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Calculation of Atomic Data for Plasma Modeling: Ionization Processes

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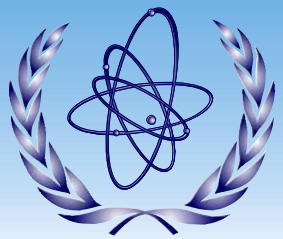


International Atomic Energy Agency

Calculation of Atomic Data for Plasma Modeling: Ionization Processes

R. Clark, D. Humbert, K. Sheikh

Nuclear Data Section

Electron impact ionization

- Process similar to excitation, incoming free electron, outgoing free electron with different energy
- However, now there are two outgoing free electrons, causes complication
- Total energy after collision is $E_T = E_i - \Delta E$, where E_T total energy after collision, E_i is the impact energy and ΔE is the ionization energy

Electron impact ionization

- This energy is distributed between the two outgoing electrons
- For a given angular momentum of one outgoing electron, there is a range of angular momenta possible for the other, depending on the angular momentum of the target state
- These considerations give rise to a very large number of possible free electron wave functions needed to solve problem

Common approximations

- Lotz formula. Well-known. Not bad accuracy for well-studied systems.
- Scaled Coulomb Born. Extension of the excitation method. Fits available. Accuracy acceptable for many systems.
- Distorted wave. Problem is now in two outgoing free wave functions, split of total energy between the two. Large increase of computational time
- Convergent close coupling (CCC) has been successfully applied to ionization

Scaled hydrogenic method

Reduced hydrogenic cross section :

$$Q_{nl}^{HR} = \left(\frac{Z}{n}\right)^4 \frac{Q_{nl}^{H}}{\pi a_0^2}$$

For complex ion,

$$Q(u) = \pi a_0^2 \left(\frac{n}{Z_{eff}}\right)^4 r_{nl} Q_{nl}^{HR}$$

Scaled hydrogenic method

Note for hydrogenic ion, ionization energy is :

$$E^I(Ryd) = \left(\frac{Z}{n}\right)^2$$

Assume similar for complex ion to arrive at :

$$Q(u) = \frac{\pi a_0^2}{\left[E^I(Ryd)\right]^2} r_{nl} Q_{nl}^{HR}(u)$$

Scaled hydrogenic method

- If scaled hydrogenic cross section, $Q_{nl}^{HR}(u)$ Is known, then cross section for arbitrary ion can be calculated
- Scaled cross sections calculated for 1s through 6g have been fitted as function of shell and impact energy
- Result is fit formula for scaled hydrogenic cross section
- Allows calculation of approximate cross section for any ion

Scaled Hydrogenic Method

Fit form used :

$$Q_{nl}^{HR}(u) = \frac{1}{u}[(C_1 + \frac{C_2 + C_3 l}{n})\ln(u) +$$

$$(C_4 + \frac{C_5 + C_6 l}{n})(1 - \frac{1}{u}) +$$

$$(C_7 + \frac{C_8 + C_9 l}{n})(1 - \frac{1}{u})^2]$$

Scaled hydrogenic

- In previous, u is the electron impact energy in threshold units
- Result is cross section for one shell of hydrogenic
- Possible to include angular coupling effects as well as mixing of target states
- The C_i are the fitting coefficients with the values:

