The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

IAEA
International Atomic Energy Agency

2028-3

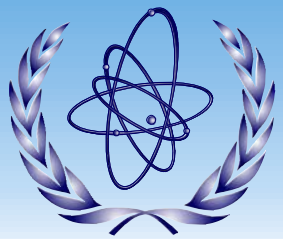
Joint ICTP/IAEA Workshop on Atomic and Molecular Data for Fusion

20 - 30 April 2009

Calculation of Atomic Data for Plasma Modeling: Electron Impact Excitation

Robert E.H. CLARK

IAEA, Div. of Physical & Chemical Science
Dept. of Nuclear Sciences & App. A-1400
Vienna
Austria



International Atomic Energy Agency

Calculation of Atomic Data for Plasma Modeling: Electron Impact Excitation

R. Clark, D. Humbert, K. Sheikh

Nuclear Data Section

Transition processes

- Excitation
- Ionization
- Autoionization
- Photoionization
- Inverse processes
- Both electron and ion impact may be important in above
- Charge transfer
- Molecular processes

General Formulation for excitation

$$Q = \sum \left| R(a,b) \right|^2$$

$$R(a,b) = \int dx_1 \ldots \int dx_{N+1} u^*(x_i) \Psi^*(x_i^{-1}) \left[\sum \frac{1}{r_{pj}} \right] u(x_j) \Psi(x_j^{-1})$$

Electron impact excitation considerations

- Requires solution of coupled equations representing target states and free electrons
- Common solution is to largely decouple to initial target and free electron, final target and free electron
- Choices are then in method of solution for target and for free electron

Common approximations

- Plane-wave-Born
- Coulomb Born
- Distorted wave
- Close coupling

Allowed and forbidden transitions

- Dipole allowed, $l_2 = l_1 \pm 1$, are generally stronger, with $l_2 = l_1 + 1$ the stronger
- Spin allowed are generally stronger, singlet-singlet or triplet-triplet
- $J_2 = J_1 \pm 1,0$ but not $J_2 = J_1 = 0$
- Mixing can change these general assumptions

Plane wave Born

- Two state method
- Free electrons are both plane wave, potential of target is completely ignored
- Cross sections can be calculated from generalized oscillator strength from target states
- Calculation is fast
- Accuracy best at high impact electron energies
- Option in structure code to calculate PWB

Coulomb Born

- Next level of approximation
- Free electrons are Coulomb functions, using Z-N bound electrons for effective charge
- Sampson et. al. calculated for hydrogenic targets, then used screening parameters to extend to complex ions
- Best for several times ionized and not many equivalent electrons

Distorted wave

- Take into account the actual potential from the target state in calculation of free electron
- Several methods for doing this, DWA, FOMBT
- Exchange effect on potential also treated in variety of ways
- Average approximation allows faster solution

Close coupling

- Solve full set of coupled equations, bound and free
- May include many high lying states, above continuum, leading to resonances
- Long computing time required
- R-Matrix theory allows solutions within limited radius, match energy solutions at boundary
- Most accurate theory

Collision strength

- Cross section generally of order of atomic dimension
- Cross section decreases with energy
- Cross section dependent on direction of transition
- Collision strength defined as:

$$Q_{ij} = \frac{\pi a_2^0}{g_i E_i (Ryd)} \Omega(i, j)$$

Rate coefficients

- Electron distribution is often Maxwellian
- Weighted integral of cross section gives rate coefficient:

$$R = \int F(E,T)\, v(E)\, \sigma(E)\, dE$$

Rate coefficients

- Can be generated from web interface
- Function of temperature, not individual electron energy
- Temperature grid automatically set by interface from range of impact energies used in cross section calculation
- Must have sufficient points for integration to make sense

Detailed balance

- In LTE, rates for upward and downward balance: $n_i R_{ij} = n_j R_{ij}$
- Populations given by energies and statistical weights (assume Maxwellian electron distribution)
- Gives relationship between cross section and inverse:

$$R_{ji} = \frac{g_i}{g_j} e^{\frac{-E}{kT}} R_{ij}$$

Resonances

- Doubly excited levels may be formed and autoionize to a singly excited level
- Consider e + $1s^2$ → 1s2p + e' as the direct excitation
- At a particular energy a capture can take place: e + $1s^2$ → 1s3dnl giving a doubly excited state

