density, approaches LTE
- Low density, goes to coronal
- Steady state, populations not changing:

$$\frac{dN_{i,j}}{dt} = 0$$

For all levels of all ion stages.

Effective rate coefficients

- Full model can involve very large problem, thousands of levels in each ion stage. Connections mean many millions of possible transitions. Solution of rate equations will be lengthy.
- Time dependent case will take longer, requiring solution in small time increments of the full rate equations.

Effective rate coefficients

- If solution is calculated over a two dimensional grid in temperature and density, solution for other temperature, density can be found; very good solution for steady state, acceptable for time dependent.
- For each calculated solution, save total population of each ion stage, total radiated power, radiated power per ion stage, total ionization and recombination rate coefficients for each ion stage. Can also store spectrum for each ion stage.

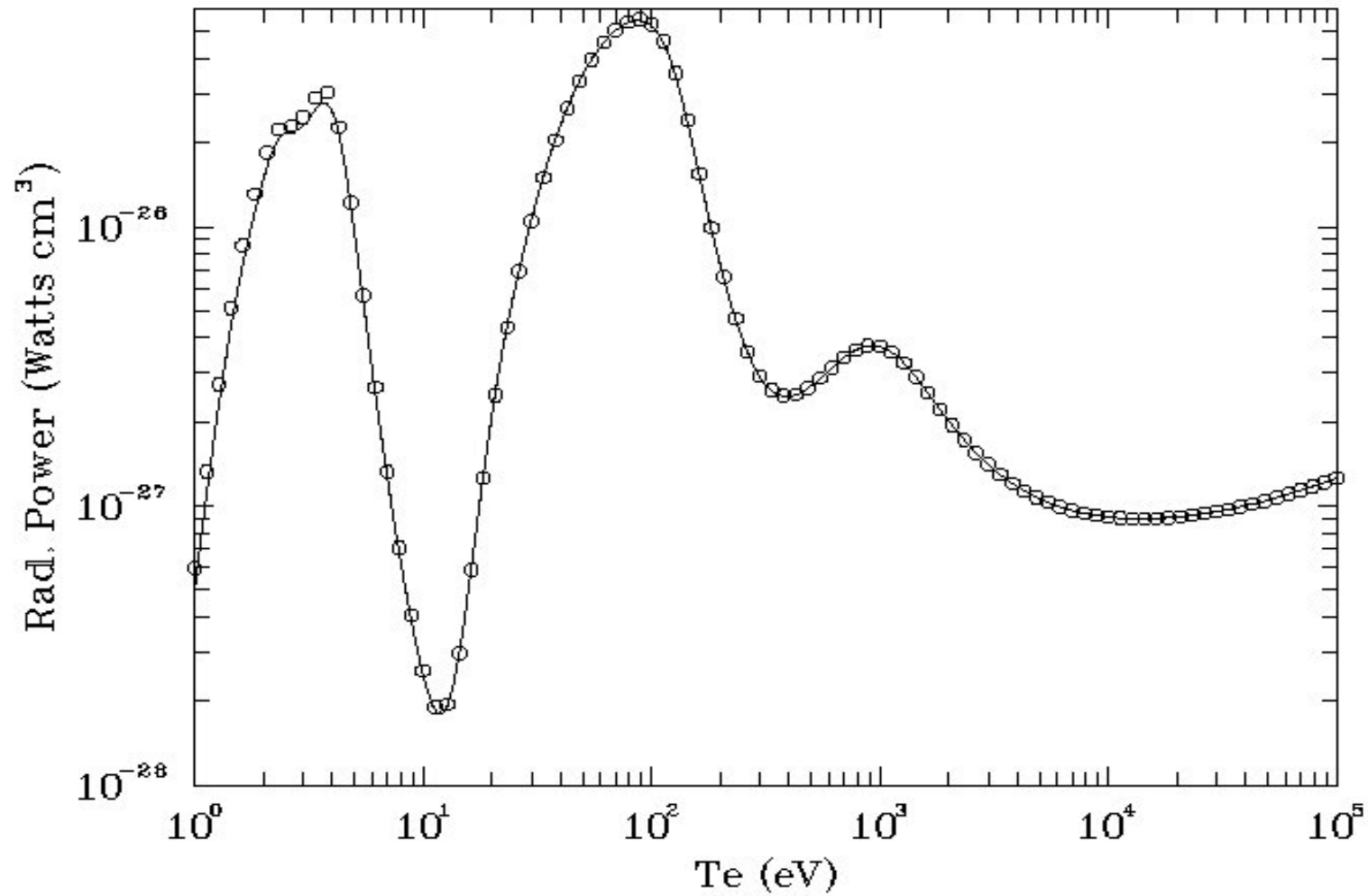
Effective rate coefficients

- For steady state solution, interpolate on total ion populations, total radiated power.
- For time dependent, interpolate on effective ionization and recombination rate coefficient. Then solve much simpler equations for ion stage populations, use with radiated power per ion stage to get total radiated power.