Fitting parameters

C_1 1.5369

C_2 0.99656

C_3 -0.61916

C_4 2.4463

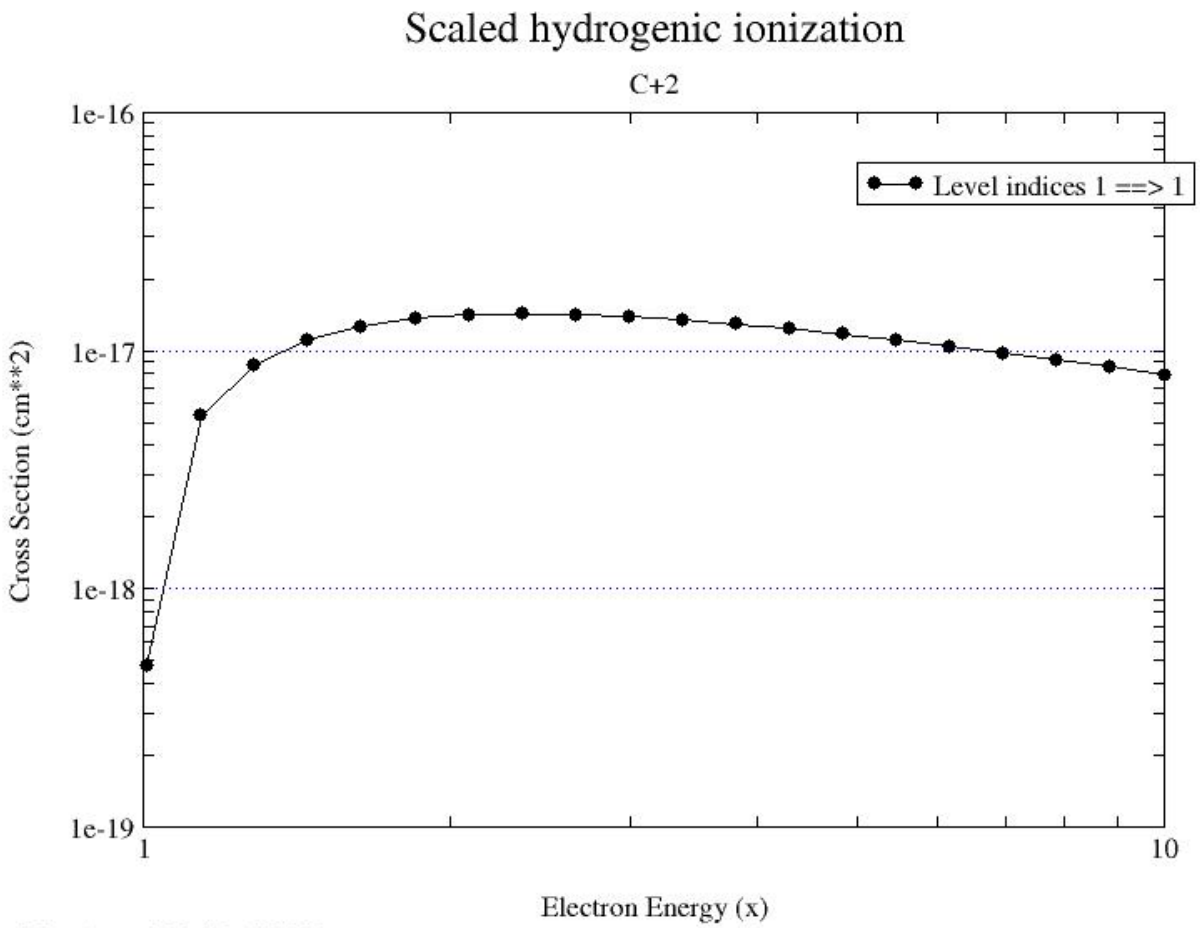
C_5 -2.4773

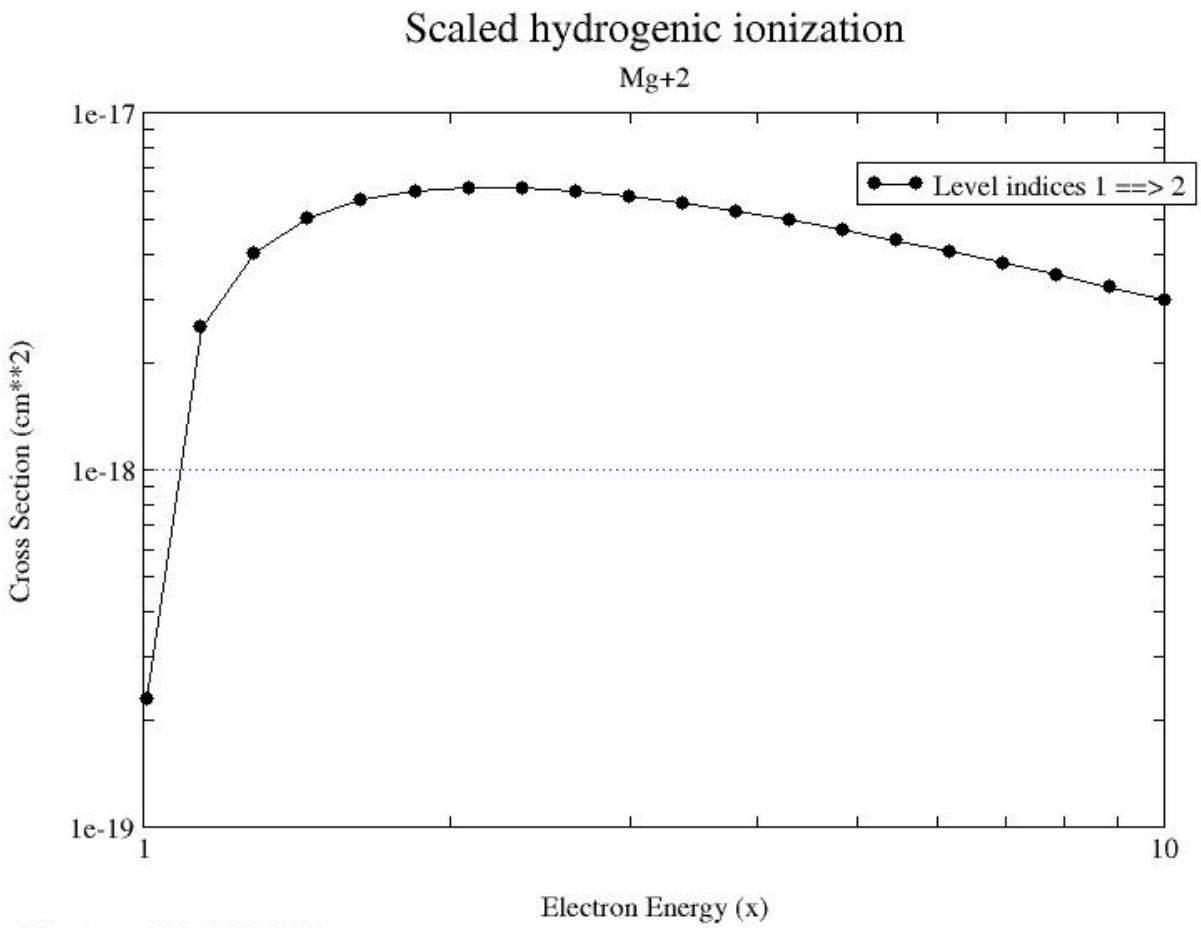
C_6 3.2151

C_7 -1.4512

C_8 1.7230

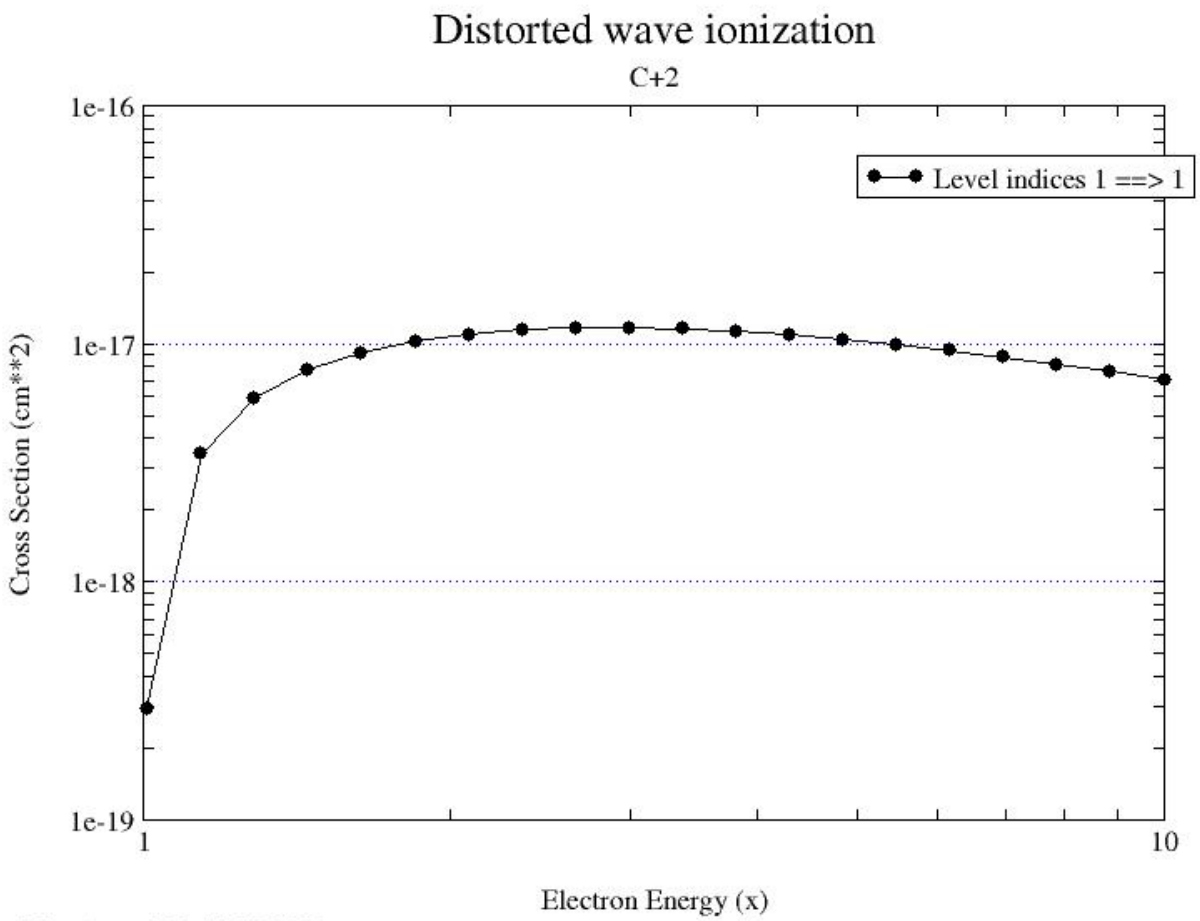
C_9 -0.47075

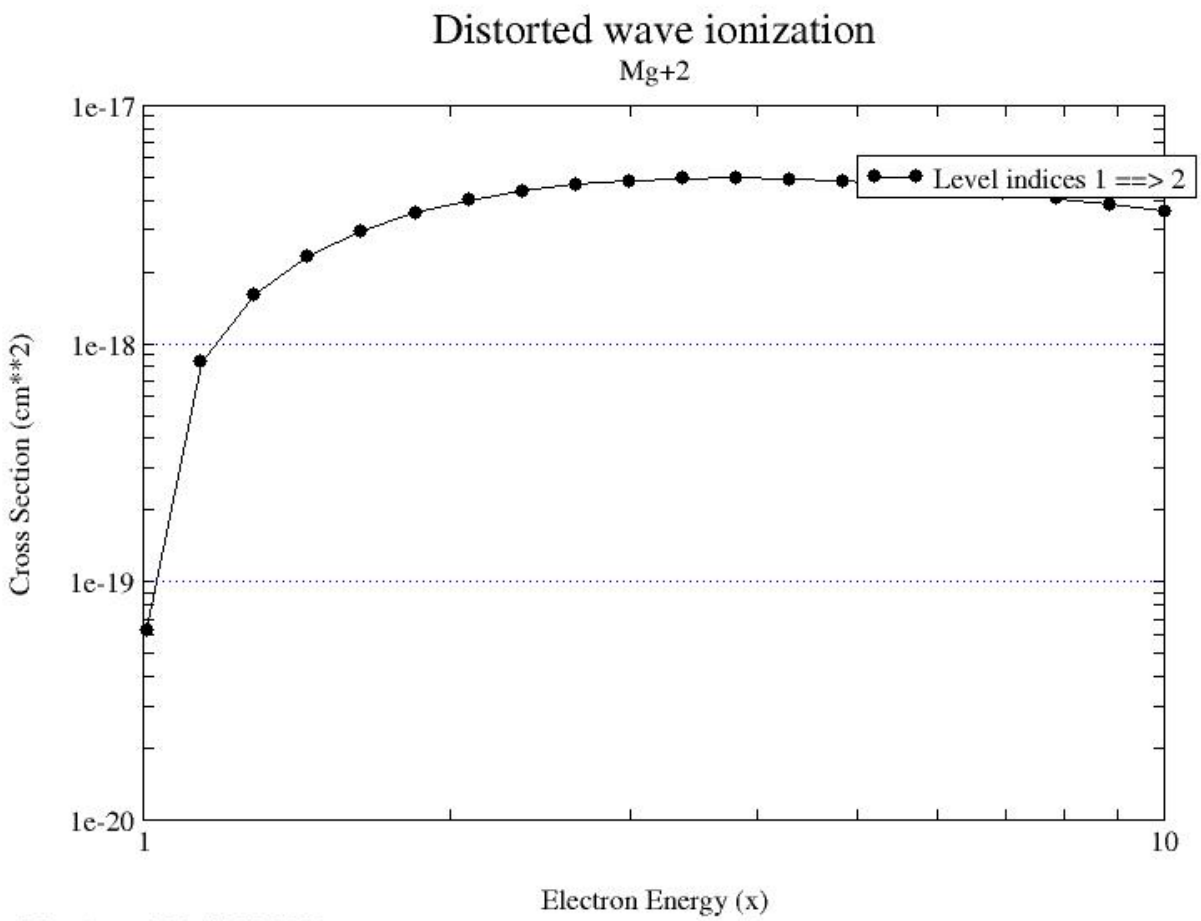




Distorted wave

- Similar to calculation for excitation
- Difficulty is now there are two outgoing free electrons
- Energy splits between two, very many free electron orbitals needed
- Perform quadrature over outgoing electron energy split
- Computational time is significant





Close coupling

- Application now made to ionization
- Convergant close coupling technique developed by Bray and Fursa has wide range of applications
- Still under development
- Difficulty handling partial filled shells

Photoionization

- Photon causes ejection of electron
- Not very likely in fusion plasmas
- Inverse process is radiative recombination
- Competes with inverse of electron impact ionization, three body recombination
- Radiative recombination is often dominant recombination mechanism

Autoionization

- May have ion suffer inner shell excitation
- Result may lie above continuum
- Result is autoionization
- Inverse process is di-electronic recombination
- Both may be very important in fusion plasmas