Resonances

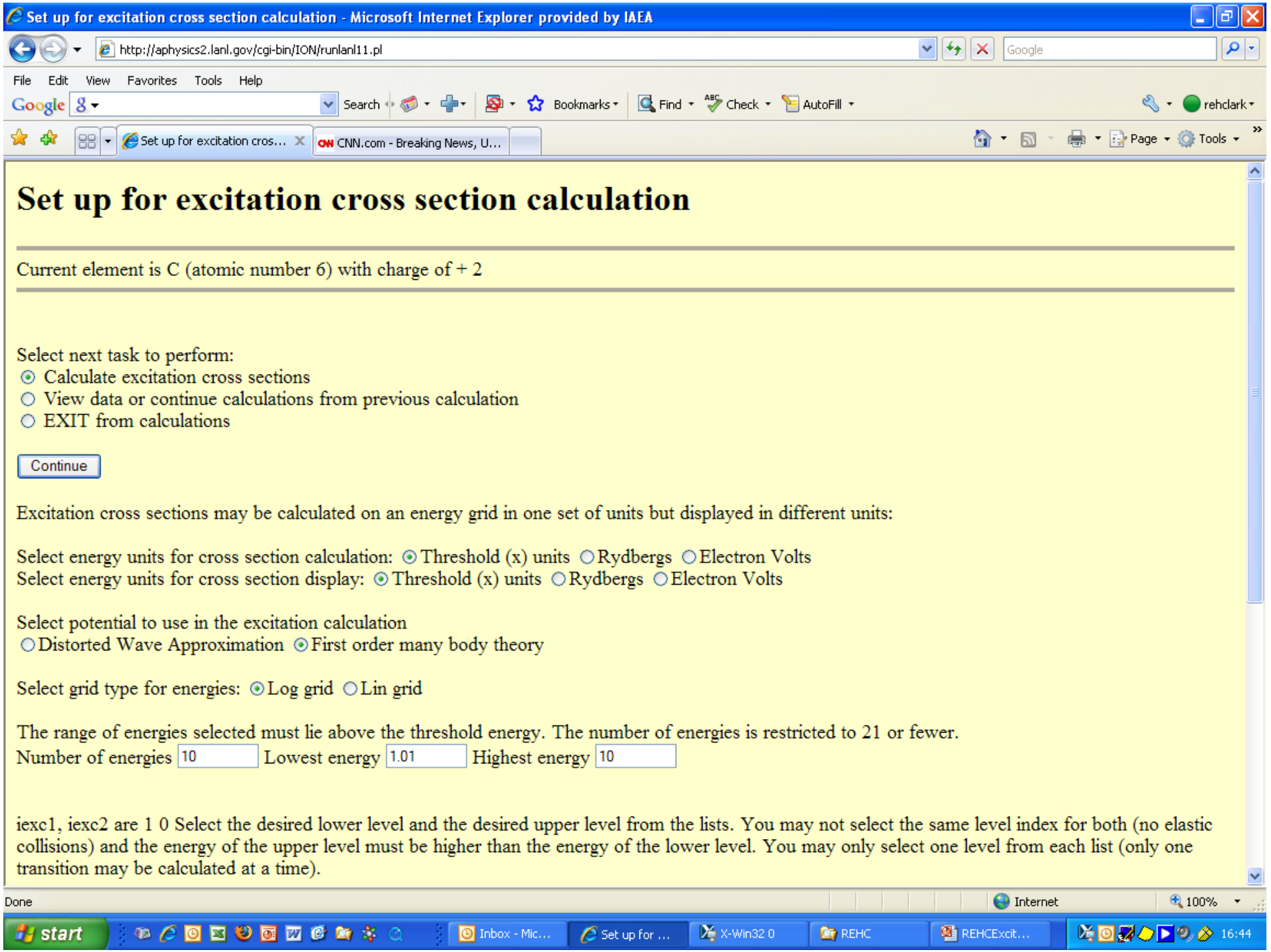
- Autoionization can proceed:
  $1s3dnl \rightarrow 1s2p + e'$
- Series takes place for different values of nl. Also, change the 3d shell to 3s, 3p, etc. Many resonances can occur
- Each resonance is at a definite, discrete energy, dictated by capture of the initial free electron into a specific state

