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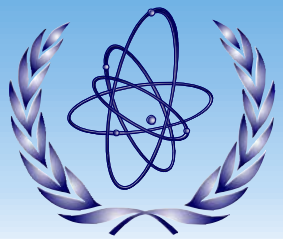
Calculation of Atomic Data for Plasma Modeling: Atomic Structure II

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: Atomic Structure II

R. Clark, D. Humbert, K. Sheikh

Nuclear Data Section

Data Obtained From Structure Code

- Energy levels
- Radial wave functions
- Effects of mixing (configuration and spin-orbit)
- Plane wave Born (PWB) collision cross sections
- Oscillator strengths
- Configuration and fine structure modes

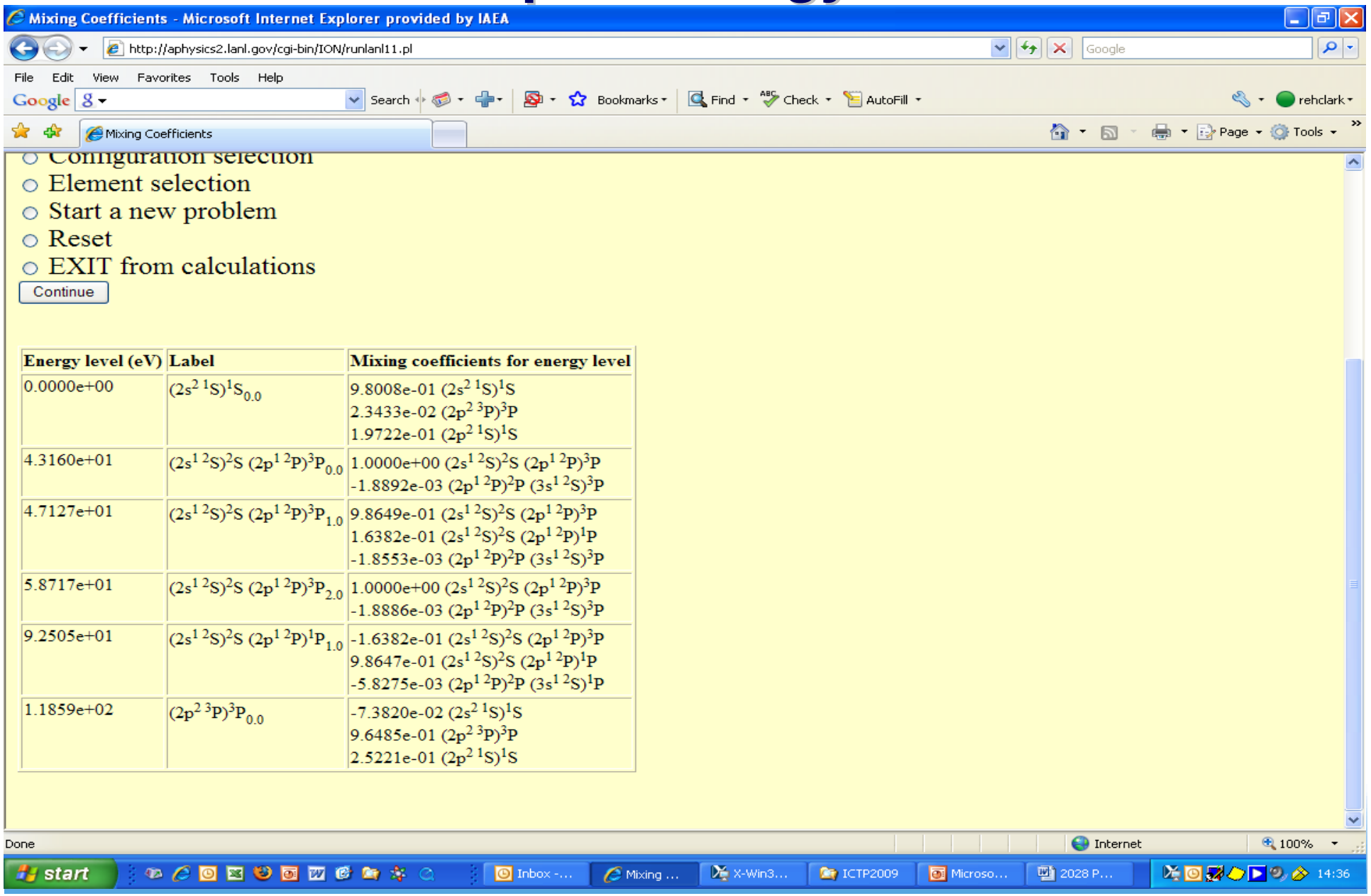
Mixing of target states

- Configurations and LS terms form basis states
- Coulomb interaction causes mixing of configurations which have the same LS terms
- Spin-orbit causes mixing of LS terms which have the same configuration
- Mixing provides better description of energy levels

Example of Configuration Mixing

- Consider Be-like ion, Fe^{+22}.
- Consider configurations $2s^2$, 2s2p, $2p^2$, 2s3p and 2p3s.
- Configuration mixing occurs due to Coulomb interaction.
- Spin-orbit causes mixing of LS terms.
- List of make-up of energy levels:

Make-up of Energy Levels



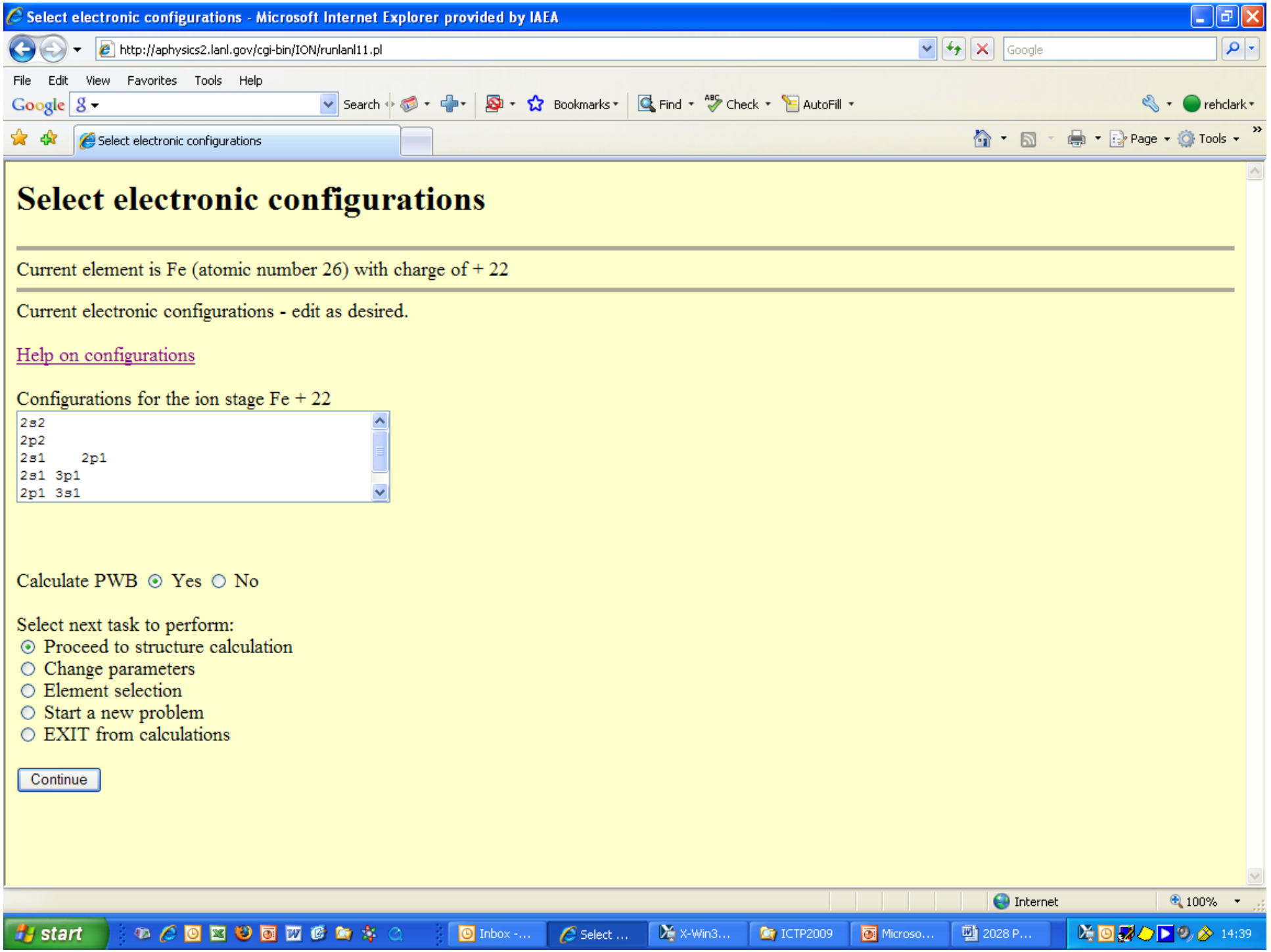
Energy level (eV)	Label	Mixing coefficients for energy level
0.0000e+00	$(2s^2\ ^1S)^1S_{0.0}$	9.8008e-01 $(2s^2\ ^1S)^1S$ 2.3433e-02 $(2p^2\ ^3P)^3P$ 1.9722e-01 $(2p^2\ ^1S)^1S$
4.3160e+01	$(2s^1\ ^2S)^2S\ (2p^1\ ^2P)^3P_{0.0}$	1.0000e+00 $(2s^1\ ^2S)^2S\ (2p^1\ ^2P)^3P$ -1.8892e-03 $(2p^1\ ^2P)^2P\ (3s^1\ ^2S)^3P$
4.7127e+01	$(2s^1\ ^2S)^2S\ (2p^1\ ^2P)^3P_{1.0}$	9.8649e-01 $(2s^1\ ^2S)^2S\ (2p^1\ ^2P)^3P$ 1.6382e-01 $(2s^1\ ^2S)^2S\ (2p^1\ ^2P)^1P$ -1.8553e-03 $(2p^1\ ^2P)^2P\ (3s^1\ ^2S)^3P$
5.8717e+01	$(2s^1\ ^2S)^2S\ (2p^1\ ^2P)^3P_{2.0}$	1.0000e+00 $(2s^1\ ^2S)^2S\ (2p^1\ ^2P)^3P$ -1.8886e-03 $(2p^1\ ^2P)^2P\ (3s^1\ ^2S)^3P$
9.2505e+01	$(2s^1\ ^2S)^2S\ (2p^1\ ^2P)^1P_{1.0}$	-1.6382e-01 $(2s^1\ ^2S)^2S\ (2p^1\ ^2P)^3P$ 9.8647e-01 $(2s^1\ ^2S)^2S\ (2p^1\ ^2P)^1P$ -5.8275e-03 $(2p^1\ ^2P)^2P\ (3s^1\ ^2S)^1P$
1.1859e+02	$(2p^2\ ^3P)^3P_{0.0}$	-7.3820e-02 $(2s^2\ ^1S)^1S$ 9.6485e-01 $(2p^2\ ^3P)^3P$ 2.5221e-01 $(2p^2\ ^1S)^1S$

Consequences of Mixing

- Configuration can allow “double electron” jumps. Since the $2s^2\ {}^1S_0$ contains some of the $2p^2\ {}^1S_0$ state, it becomes possible to have a non-zero probability for a transition to occur between those states.
- LS term mixing can cause radiative transitions between “spin-forbidden” states

Mixing effects on PWB

- Consider the transition in the He-like iron transition $2s^2\ {}^1S_0 \rightarrow 2p^2\ {}^3P_0$.
- This would normally be a forbidden transition for PWB for two reasons: It is a double electron jump and it is spin forbidden
- The calculation shows the PWB, while small, is non zero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http://aphysics2.lanl.gov/cgi-bin/ION/runlanl11.pl
Google
File Edit View Favorites Tools Help
Search Bookmarks Find Check AutoFill rehclark
Select electronic configurations
Page Tools
Select electronic configurations
Current element is Fe (atomic number 26) with charge of + 22
Current electronic configurations - edit as desired.
Help on configurations
Configurations for the ion stage Fe + 22
2s2
2p2
2s1 2p1
2s1 3p1
2p1 3s1
Calculate PWB Yes No
Select next task to perform:
Proceed to structure calculation
Change parameters
Element selection
Start a new problem
EXIT from calculations
Continue
Internet
100%
start
Inbox -...
Select ...
X-Win3...
ICTP2009
Microso...
2028 P...
14:39

Continue

Current element is Fe (atomic number 26) with charge of + 22

ALADDIN file for PWB transitions

JPEG file(new window)