- May be calculated with DW theory, or automatically generated with CC methods

Levels of Mg + 1

Energy (eV)	Stat. Wt.	Level
0.0000e+00	2	$(2p^6\ ^1S)^1S\ (3s^1\ ^2S)^2S_{0.5}$
4.4725e+00	2	$(2p^6\ ^1S)^1S\ (3p^1\ ^2P)^2P_{0.5}$
4.4812e+00	4	$(2p^6\ ^1S)^1S\ (3p^1\ ^2P)^2P_{1.5}$
9.1187e+00	4	$(2p^6\ ^1S)^1S\ (3d^1\ ^2D)^2D_{1.5}$
9.1187e+00	6	$(2p^6\ ^1S)^1S\ (3d^1\ ^2D)^2D_{2.5}$
4.9418e+01	4	$(2p^5\ ^2P)^2P\ (3s^2\ ^1S)^2P_{1.5}$
4.9689e+01	2	$(2p^5\ ^2P)^2P\ (3s^2\ ^1S)^2P_{0.5}$
5.2834e+01	4	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3p^1\ ^2P)^4S_{1.5}$
5.3212e+01	8	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3p^1\ ^2P)^4D_{3.5}$
5.3275e+01	6	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3p^1\ ^2P)^4D_{2.5}$
5.3341e+01	4	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3p^1\ ^2P)^4D_{1.5}$
5.3401e+01	2	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3p^1\ ^2P)^4D_{0.5}$
5.3539e+01	6	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3p^1\ ^2P)^4P_{2.5}$
5.3613e+01	4	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3p^1\ ^2P)^4P_{1.5}$
5.3659e+01	2	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3p^1\ ^2P)^4P_{0.5}$
5.3768e+01	4	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^1P\ (3p^1\ ^2P)^2D_{1.5}$
5.3863e+01	6	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^1P\ (3p^1\ ^2P)^2D_{2.5}$