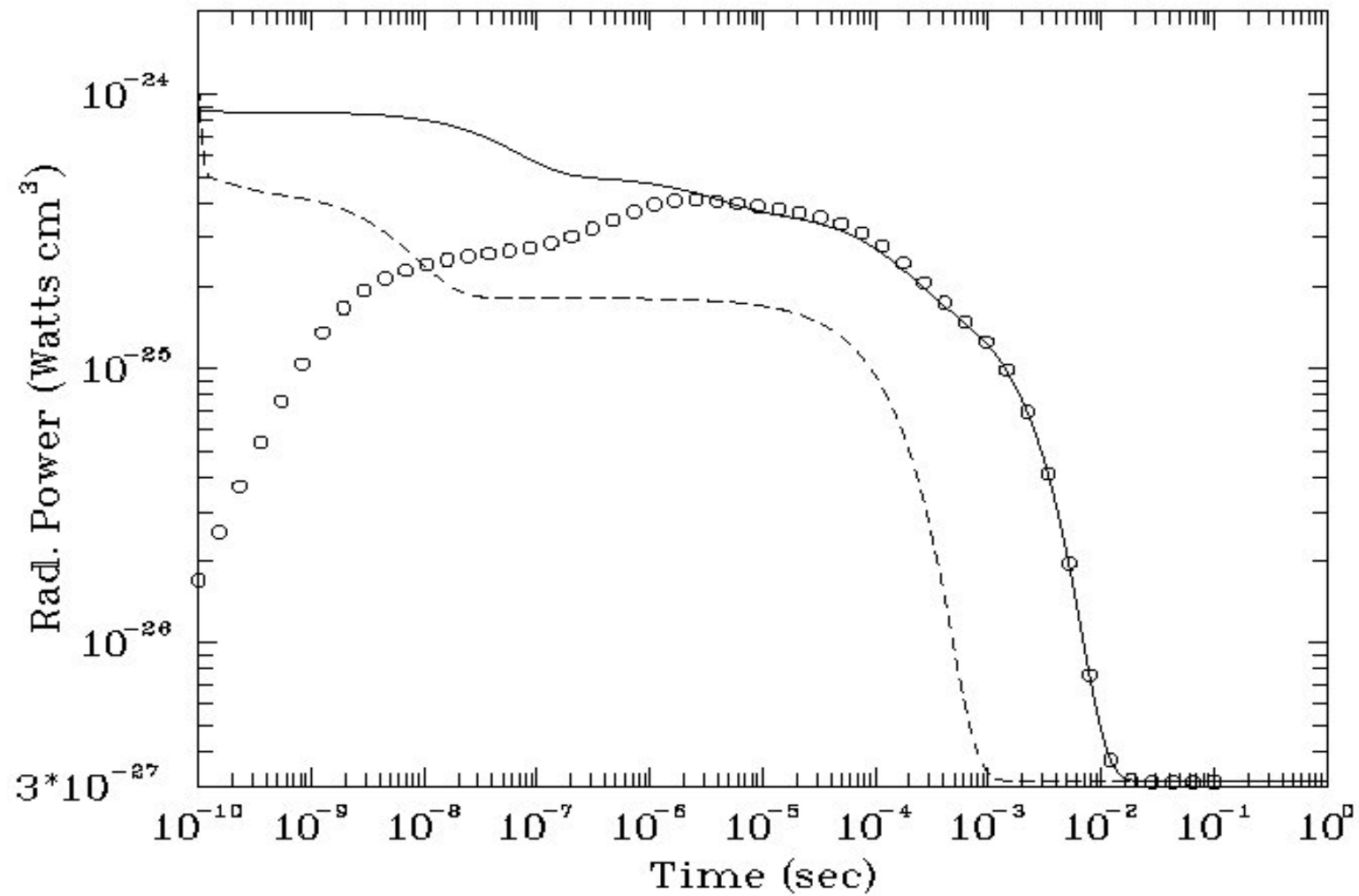
Effective rate coefficients

- **Steady state solution is very good.**
- **Time dependent is good for overall time behaviour, not so good for early times far from steady state.**

Steady state example



Time dependant example



Types of Time Dependent Problems

- Initial equilibrium populations with changing temperature/densities.