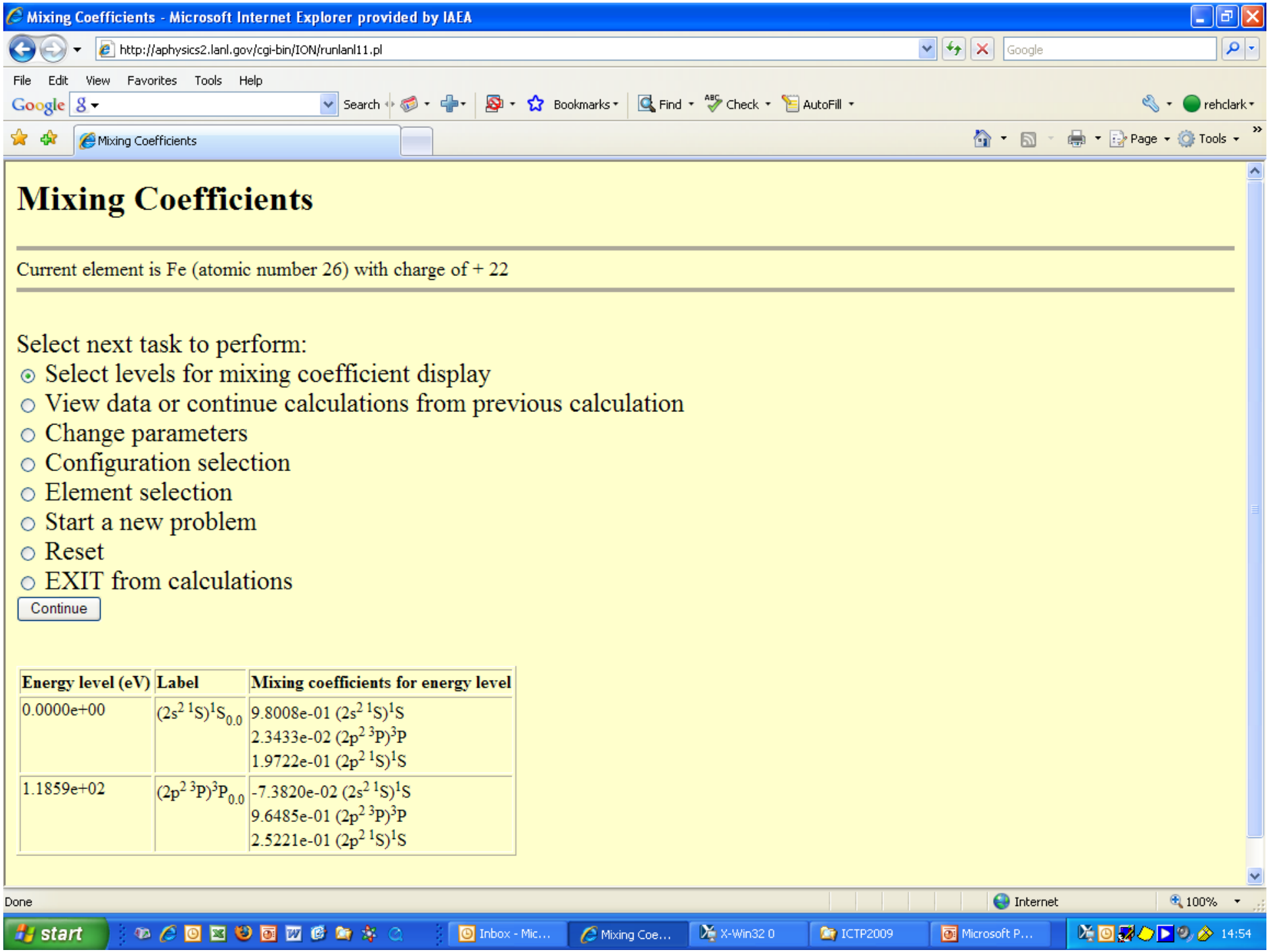
Energy (x) Collision Strength

Transition is $(2s^2\ ^1S)^1S_{0.0}$ ==> $(2p^2\ ^3P)^3P_{0.0}$ with transition energy of 1.1859e+02 eV

1.0100e+00 3.1607e-04
1.4260e+00 3.3530e-04
2.0132e+00 3.7385e-04
2.8423e+00 4.3363e-04
4.0129e+00 5.1082e-04
5.6655e+00 5.9731e-04
7.9988e+00 6.8297e-04
1.1293e+01 7.5892e-04
1.5944e+01 8.2014e-04
2.2510e+01 8.6620e-04
3.1781e+01 8.9926e-04
4.4868e+01 9.2239e-04
6.3348e+01 9.3832e-04
8.9440e+01 9.5005e-04
1.2627e+02 9.5766e-04
1.7827e+02 9.6341e-04
2.5169e+02 9.6734e-04
3.5534e+02 9.6997e-04
5.0169e+02 9.7276e-04
7.0830e+02 9.7370e-04
9.9997e+02 9.7429e-04

Mixing effects on PWB

- Neither the $2s^2\ {}^1S_0$ nor the $2p^2\ {}^3P_0$ level is a pure level. Mixing of the configurations occurs due to the coulomb interaction and mixing of the singlet and triplet comes in through the spin-orbit interaction, allowing this transition to occur.
- Such effects are important, they often open a channel for population or de-population of levels in a plasma calculation



Mixing Coefficients

Current element is Fe (atomic number 26) with charge of + 22

Select next task to perform:

- (•) Select levels for mixing coefficient display
- ( ) View data or continue calculations from previous calculation
- ( ) Change parameters
- ( ) Configuration selection
- ( ) Element selection
- ( ) Start a new problem
- ( ) Reset
- ( ) EXIT from calculations

Continue

Energy level (eV)	Label	Mixing coefficients for energy level
0.0000e+00	$(2s^2\ ^1S)^1S_{0.0}$	9.8008e-01 $(2s^2\ ^1S)^1S$ 2.3433e-02 $(2p^2\ ^3P)^3P$ 1.9722e-01 $(2p^2\ ^1S)^1S$
1.1859e+02	$(2p^2\ ^3P)^3P_{0.0}$	-7.3820e-02 $(2s^2\ ^1S)^1S$ 9.6485e-01 $(2p^2\ ^3P)^3P$ 2.5221e-01 $(2p^2\ ^1S)^1S$

Mixing effects on oscillator strength

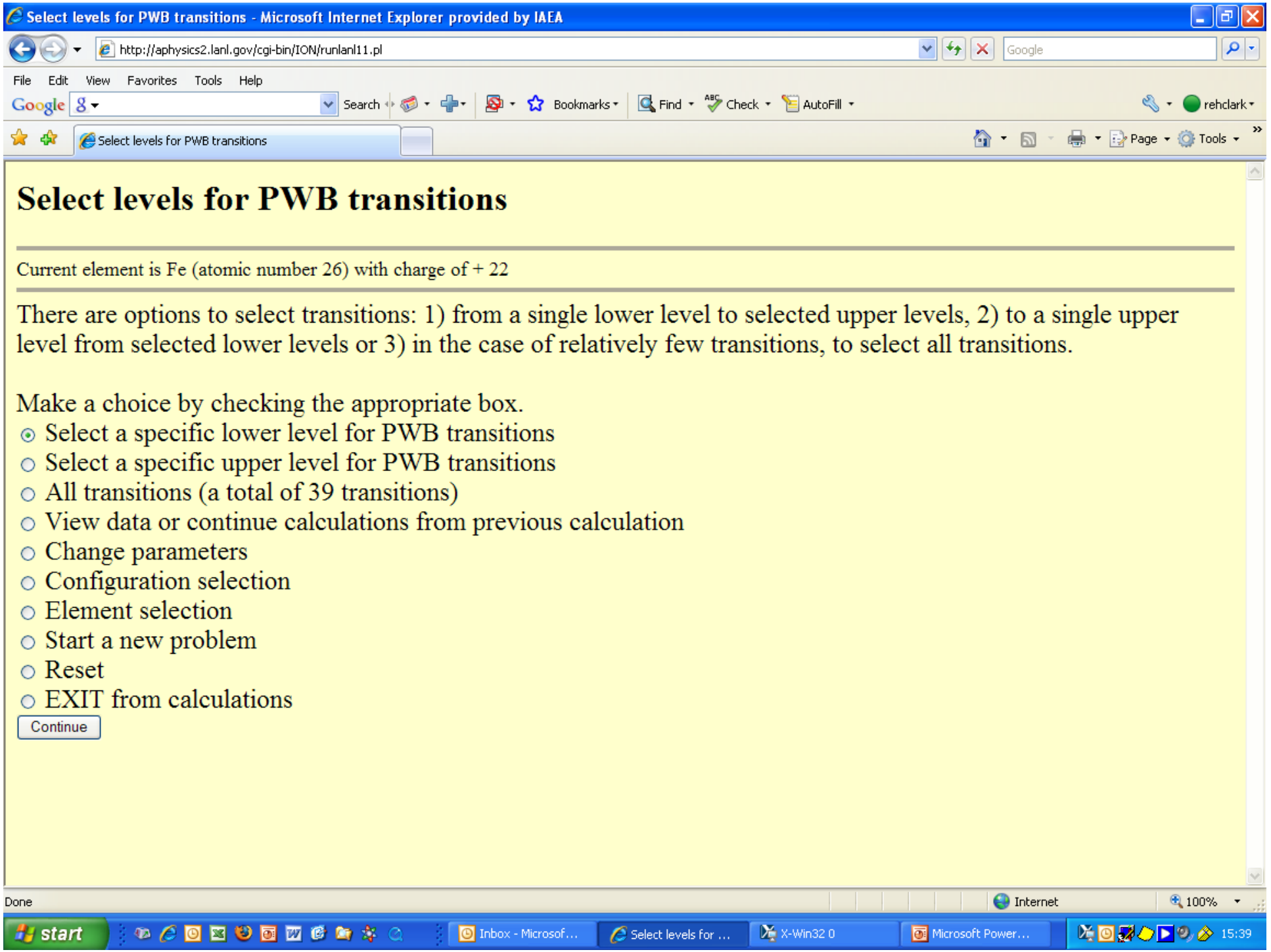
- Consider He-like transition $1s^2 \rightarrow 1s2p\,^3P_1$.
- The $1s2p\,^3P_1$ is actually a mixture of $^1P_1$ and $^3P_1$ with the mixing varying with nuclear charge. For C, they mixing coefficients are 0.99995 and 0.00041, while for Fe they are 0.95922 and 0.28266.
- For carbon this is a forbidden transition, gf = 1.1851e-05