5.3895e+01	2	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^1P\ (3p^1\ ^2P)^2P_{0.5}$

6.0575e+01	6	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^1P\ (3d^1\ ^2D)^2F_{2.5}$
6.0620e+01	4	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^1P\ (3d^1\ ^2D)^2P_{1.5}$
6.0662e+01	8	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^1P\ (3d^1\ ^2D)^2F_{3.5}$
6.0709e+01	2	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^1P\ (3d^1\ ^2D)^2P_{0.5}$
6.0724e+01	6	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^1P\ (3d^1\ ^2D)^2D_{2.5}$
6.0724e+01	4	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^1P\ (3d^1\ ^2D)^2D_{1.5}$
6.1111e+01	2	$(2p^5\ ^2P)^2P\ (3p^2\ ^3P)^2P_{0.5}$
6.1167e+01	4	$(2p^5\ ^2P)^2P\ (3p^2\ ^3P)^2P_{1.5}$
6.2601e+01	8	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3d^1\ ^2D)^2F_{3.5}$
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6.2762e+01	4	$(2p^5\ ^2P)^2P\ (3p^2\ ^1S)^2P_{1.5}$
6.2936e+01	4	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3d^1\ ^2D)^2D_{1.5}$
6.2970e+01	6	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3d^1\ ^2D)^2D_{2.5}$
6.2991e+01	2	$(2p^5\ ^2P)^2P\ (3p^2\ ^1S)^2P_{0.5}$
6.3217e+01	2	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3d^1\ ^2D)^2P_{0.5}$
6.3350e+01	4	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3d^1\ ^2D)^2P_{1.5}$