Resources on the web

- Several electronic databases searched by GENIE
- LANL codes use DWA or FOMBT for electron impact excitation, configuration or fine structure
- Average approximation on A+M Unit home page for electron impact in configuration mode only
- Heavy particle collisions on Unit home page, bare nucleus on hydrogenic ion

LANL calculations

- Generate atomic structure, files are saved
- Select energy parameters
- Select potential
- Select transition


Set up for excitation cross section calculation - Microsoft Internet Explorer provided by IAEA
http://aphysics2.lanl.gov/cgi-bin/ION/runlanl11.pl
File Edit View Favorites Tools Help
Set up for excitation cros...
CNN.com - Breaking News, U...
Set up for excitation cross section calculation
Current element is C (atomic number 6) with charge of + 2
Select next task to perform:
Calculate excitation cross sections
View data or continue calculations from previous calculation
EXIT from calculations
Continue
Excitation cross sections may be calculated on an energy grid in one set of units but displayed in different units:
Select energy units for cross section calculation: Threshold (x) units Rydbergs Electron Volts
Select energy units for cross section display: Threshold (x) units Rydbergs Electron Volts
Select potential to use in the excitation calculation
Distorted Wave Approximation First order many body theory
Select grid type for energies: Log grid Lin grid
The range of energies selected must lie above the threshold energy. The number of energies is restricted to 21 or fewer.
Number of energies 10 Lowest energy 1.01 Highest energy 10
iexc1, iexc2 are 1 0 Select the desired lower level and the desired upper level from the lists. You may not select the same level index for both (no elastic collisions) and the energy of the upper level must be higher than the energy of the lower level. You may only select one level from each list (only one transition may be calculated at a time).
Done
Internet
100%
start
Inbox - Mic...
Set up for ...
X-Win32 0
REHC
REHCExcit...
16:44

Set up for excitation cross section calculation - Microsoft Internet Explorer provided by IAEA

http://aphysics2.lanl.gov/cgi-bin/ION/runlanl11.pl

File Edit View Favorites Tools Help

Google Search Bookmarks Find Check AutoFill rehclark

Set up for excitation cros... CNN.com - Breaking News, U...

Page Tools

Select potential to use in the excitation calculation

○ Distorted Wave Approximation ◉ First order many body theory

Select grid type for energies: ◉ Log grid ○ Lin grid

The range of energies selected must lie above the threshold energy. The number of energies is restricted to 21 or fewer.

Number of energies 10 Lowest energy 1.01 Highest energy 10

iexc1, iexc2 are 1 0 Select the desired lower level and the desired upper level from the lists. You may not select the same level index for both (no elastic collisions) and the energy of the upper level must be higher than the energy of the lower level. You may only select one level from each list (only one transition may be calculated at a time).