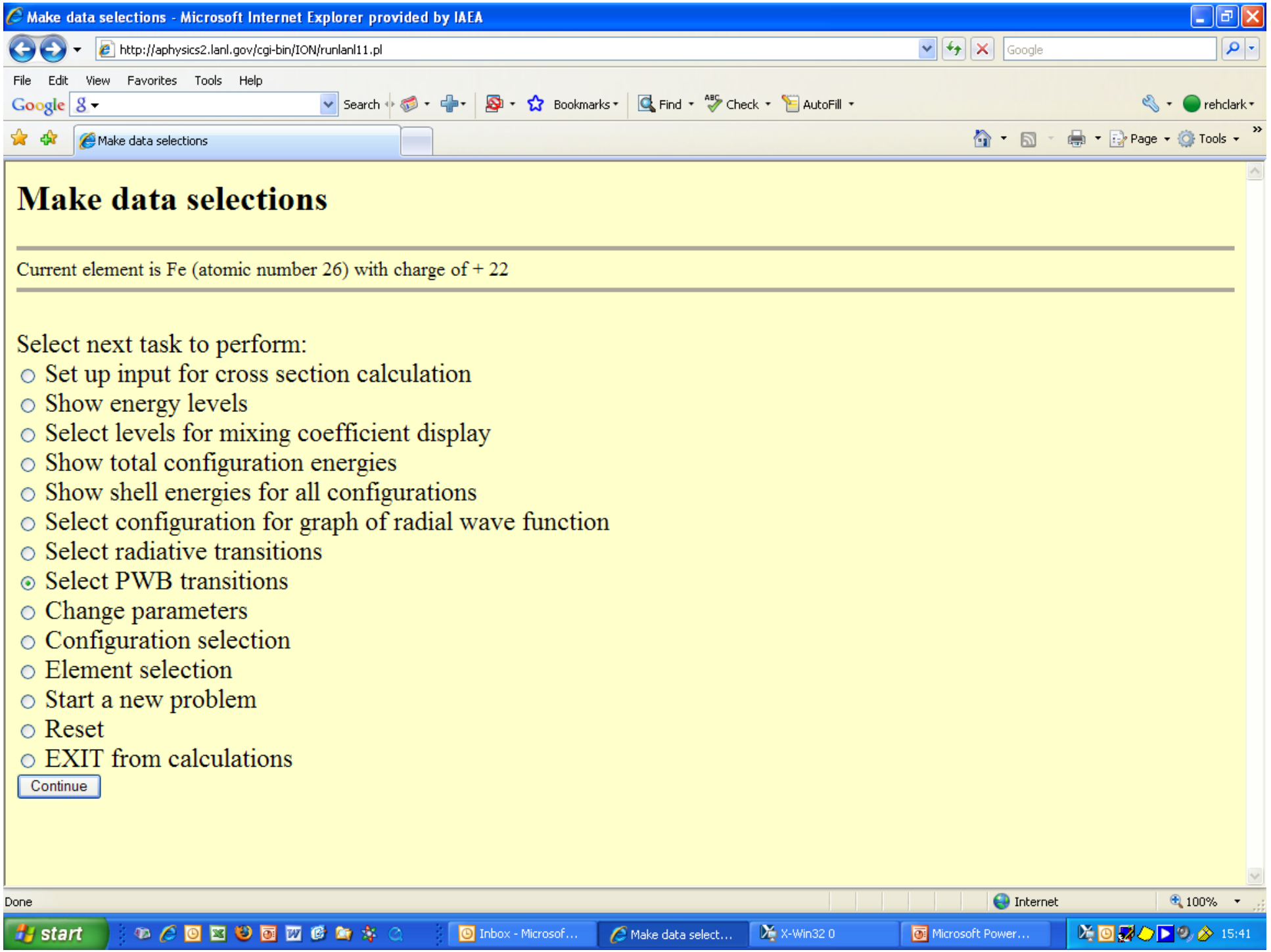
Mixing effects on oscillator strength

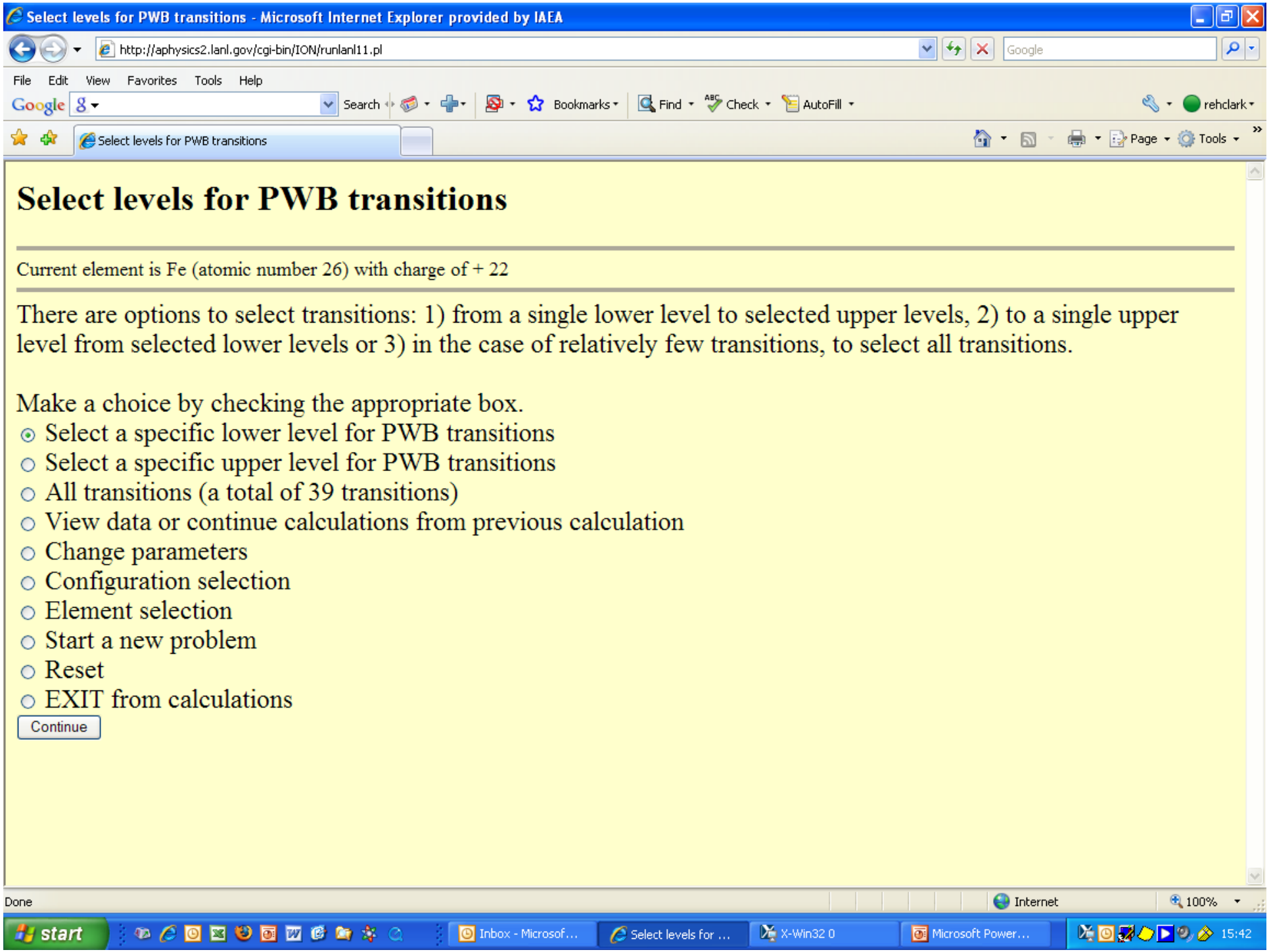
- For iron it is allowed, gf = 6.3684e-02
- This makes a difference in radiated power and for ionization balance
- For carbon, electron configuration over-estimates radiated power, underestimates ionization rates
- For iron, configuration model is better