- Initial ion stage out of equilibrium. Two cases; ionizing plasma, recombining plasma.
- At long time interval, should go to steady state solution, use as check on time dependent calculation.
- From A+M page, click on RATES

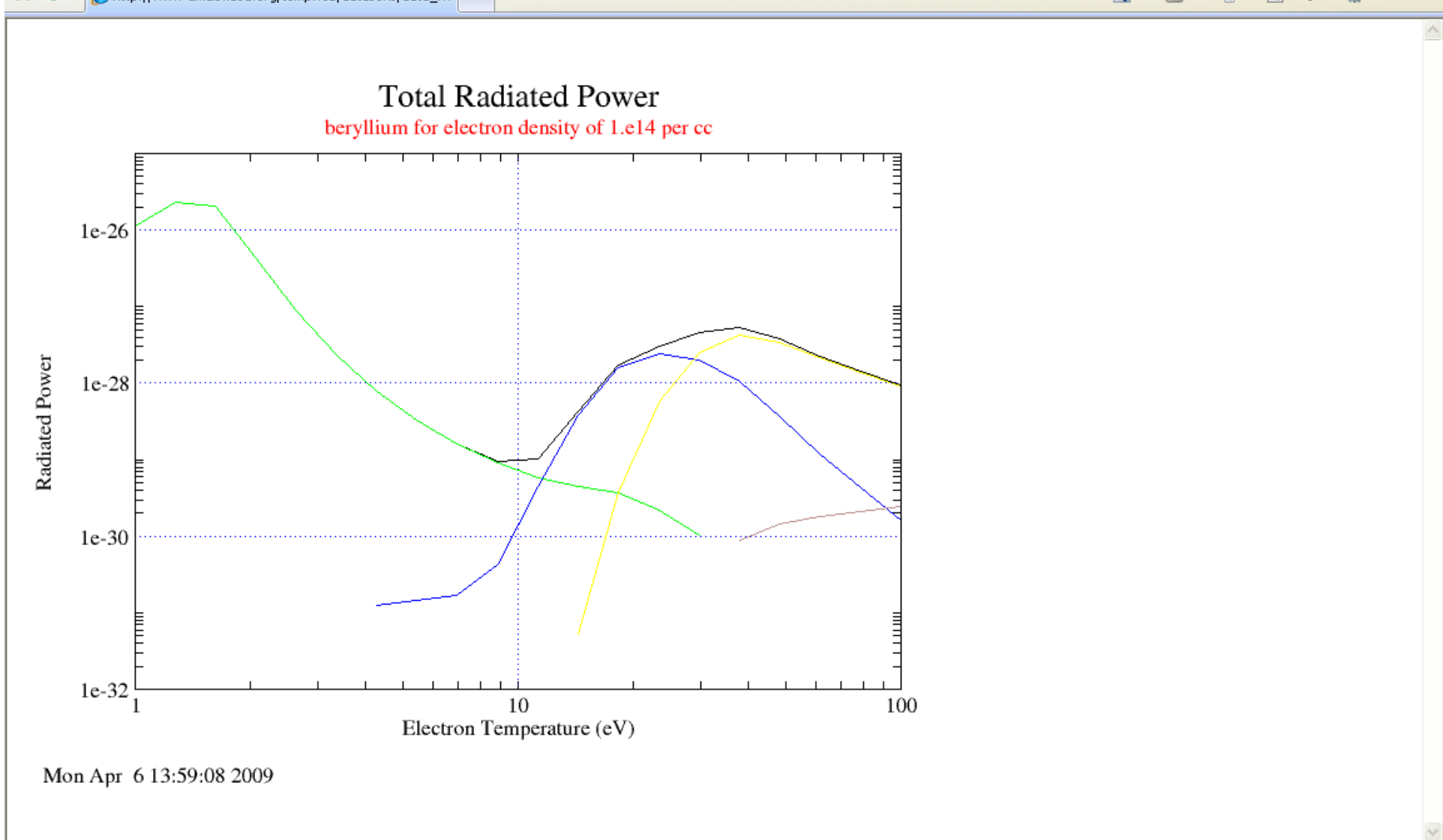
Sensitivity of CR results to data errors