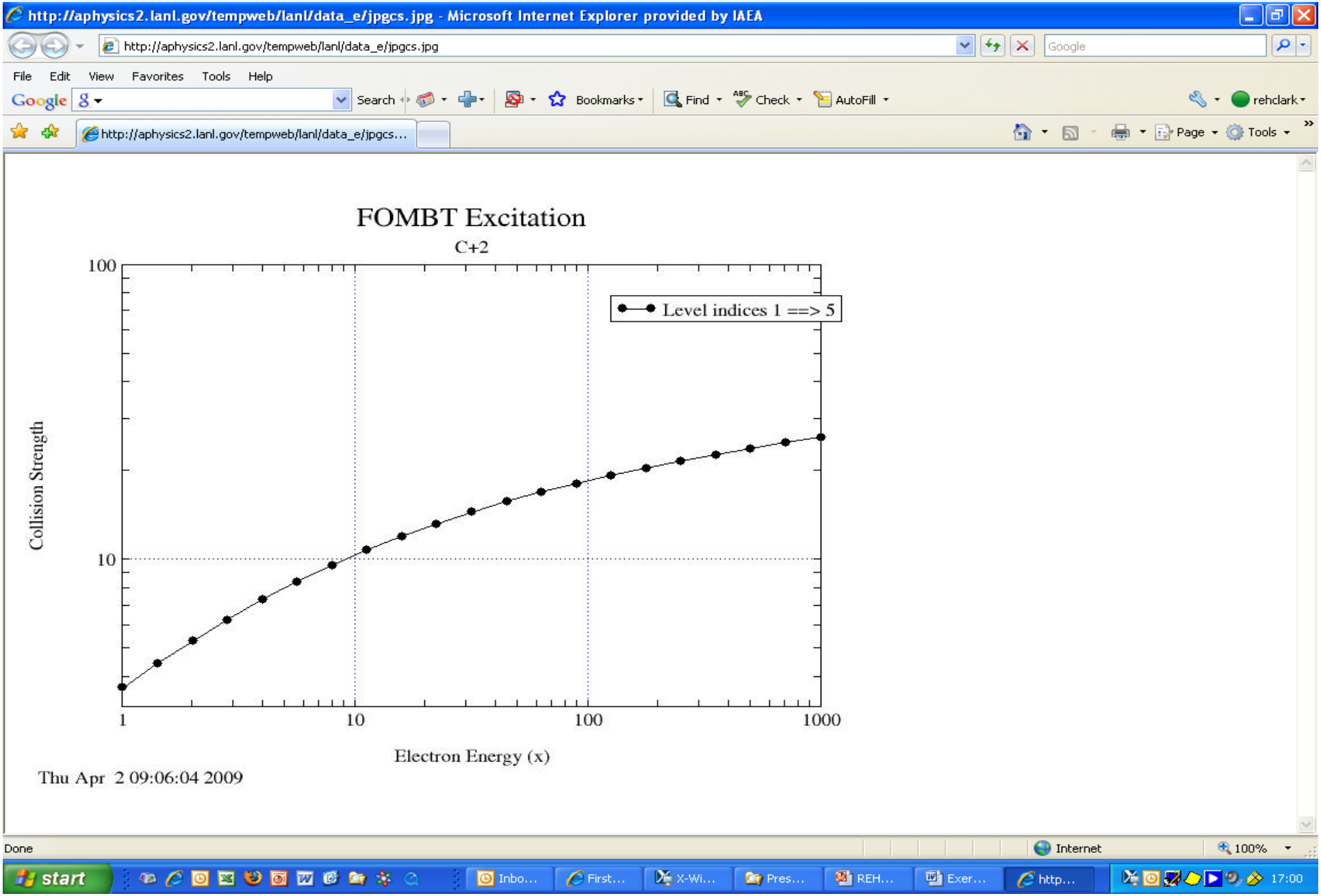
Lower level	Upper level
0.0000e+00 (2s2 1S)1S0.0	All levels
6.4463e+00 (2s1 2S)2S (2p1 2P)3P0.0	0.0000e+00 (2s2 1S)1S0.0
6.4497e+00 (2s1 2S)2S (2p1 2P)3P1.0	6.4463e+00 (2s1 2S)2S (2p1 2P)3P0.0
6.4566e+00 (2s1 2S)2S (2p1 2P)3P2.0	6.4497e+00 (2s1 2S)2S (2p1 2P)3P1.0
1.2871e+01 (2s1 2S)2S (2p1 2P)1P1.0	6.4566e+00 (2s1 2S)2S (2p1 2P)3P2.0
1.7051e+01 (2p2 3P)3P0.0	1.2871e+01 (2s1 2S)2S (2p1 2P)1P1.0
1.7054e+01 (2p2 3P)3P1.0	1.7051e+01 (2p2 3P)3P0.0
1.7061e+01 (2p2 3P)3P2.0	1.7054e+01 (2p2 3P)3P1.0
1.8597e+01 (2p2 1D)1D2.0	1.7061e+01 (2p2 3P)3P2.0
2.2933e+01 (2p2 1S)1S0.0	1.8597e+01 (2p2 1D)1D2.0
2.9622e+01 (2s1 2S)2S (3s1 2S)3S1.0	2.2933e+01 (2p2 1S)1S0.0