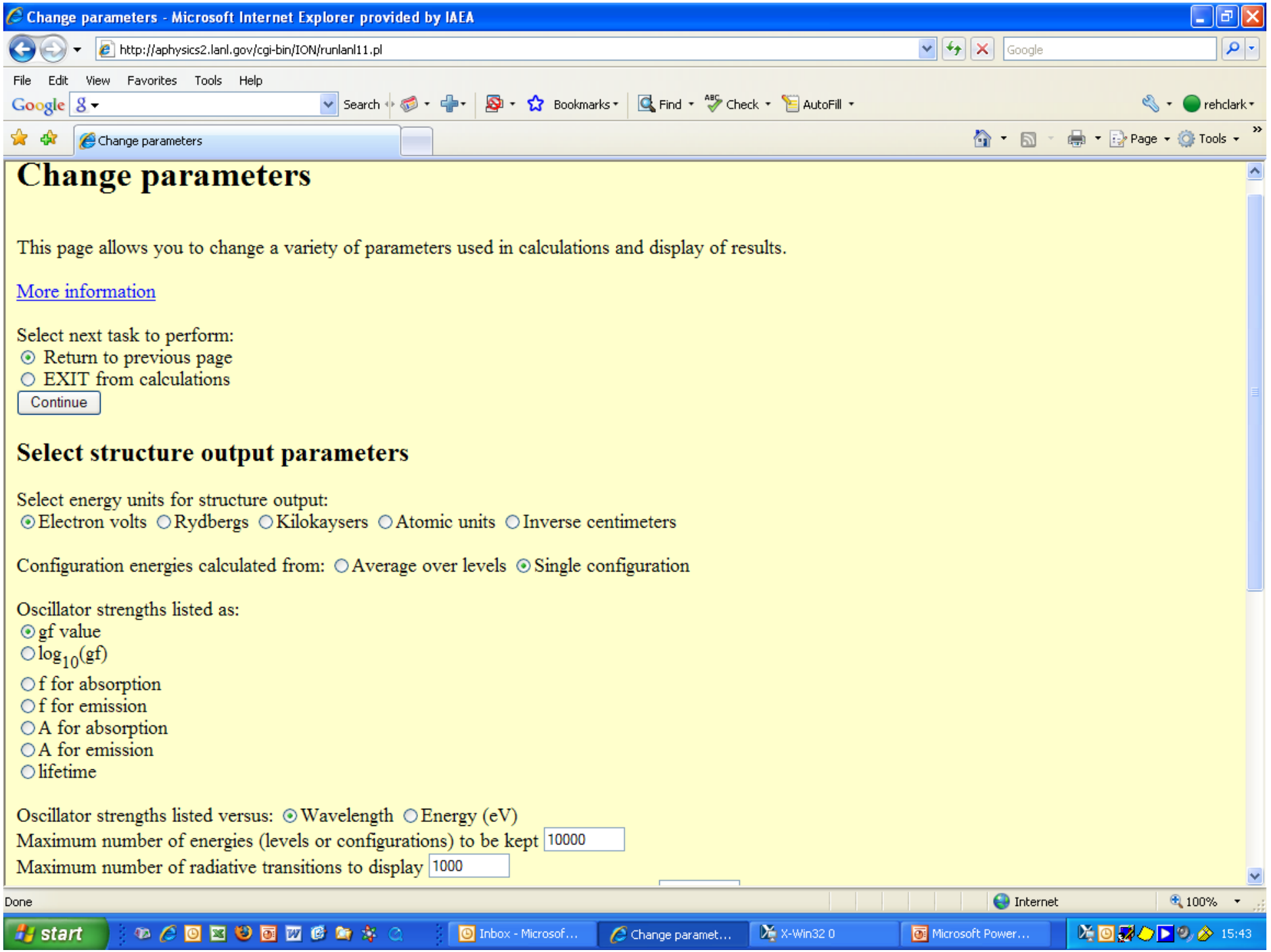
Selecting data for display

- All available data are listed by type
- Selection of data type allows selection by transition, lower and upper levels
- For small number of transitions, all may be viewed simultaneously
- Parameters can be changed at any time


Select levels for PWB transitions - Microsoft Internet Explorer provided by IAEA
http://aphysics2.lanl.gov/cgi-bin/ION/runlanl11.pl
File Edit View Favorites Tools Help
Select levels for PWB transitions
Select levels for PWB transitions
Current element is Fe (atomic number 26) with charge of + 22
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 lower level for PWB transitions
Select a specific upper level for PWB transitions
All transitions (a total of 39 transitions)
View data or continue calculations from previous calculation
Change parameters
Configuration selection
Element selection
Start a new problem
Reset
EXIT from calculations
Continue
Done
Internet
100%
start
15:39


Make data selections - Microsoft Internet Explorer provided by IAEA
http://aphysics2.lanl.gov/cgi-bin/ION/runlanl11.pl
Google
File Edit View Favorites Tools Help
Search Bookmarks Find Check AutoFill rehclark
Make data selections
Page Tools
Make data selections
Current element is Fe (atomic number 26) with charge of + 22
Select next task to perform:
Set up input for cross section calculation
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
Change parameters
Configuration selection
Element selection
Start a new problem
Reset
EXIT from calculations
Continue
Done
Internet
100%
start
Inbox - Microsof...
Make data select...
X-Win32 0
Microsoft Power...
15:41


Select levels for PWB transitions - Microsoft Internet Explorer provided by IAEA
http://aphysics2.lanl.gov/cgi-bin/ION/runlanl11.pl
File Edit View Favorites Tools Help
Select levels for PWB transitions
Select levels for PWB transitions
Current element is Fe (atomic number 26) with charge of + 22
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 lower level for PWB transitions
Select a specific upper level for PWB transitions
All transitions (a total of 39 transitions)
View data or continue calculations from previous calculation
Change parameters
Configuration selection
Element selection
Start a new problem
Reset
EXIT from calculations
Continue
Done
Internet
100%
start
Inbox - Microsof...
Select levels for ...
X-Win32 0
Microsoft Power...
15:42