Levels of Mg + 2

Energy (eV)	Stat. Wt.	Level
1.5354e+01	1	$(2p^6\ ^1S)^1S_{0.0}$

Current element is Mg (atomic number 12) with charge of + 1

Help on configuration energies

Shell energies of Mg + 1 **Energy (eV) Shell**	**Shell energies of Mg + 2** **Energy (eV) Shell**
Shell energies for 3s 1.3469e+03 $1s^2$ 1.1259e+02 $2s^2$ 7.1853e+01 $2p^6$ 1.5213e+01 3s Total configuration energy is 0.0000e+00 Stat. Wt. is 2 Shell energies for 3p 1.3488e+03 $1s^2$ 1.1434e+02 $2s^2$ 7.3786e+01 $2p^6$ 1.0751e+01 3p Total configuration energy is 4.4510e+00 Stat. Wt. is 6 Shell energies for 3d 1.3519e+03 $1s^2$ 1.1721e+02 $2s^2$ 7.6638e+01 $2p^6$ 6.2349e+00 3d Total configuration energy is 8.9633e+00 Stat. Wt. is 10	Shell energies for 1.3581e+03 $1s^2$ 1.2342e+02 $2s^2$ 8.2845e+01 $2p^6$ Total configuration energy is 1.5198e+01 Stat. Wt. is 1

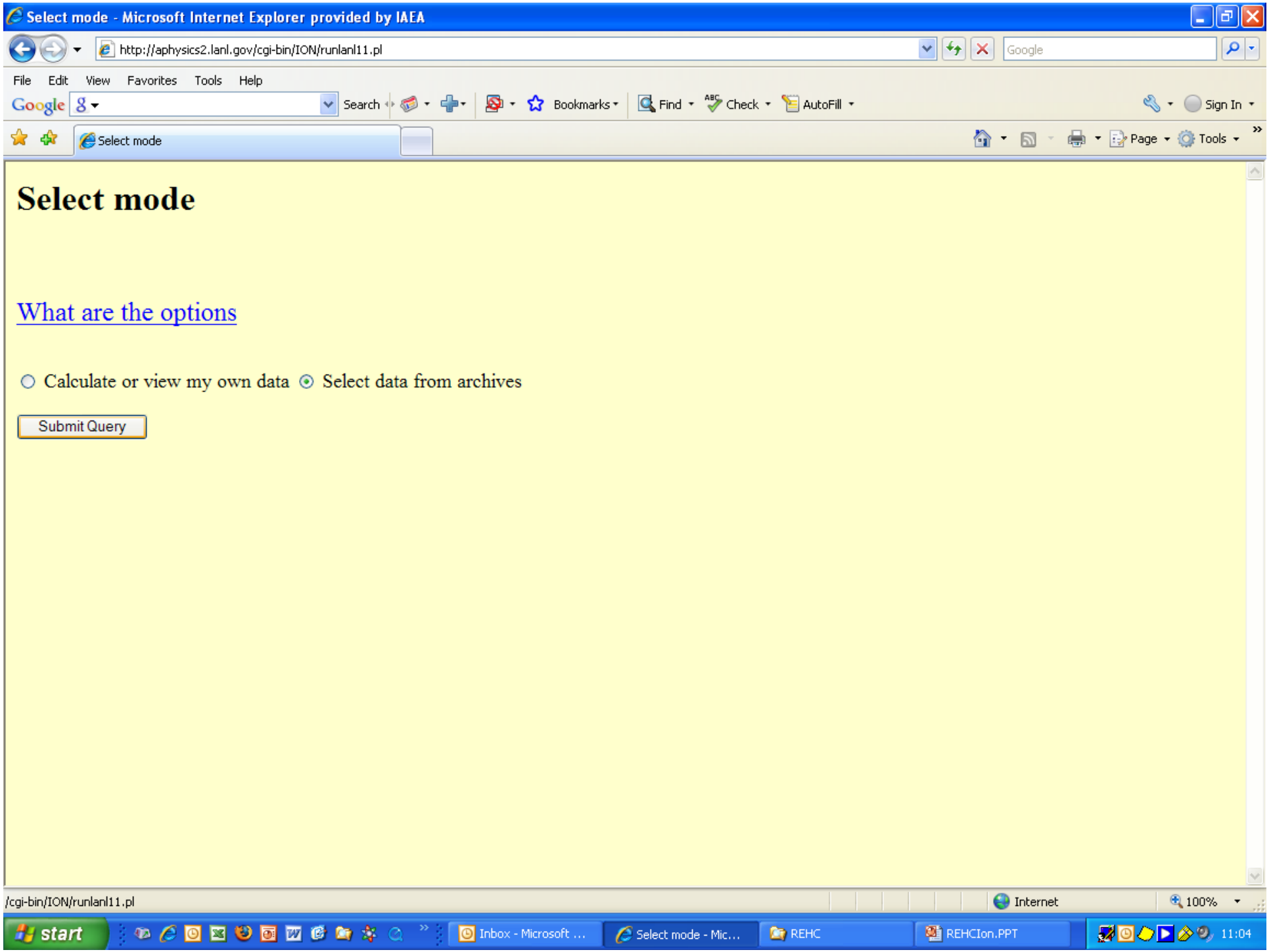
AUTOIONIZATION

JPEG file(new window)