3.0754e+01 (2s1 2S)2S (3s1 2S)1S0.0	2.9622e+01 (2s1 2S)2S (3s1 2S)3S1.0
3.2302e+01 (2s1 2S)2S (3p1 2P)1P1.0	3.0754e+01 (2s1 2S)2S (3s1 2S)1S0.0
3.2329e+01 (2s1 2S)2S (3p1 2P)3P0.0	3.2302e+01 (2s1 2S)2S (3p1 2P)1P1.0
3.2329e+01 (2s1 2S)2S (3p1 2P)3P1.0	3.2329e+01 (2s1 2S)2S (3p1 2P)3P0.0
3.2331e+01 (2s1 2S)2S (3p1 2P)3P2.0	3.2329e+01 (2s1 2S)2S (3p1 2P)3P1.0
3.3592e+01 (2s1 2S)2S (3d1 2D)3D1.0	3.2331e+01 (2s1 2S)2S (3p1 2P)3P2.0
3.3593e+01 (2s1 2S)2S (3d1 2D)3D2.0	3.3592e+01 (2s1 2S)2S (3d1 2D)3D1.0
3.3593e+01 (2s1 2S)2S (3d1 2D)3D3.0	3.3593e+01 (2s1 2S)2S (3d1 2D)3D2.0
3.4531e+01 (2s1 2S)2S (3d1 2D)1D2.0	3.3593e+01 (2s1 2S)2S (3d1 2D)3D3.0