Change parameters - Microsoft Internet Explorer provided by IAEA
http://aphysics2.lanl.gov/cgi-bin/ION/runlanl11.pl
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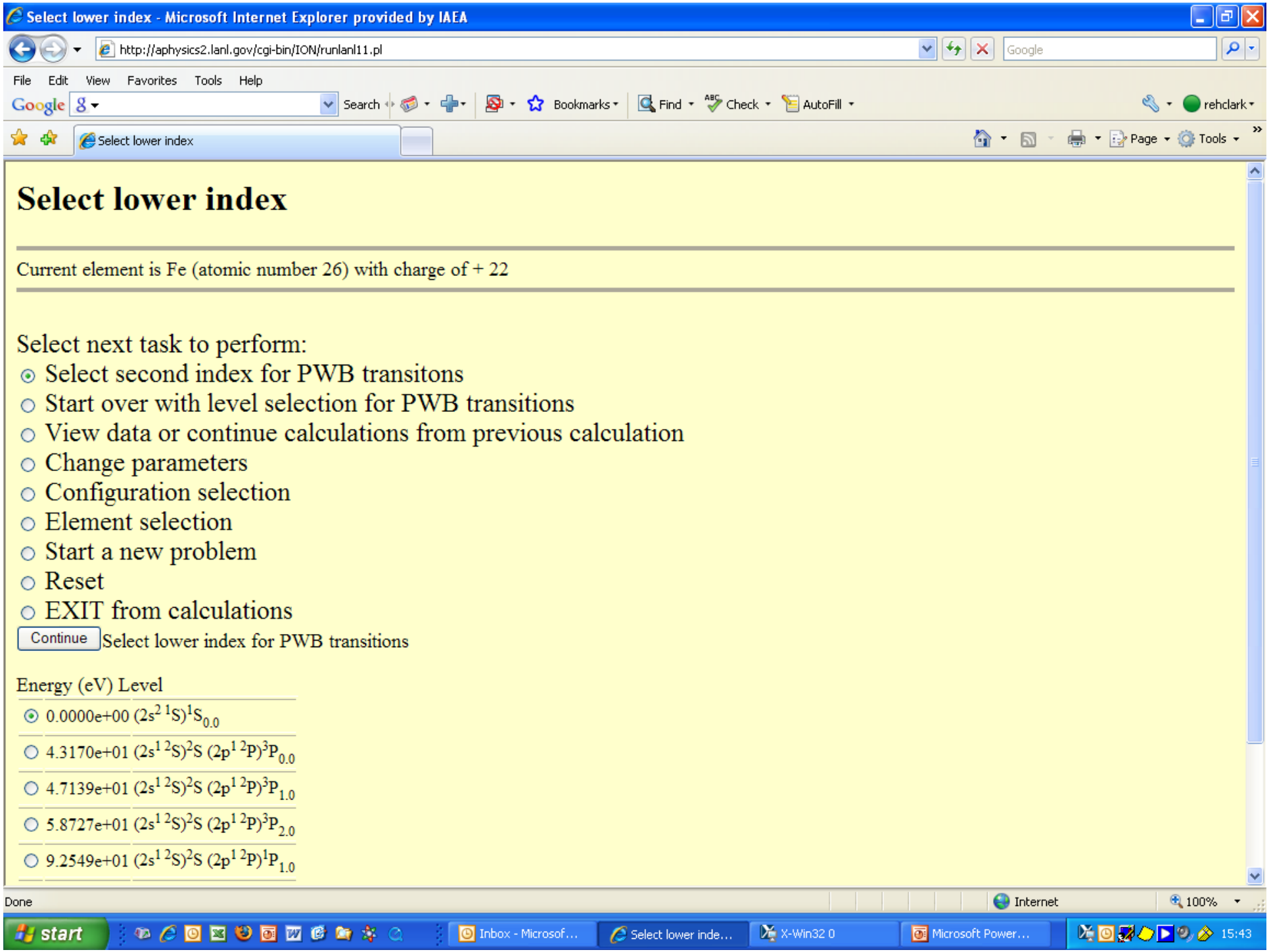
File Edit View Favorites Tools Help
Search Bookmarks Find Check AutoFill rehclark
Change parameters
Page Tools
Change parameters
This page allows you to change a variety of parameters used in calculations and display of results.
More information
Select next task to perform:
Return to previous page
EXIT from calculations
Continue
Select structure output parameters
Select energy units for structure output:
Electron volts Rydbergs Kilokaysers Atomic units Inverse centimeters
Configuration energies calculated from: Average over levels Single configuration
Oscillator strengths listed as:
gf value
log10(gf)
f for absorption
f for emission
A for absorption
A for emission
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
Done
Internet
100%
start
Inbox - Microsof...
Change paramet...
X-Win32 0
Microsoft Power...
15:43


Select lower index - Microsoft Internet Explorer provided by IAEA
http://aphysics2.lanl.gov/cgi-bin/ION/runlanl11.pl
Google
File Edit View Favorites Tools Help
Search Bookmarks Find Check AutoFill rehclark
Select lower index
Page Tools
Select lower index
Current element is Fe (atomic number 26) with charge of + 22
Select next task to perform:
Select second index for PWB transitons
Start over with level selection for PWB transitions
View data or continue calculations from previous calculation
Change parameters
Configuration selection
Element selection
Start a new problem
Reset
EXIT from calculations
Continue
Select lower index for PWB transitions
Energy (eV) Level
0.0000e+00 (2s2 1S)1S0.0
4.3170e+01 (2s1 2S)2S (2p1 2P)3P0.0
4.7139e+01 (2s1 2S)2S (2p1 2P)3P1.0
5.8727e+01 (2s1 2S)2S (2p1 2P)3P2.0
9.2549e+01 (2s1 2S)2S (2p1 2P)1P1.0
Done
Internet
100%
start
Inbox - Microsof...
Select lower inde...
X-Win32 0
Microsoft Power...
15:43

Select second level index for PWB transitions

Current element is Fe (atomic number 26) with charge of + 22

Select next task to perform:

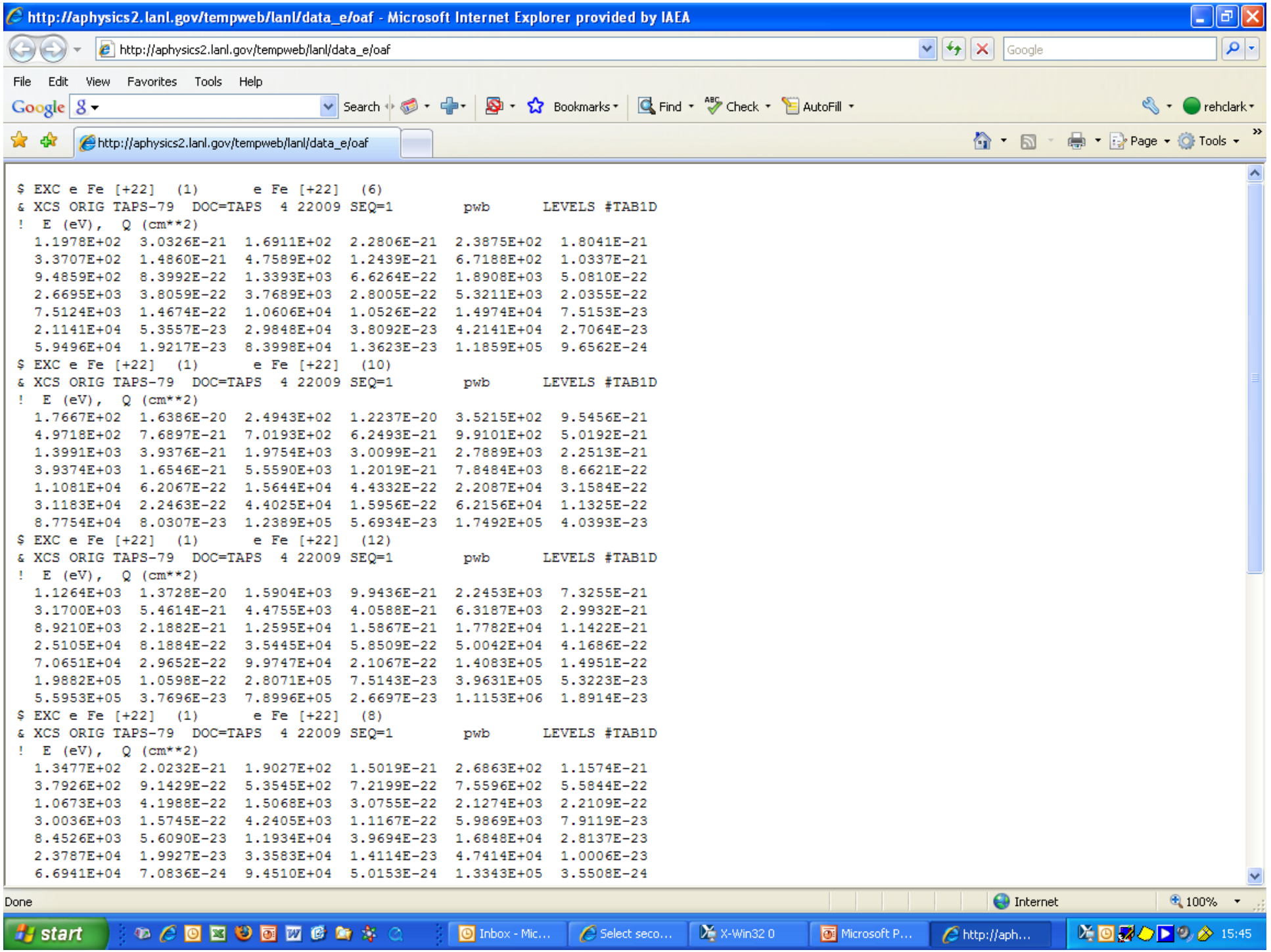
- (•) Display the selected PWB transitions
- ( ) Start over with level selection for PWB transitions
- ( ) View data or continue calculations from previous calculation
- ( ) Change parameters
- ( ) Configuration selection
- ( ) Element selection
- ( ) Start a new problem
- ( ) Reset
- ( ) EXIT from calculations