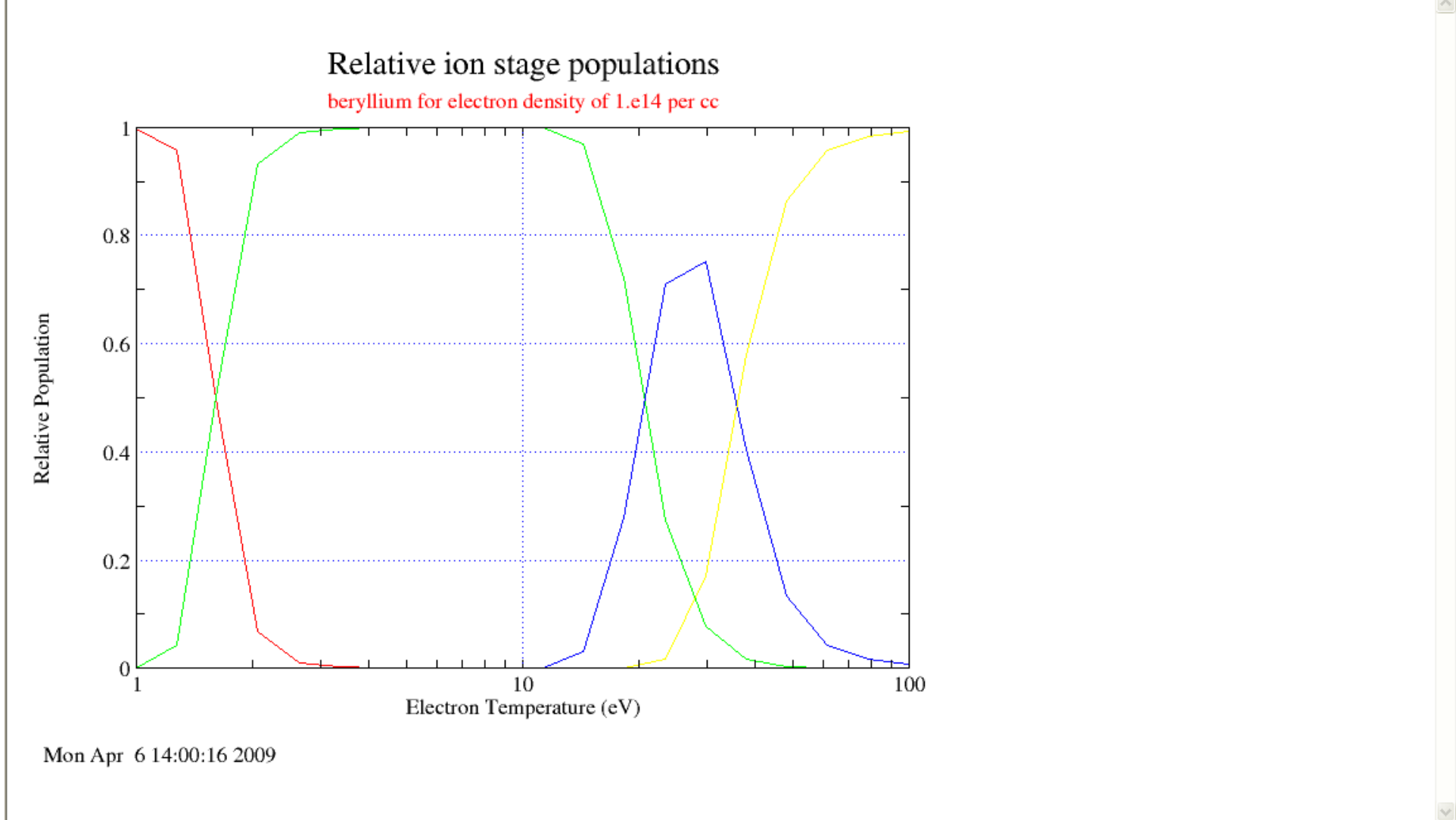
- **Many large scale properties of plasma relatively insensitive to details of calculation**
- **Most important aspect is building a complete set of data**
- **If processes are missing, disaster can occur; population builds up artificially and all results can be wrong**
- **Data should be consistent with same set of basis functions used**