Continue

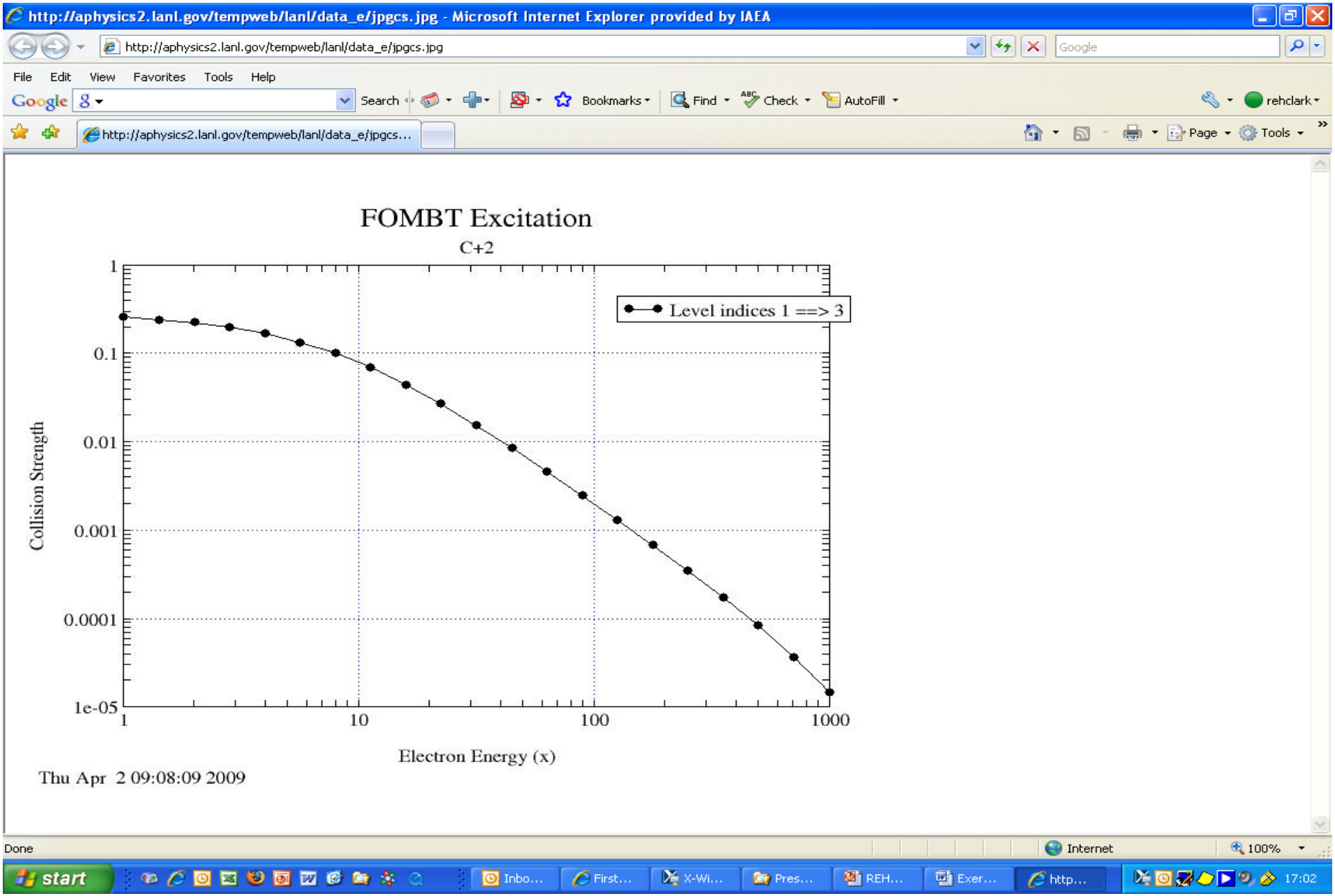
Done Internet 100%

start Inbox - Mic... Set up for ... X-Win32 