Continue

Select second index for PWB. (A total of 7 transitions were found)

Transitions will be between $(2s^2\ ^1S)^1S_{0.0}$ (energy of 0.0000e+00 eV) and your choice from the list. You may also access an ALADDIN formatted file of the 7 transitions by clicking here.

Energy (eV)	Level
(•)	All levels (7 transitions)
( ) 4.7139e+01	$(2s^1\ ^2S)^2S\ (2p^1\ ^2P)^3P_{1.0}$
( ) 9.2549e+01	$(2s^1\ ^2S)^2S\ (2p^1\ ^2P)^1P_{1.0}$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http://aphysics2.lanl.gov/tempweb/lanl/data_e/oaf
File Edit View Favorites Tools Help
Search Bookmarks Find Check AutoFill rehclark
Page Tools
$ EXC e Fe [+22] (1) e Fe [+22] (6)
& XCS ORIG TAPS-79 DOC=TAPS 4 22009 SEQ=1 pwb LEVELS #TAB1D
! E (eV), Q (cm**2)
1.1978E+02 3.0326E-21 1.6911E+02 2.2806E-21 2.3875E+02 1.8041E-21
3.3707E+02 1.4860E-21 4.7589E+02 1.2439E-21 6.7188E+02 1.0337E-21
9.4859E+02 8.3992E-22 1.3393E+03 6.6264E-22 1.8908E+03 5.0810E-22
2.6695E+03 3.8059E-22 3.7689E+03 2.8005E-22 5.3211E+03 2.0355E-22
7.5124E+03 1.4674E-22 1.0606E+04 1.0526E-22 1.4974E+04 7.5153E-23
2.1141E+04 5.3557E-23 2.9848E+04 3.8092E-23 4.2141E+04 2.7064E-23
5.9496E+04 1.9217E-23 8.3998E+04 1.3623E-23 1.1859E+05 9.6562E-24
$ EXC e Fe [+22] (1) e Fe [+22] (10)
& XCS ORIG TAPS-79 DOC=TAPS 4 22009 SEQ=1 pwb LEVELS #TAB1D
! E (eV), Q (cm**2)
1.7667E+02 1.6386E-20 2.4943E+02 1.2237E-20 3.5215E+02 9.5456E-21
4.9718E+02 7.6897E-21 7.0193E+02 6.2493E-21 9.9101E+02 5.0192E-21
1.3991E+03 3.9376E-21 1.9754E+03 3.0099E-21 2.7889E+03 2.2513E-21
3.9374E+03 1.6546E-21 5.5590E+03 1.2019E-21 7.8484E+03 8.6621E-22
1.1081E+04 6.2067E-22 1.5644E+04 4.4332E-22 2.2087E+04 3.1584E-22
3.1183E+04 2.2463E-22 4.4025E+04 1.5956E-22 6.2156E+04 1.1325E-22
8.7754E+04 8.0307E-23 1.2389E+05 5.6934E-23 1.7492E+05 4.0393E-23
$ EXC e Fe [+22] (1) e Fe [+22] (12)
& XCS ORIG TAPS-79 DOC=TAPS 4 22009 SEQ=1 pwb LEVELS #TAB1D
! E (eV), Q (cm**2)
1.1264E+03 1.3728E-20 1.5904E+03 9.9436E-21 2.2453E+03 7.3255E-21
3.1700E+03 5.4614E-21 4.4755E+03 4.0588E-21 6.3187E+03 2.9932E-21
8.9210E+03 2.1882E-21 1.2595E+04 1.5867E-21 1.7782E+04 1.1422E-21
2.5105E+04 8.1884E-22 3.5445E+04 5.8509E-22 5.0042E+04 4.1686E-22
7.0651E+04 2.9652E-22 9.9747E+04 2.1067E-22 1.4083E+05 1.4951E-22
1.9882E+05 1.0598E-22 2.8071E+05 7.5143E-23 3.9631E+05 5.3223E-23
5.5953E+05 3.7696E-23 7.8996E+05 2.6697E-23 1.1153E+06 1.8914E-23
$ EXC e Fe [+22] (1) e Fe [+22] (8)
& XCS ORIG TAPS-79 DOC=TAPS 4 22009 SEQ=1 pwb LEVELS #TAB1D
! E (eV), Q (cm**2)
1.3477E+02 2.0232E-21 1.9027E+02 1.5019E-21 2.6863E+02 1.1574E-21
3.7926E+02 9.1429E-22 5.3545E+02 7.2199E-22 7.5596E+02 5.5844E-22
1.0673E+03 4.1988E-22 1.5068E+03 3.0755E-22 2.1274E+03 2.2109E-22
3.0036E+03 1.5745E-22 4.2405E+03 1.1167E-22 5.9869E+03 7.9119E-23
8.4526E+03 5.6090E-23 1.1934E+04 3.9694E-23 1.6848E+04 2.8137E-23
2.3787E+04 1.9927E-23 3.3583E+04 1.4114E-23 4.7414E+04 1.0006E-23
6.6941E+04 7.0836E-24 9.4510E+04 5.0153E-24 1.3343E+05 3.5508E-24
Done
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Select seco...
X-Win32 0
Microsoft P...
http://aph...
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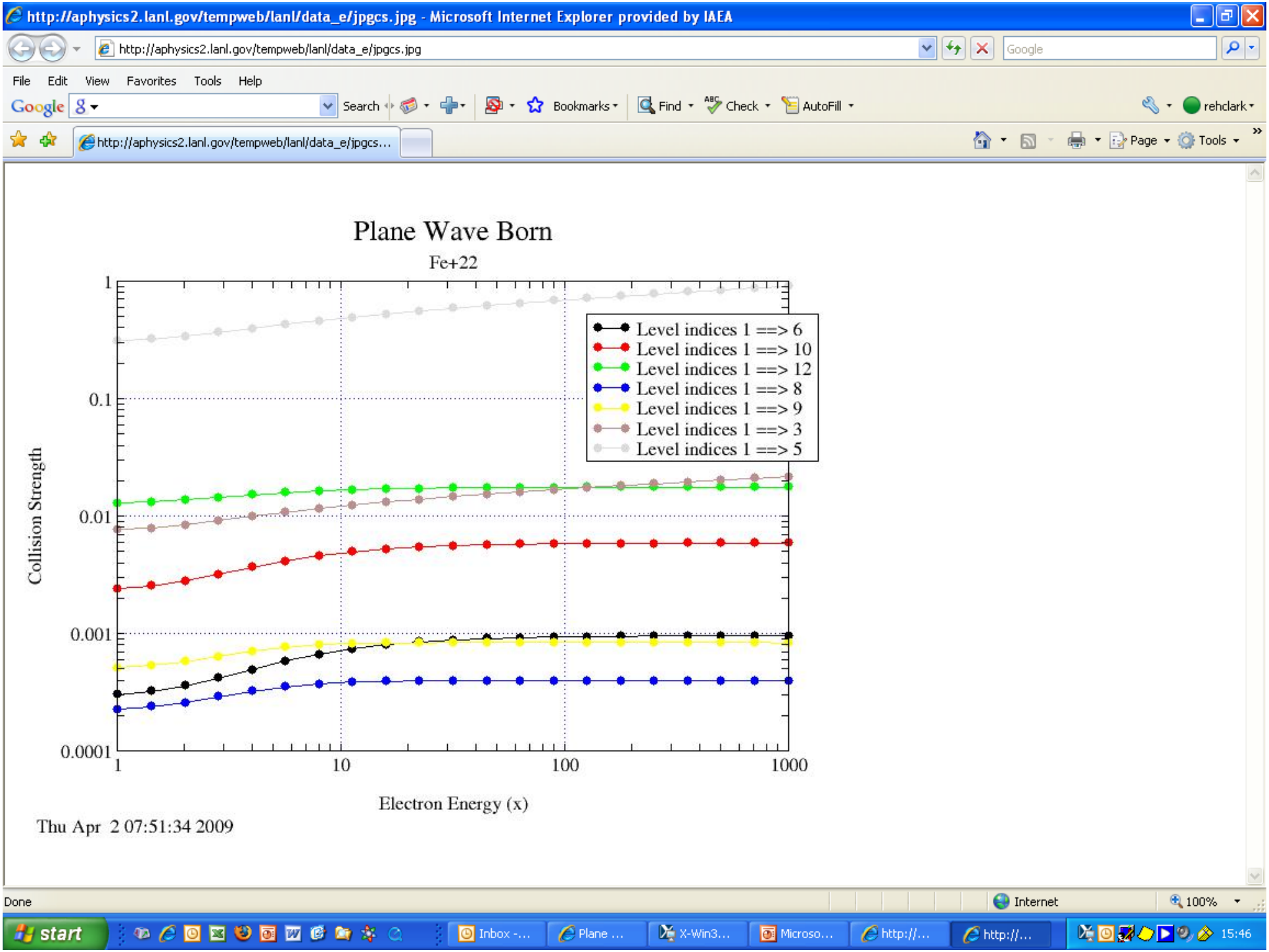
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File Edit View Favorites Tools Help
Search Bookmarks Find Check AutoFill rehclark
http://aphysics2.lanl.gov/tempweb/lanl/data_e/jpgcs...
Page Tools
Plane Wave Born
Fe+22
Collision Strength
1
0.1
0.01
0.001
0.0001
1
10
100
1000
Electron Energy (x)
Level indices 1 ==> 6
Level indices 1 ==> 10
Level indices 1 ==> 12
Level indices 1 ==> 8
Level indices 1 ==> 9
Level indices 1 ==> 3
Level indices 1 ==> 5
Thu Apr 2 07:51:34 2009
Done
Internet
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Inbox -...
Plane ...
X-Win3...
Microso...
http://...
http://...
15:46