Sensitivity of CR results to data errors

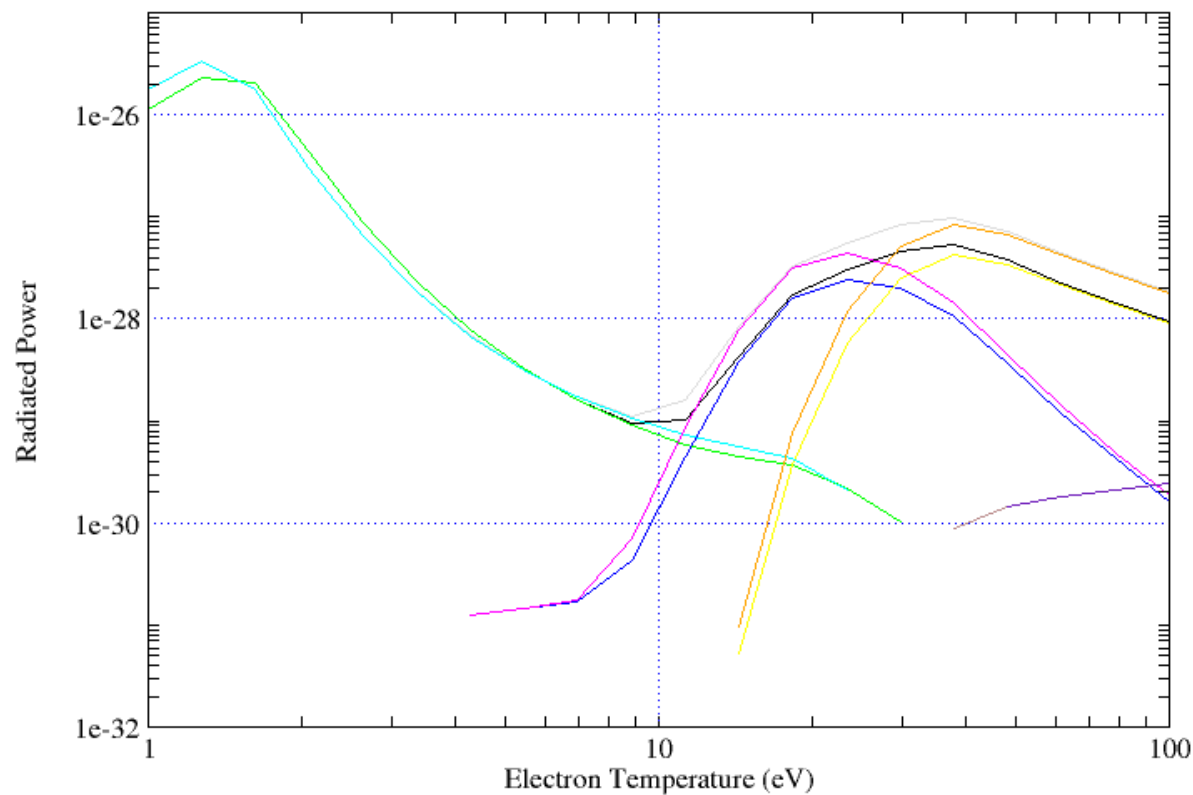
- **URL:**
<http://www-amdis.iaea.org/DATASENS/>
- **First run baseline model**
- **May choose to view baseline results**
- **Have option to modify all data: select multiplier for each type of data and apply either in random manner, or uniformly**
- **Recalculate and compare results**