0 REHC REHCExcit... 16:44

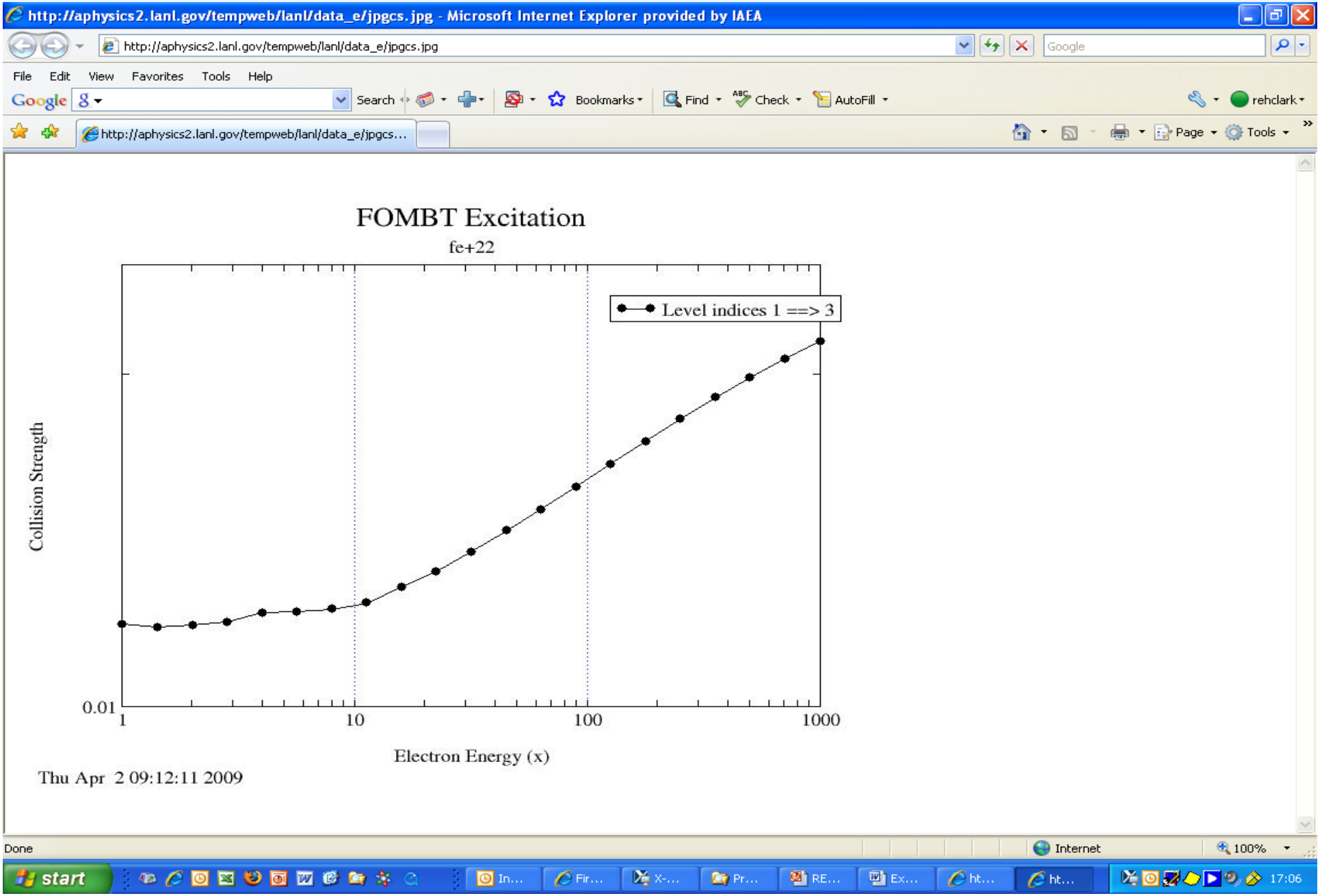
$C^{+2}\ 2s^2\ ^1S_0 \rightarrow 2s2p\ ^1P_1$