Energy eV	Transition	AI Rate
3.8047e+01	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3p^1\ ^2P)^4D_{0.5}$ -- $(2p^6\ ^1S)^1S_{0.0}$	1.3459e+09
3.8305e+01	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3p^1\ ^2P)^4P_{0.5}$ -- $(2p^6\ ^1S)^1S_{0.0}$	1.6541e+11
3.8541e+01	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^1P\ (3p^1\ ^2P)^2P_{0.5}$ -- $(2p^6\ ^1S)^1S_{0.0}$	5.4758e+10
3.9512e+01	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^1P\ (3p^1\ ^2P)^2S_{0.5}$ -- $(2p^6\ ^1S)^1S_{0.0}$	1.3030e+13
4.1598e+01	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3p^1\ ^2P)^2P_{0.5}$ -- $(2p^6\ ^1S)^1S_{0.0}$	3.3172e+12
4.2140e+01	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3p^1\ ^2P)^2S_{0.5}$ -- $(2p^6\ ^1S)^1S_{0.0}$	6.2930e+13
3.7987e+01	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3p^1\ ^2P)^4D_{1.5}$ -- $(2p^6\ ^1S)^1S_{0.0}$	1.5674e+09
3.8259e+01	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3p^1\ ^2P)^4P_{1.5}$ -- $(2p^6\ ^1S)^1S_{0.0}$	6.6580e+09
3.8413e+01	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^1P\ (3p^1\ ^2P)^2D_{1.5}$ -- $(2p^6\ ^1S)^1S_{0.0}$	3.2325e+10
3.8602e+01	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^1P\ (3p^1\ ^2P)^2P_{1.5}$ -- $(2p^6\ ^1S)^1S_{0.0}$	7.9359e+08
4.1343e+01	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3p^1\ ^2P)^2D_{1.5}$ -- $(2p^6\ ^1S)^1S_{0.0}$	2.2132e+12
4.1558e+01	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3p^1\ ^2P)^2P_{1.5}$ -- $(2p^6\ ^1S)^1S_{0.0}$	1.1169e+12
3.7921e+01	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3p^1\ ^2P)^4D_{2.5}$ -- $(2p^6\ ^1S)^1S_{0.0}$	1.1165e+09
3.8185e+01	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3p^1\ ^2P)^4P_{2.5}$ -- $(2p^6\ ^1S)^1S_{0.0}$	3.9190e+09
3.8509e+01	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^1P\ (3p^1\ ^2P)^2D_{2.5}$ -- $(2p^6\ ^1S)^1S_{0.0}$	3.2099e+10
4.1189e+01	$(2p^5\ ^2P)^2P\ (3s^1\ ^2S)^3P\ (3p^1\ ^2P)^2D_{2.5}$ -- $(2p^6\ ^1S)^1S_{0.0}$	3.3343e+12
3.4335e+01	$(2p^5\ ^2P)^2P\ (3s^2\ ^1S)^2P_{0.5}$ -- $(2p^6\ ^1S)^1S_{0.0}$	1.2827e+12