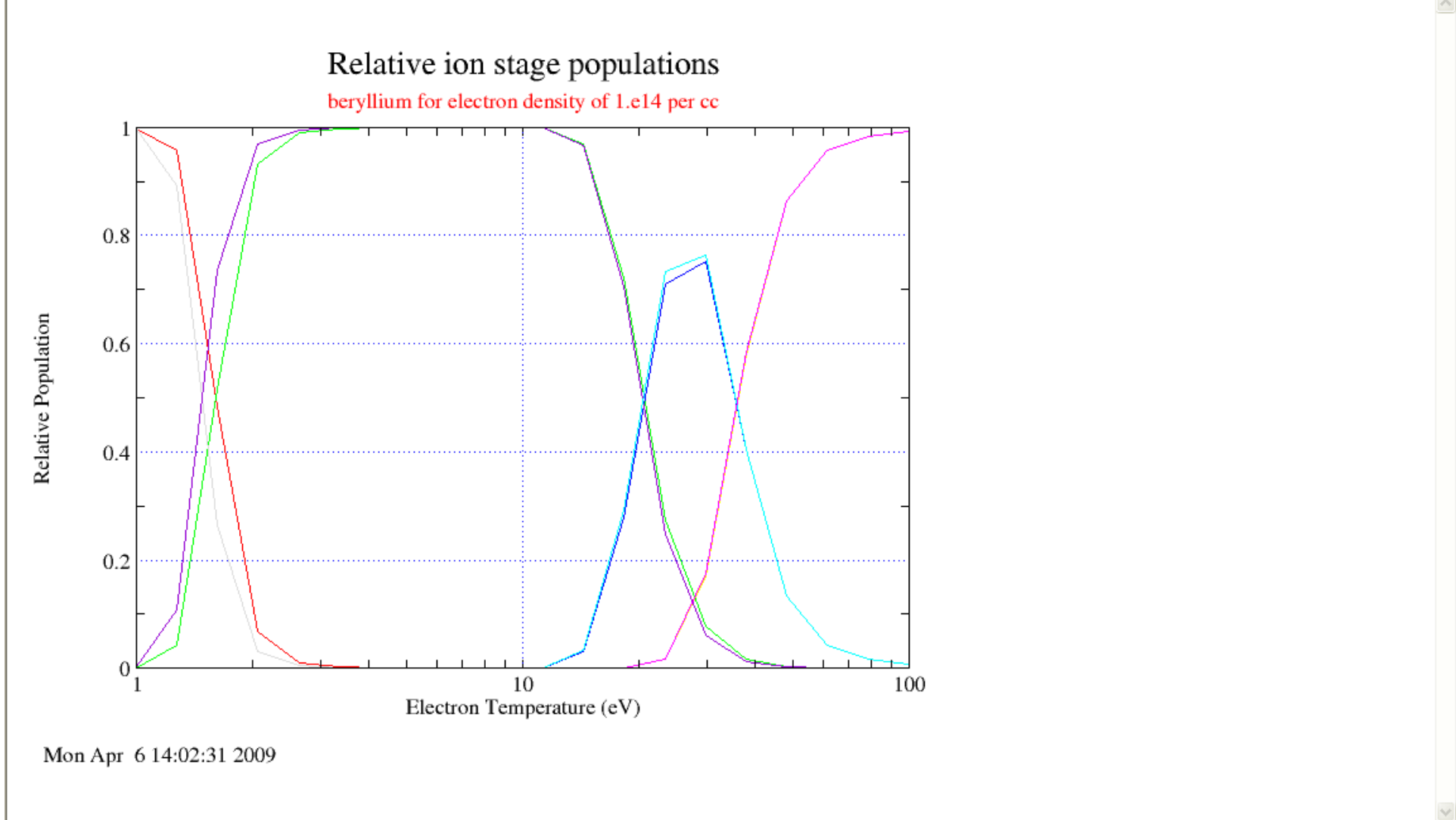


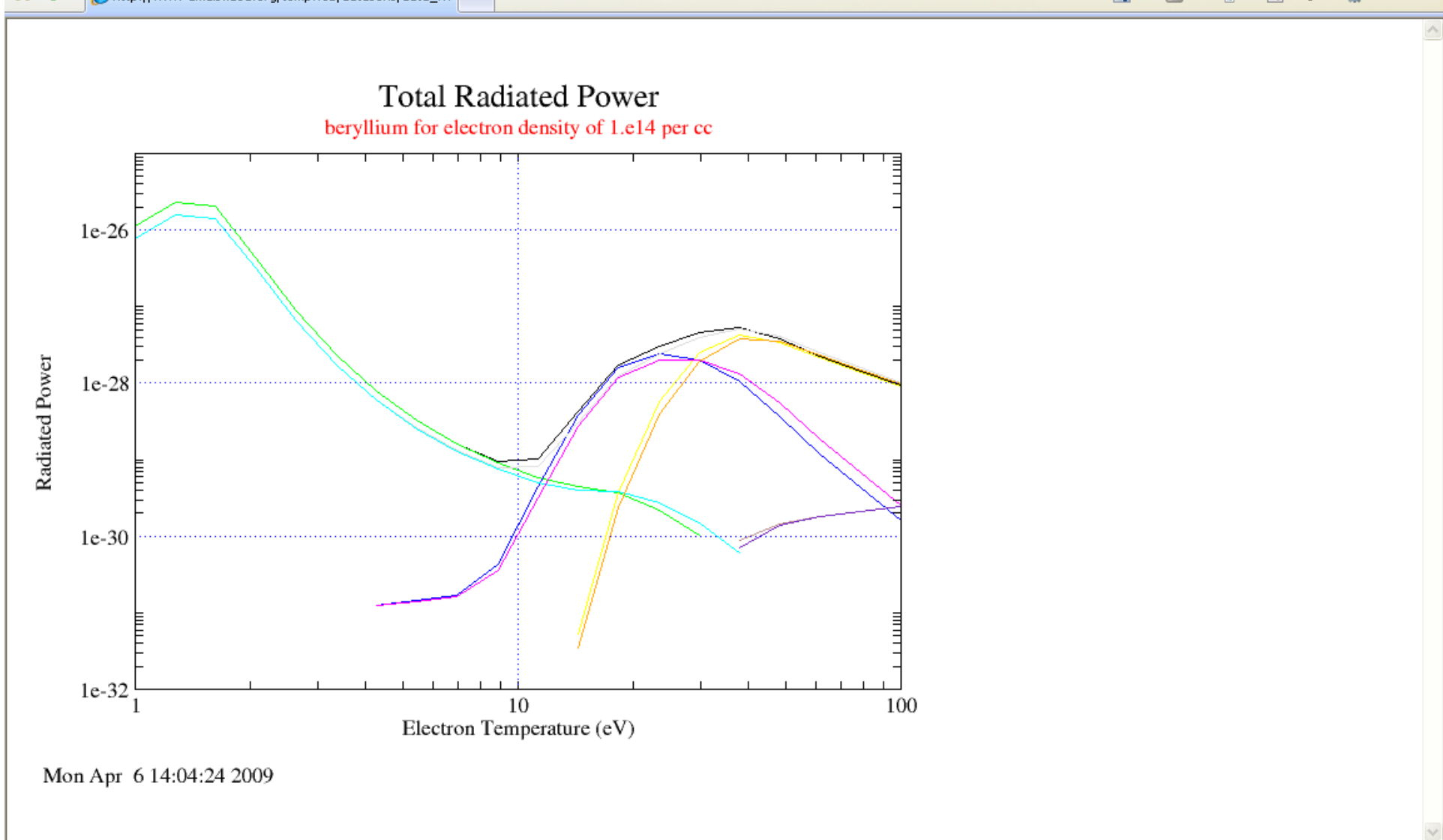
Total Radiated Power

beryllium for electron density of 1.e14 per cc



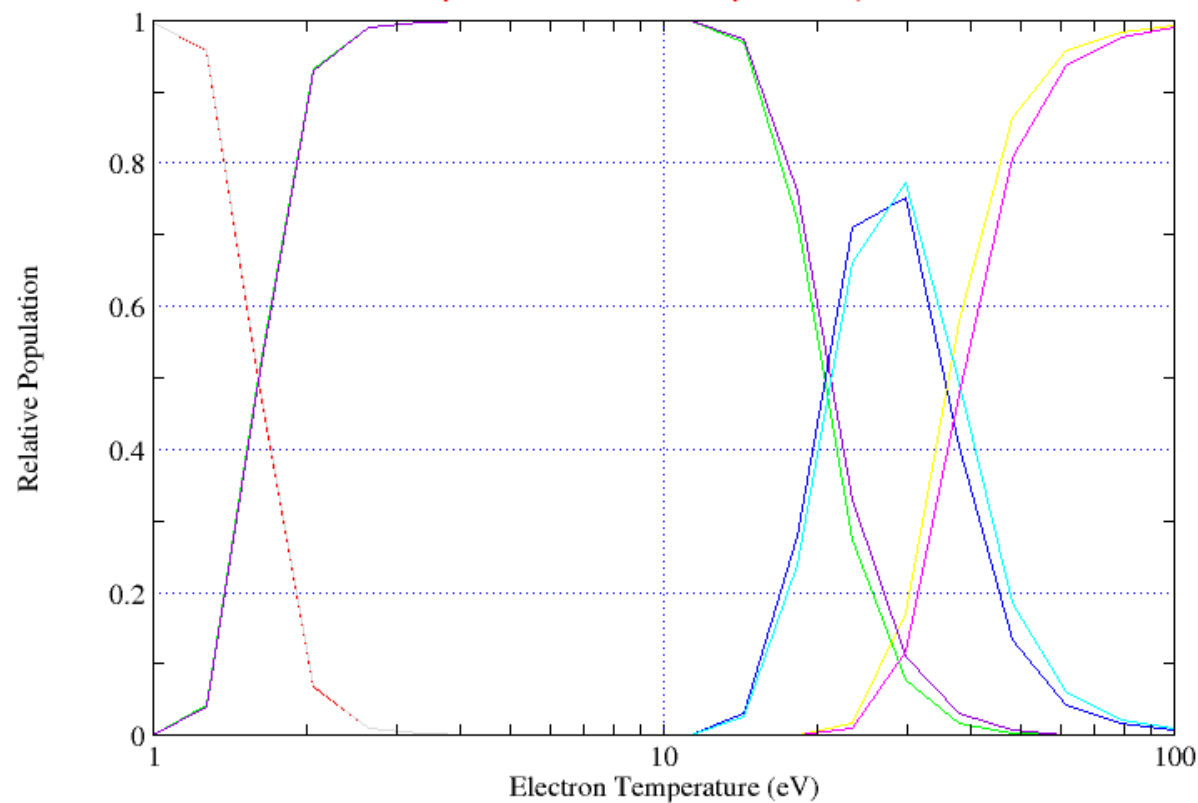
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Relative ion stage populations

beryllium for electron density of $1.e14$ per cc



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General conclusions

- **Random errors of a factor of two do not make such large error in overall plasma parameters**
- **Systematic errors in data are more important**
- **Specific spectral data were not shown, in general they are more sensitive to data errors**

General conclusions

- **Complete and consistent data set is most important**
- **Many resources for data exist**
- **More resources are being added**
- **Universal data exchange mechanism is under development**