$C^{+2}\ 2s^2\ {}^1S_0 \rightarrow 2s2p\ {}^3P_1$

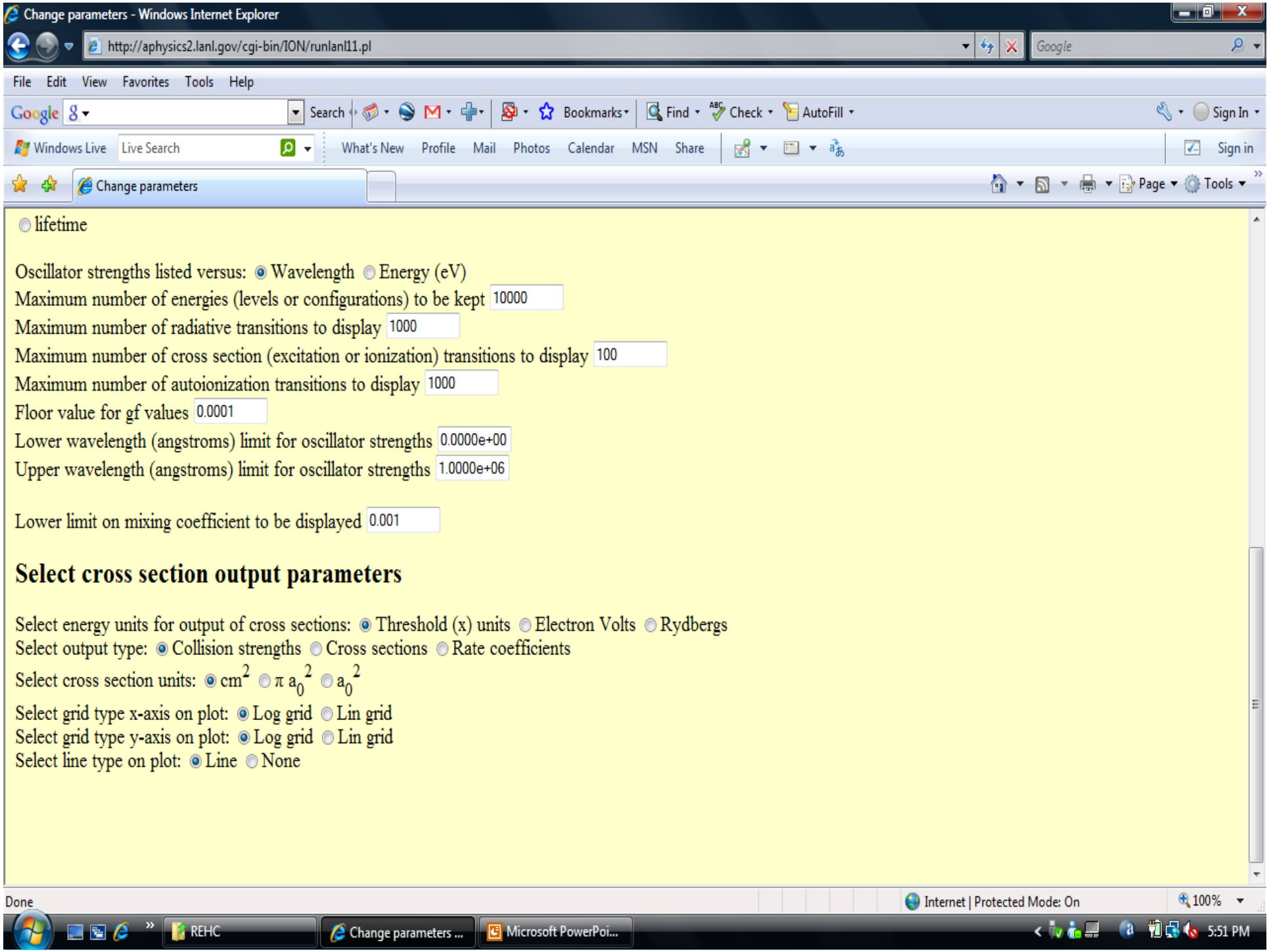


$Fe^{+22}\ 2s^2\ {}^1S_0 \rightarrow 2s2p\ {}^3P_1$



Why the difference

- It is seen that the $2s^2\ {}^1S_0 \rightarrow 2s2p\ {}^1P_1$ collision strength rises with energy
- The $2s^2\ {}^1S_0 \rightarrow 2s2p\ {}^3P_1$ is a spin forbidden transition in LS coupling
- For C^{+2} there is little spin-orbit mixing, it is a spin forbidden transition
- For Fe^{+22} there is considerable spin-orbit mixing, so there is an allowed component that rises at high energy


Change parameters - Windows Internet Explorer
http://aphysics2.lanl.gov/cgi-bin/ION/runlanl11.pl
File Edit View Favorites Tools Help
Change parameters
lifetime
Oscillator strengths listed versus: Wavelength Energy (eV)
Maximum number of energies (levels or configurations) to be kept 10000
Maximum number of radiative transitions to display 1000
Maximum number of cross section (excitation or ionization) transitions to display 100
Maximum number of autoionization transitions to display 1000
Floor value for gf values 0.0001
Lower wavelength (angstroms) limit for oscillator strengths 0.0000e+00
Upper wavelength (angstroms) limit for oscillator strengths 1.0000e+06
Lower limit on mixing coefficient to be displayed 0.001
Select cross section output parameters
Select energy units for output of cross sections: Threshold (x) units Electron Volts Rydbergs
Select output type: Collision strengths Cross sections Rate coefficients
Select cross section units: cm2 π a0 2 a0 2
Select grid type x-axis on plot: Log grid Lin grid
Select grid type y-axis on plot: Log grid Lin grid
Select line type on plot: Line None
Done
Internet | Protected Mode: On
100%
REHC
Change parameters ...
Microsoft PowerPoi...
5:51 PM

Summary

- Interface allows user to calculate excitation between selected levels
- Results in graphical, ALADDIN format
- Cross sections, collision strength or rate coefficients available
- DWA or FOMBT for potential