Data from archives

- Choice is made on opening page
- Select element from list
- Select particular model, normally only one, can be more
- Select ion
- Can now view data, but cannot add to these files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Search Bookmarks Find Check AutoFill Sign In
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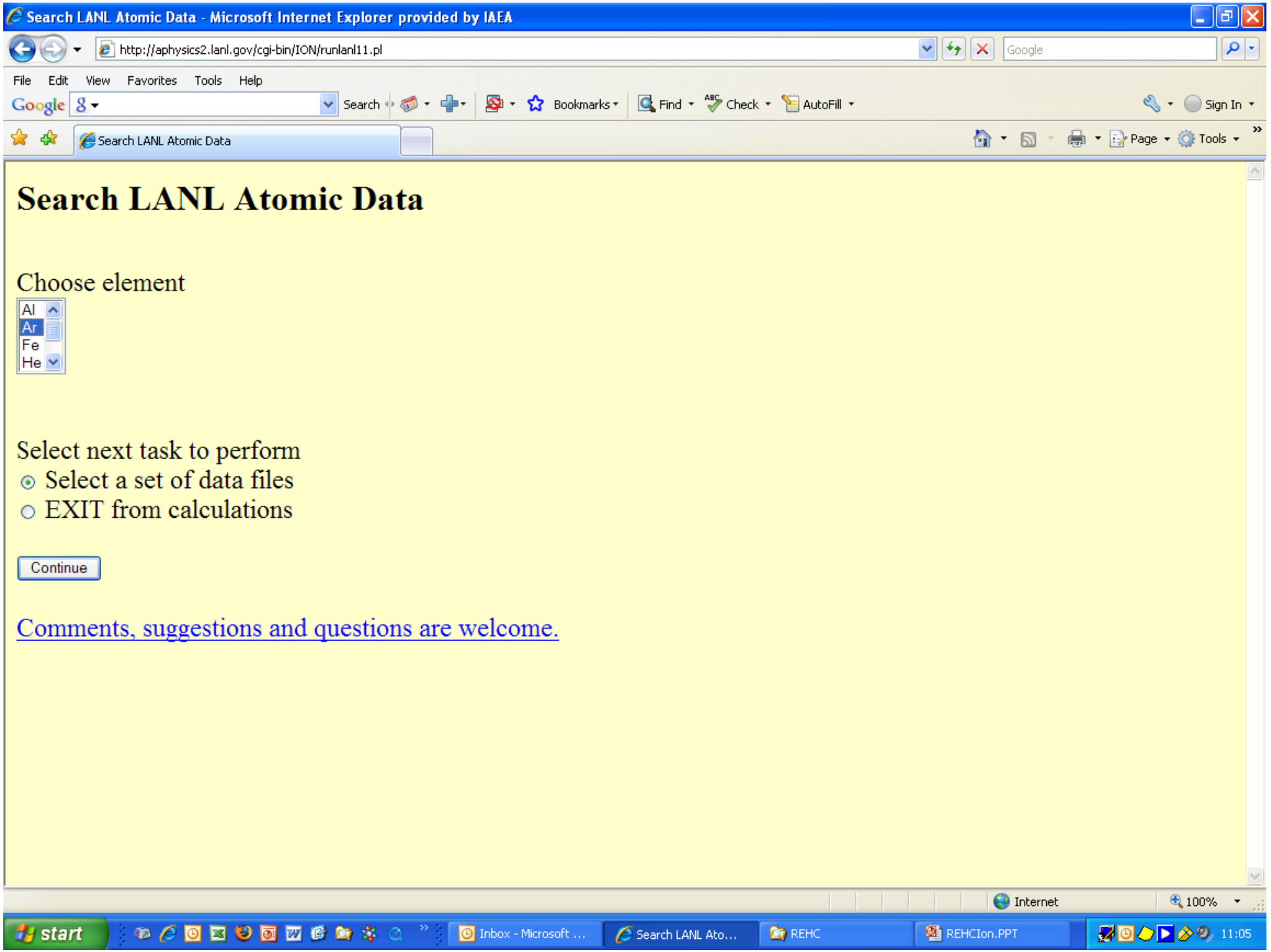
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Comments, suggestions and questions are welcome.
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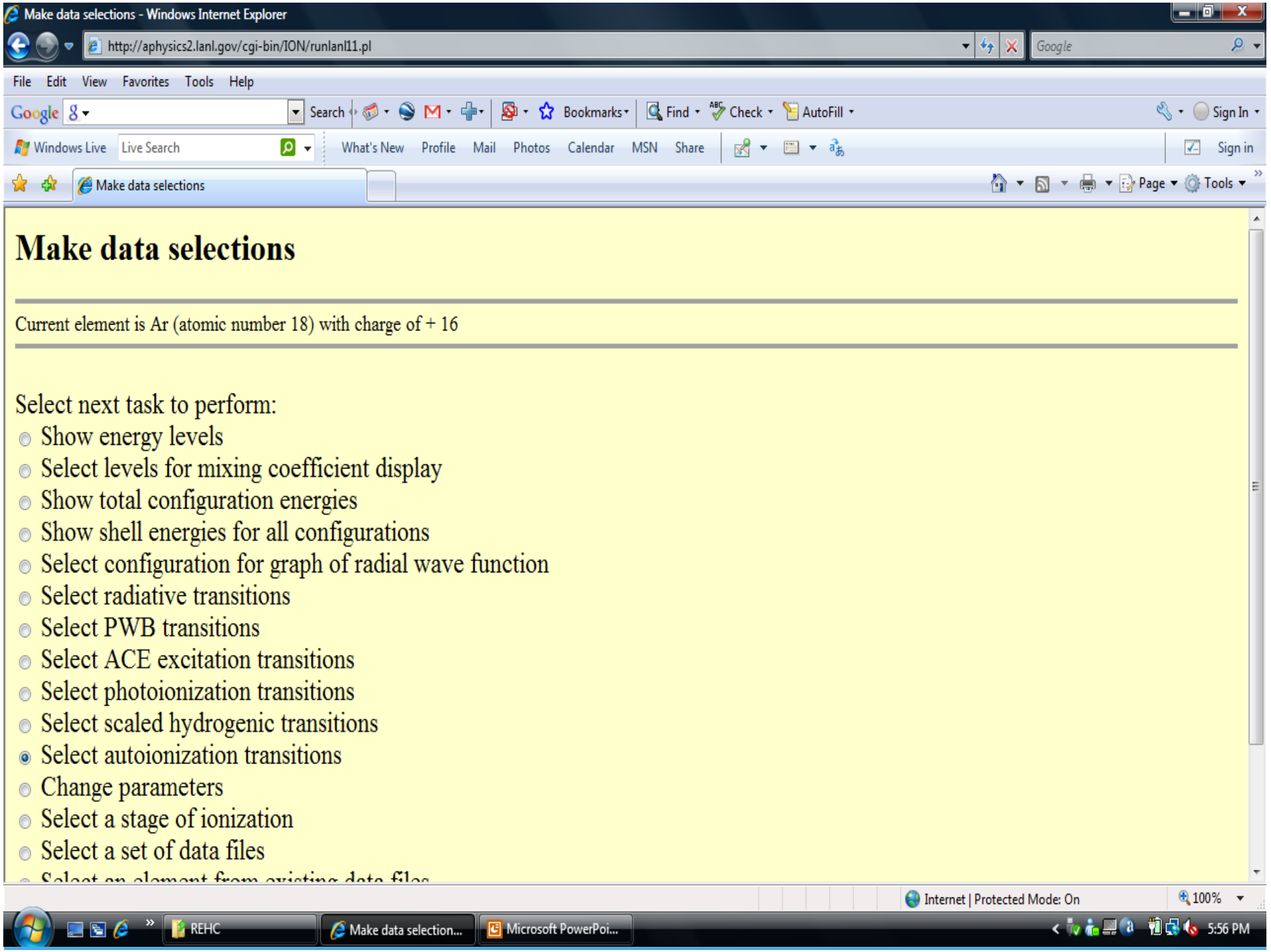
Make data selections - Windows Internet Explorer
http://aphysics2.lanl.gov/cgi-bin/ION/runlanl11.pl
Google
File Edit View Favorites Tools Help
Search
Bookmarks
Find
Check
AutoFill
Sign In
Windows Live
Live Search
What's New
Profile
Mail
Photos
Calendar
MSN
Share
Sign in
Make data selections
Page
Tools
Make data selections
Current element is Ar (atomic number 18) with charge of + 16
Select next task to perform:
Show energy levels
Select levels for mixing coefficient display
Show total configuration energies
Show shell energies for all configurations
Select configuration for graph of radial wave function
Select radiative transitions
Select PWB transitions
Select ACE excitation transitions
Select photoionization transitions
Select scaled hydrogenic transitions
Select autoionization transitions
Change parameters
Select a stage of ionization
Select a set of data files
Internet | Protected Mode: On
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REHC
Make data selection...
Microsoft PowerPoi...
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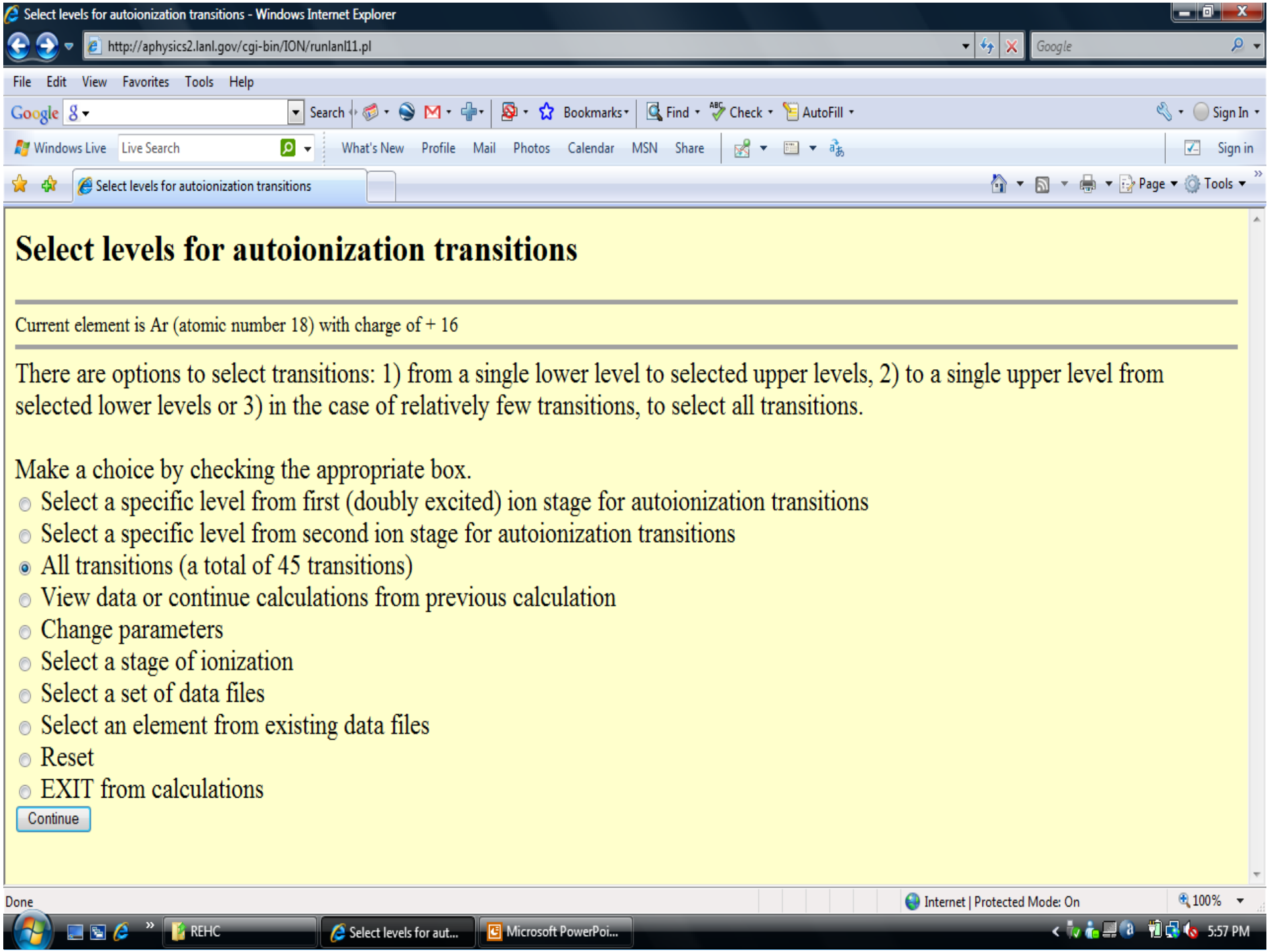
Select levels for autoionization transitions - Windows Internet Explorer
http://aphysics2.lanl.gov/cgi-bin/ION/runlanl11.pl
File Edit View Favorites Tools Help
Select levels for autoionization transitions
Select levels for autoionization transitions
Current element is Ar (atomic number 18) with charge of + 16
There are options to select transitions: 1) from a single lower level to selected upper levels, 2) to a single upper level from selected lower levels or 3) in the case of relatively few transitions, to select all transitions.
Make a choice by checking the appropriate box.
Select a specific level from first (doubly excited) ion stage for autoionization transitions
Select a specific level from second ion stage for autoionization transitions
All transitions (a total of 45 transitions)
View data or continue calculations from previous calculation
Change parameters
Select a stage of ionization
Select a set of data files
Select an element from existing data files
Reset
EXIT from calculations
Continue
Done
Internet | Protected Mode: On
100%
REHC
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Summary

- Interface allows calculation of electron impact ionization, photoionization and autoionization
- Scaled hydrogenic, binary encounter of DW
- Graphical and files of data available
- Archived data available