Oscillator strengths for Fe + 22

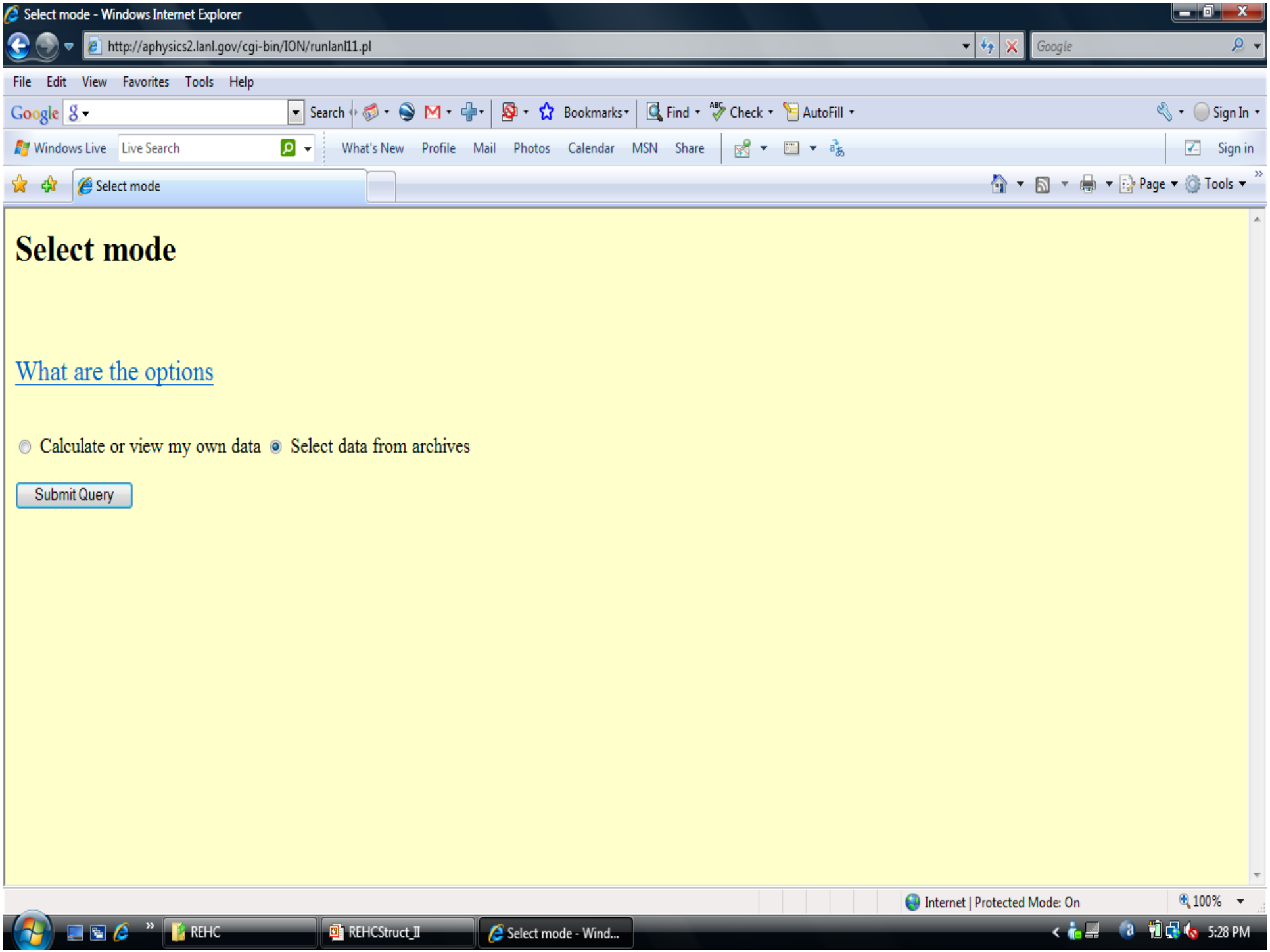
JPEG file(new window)

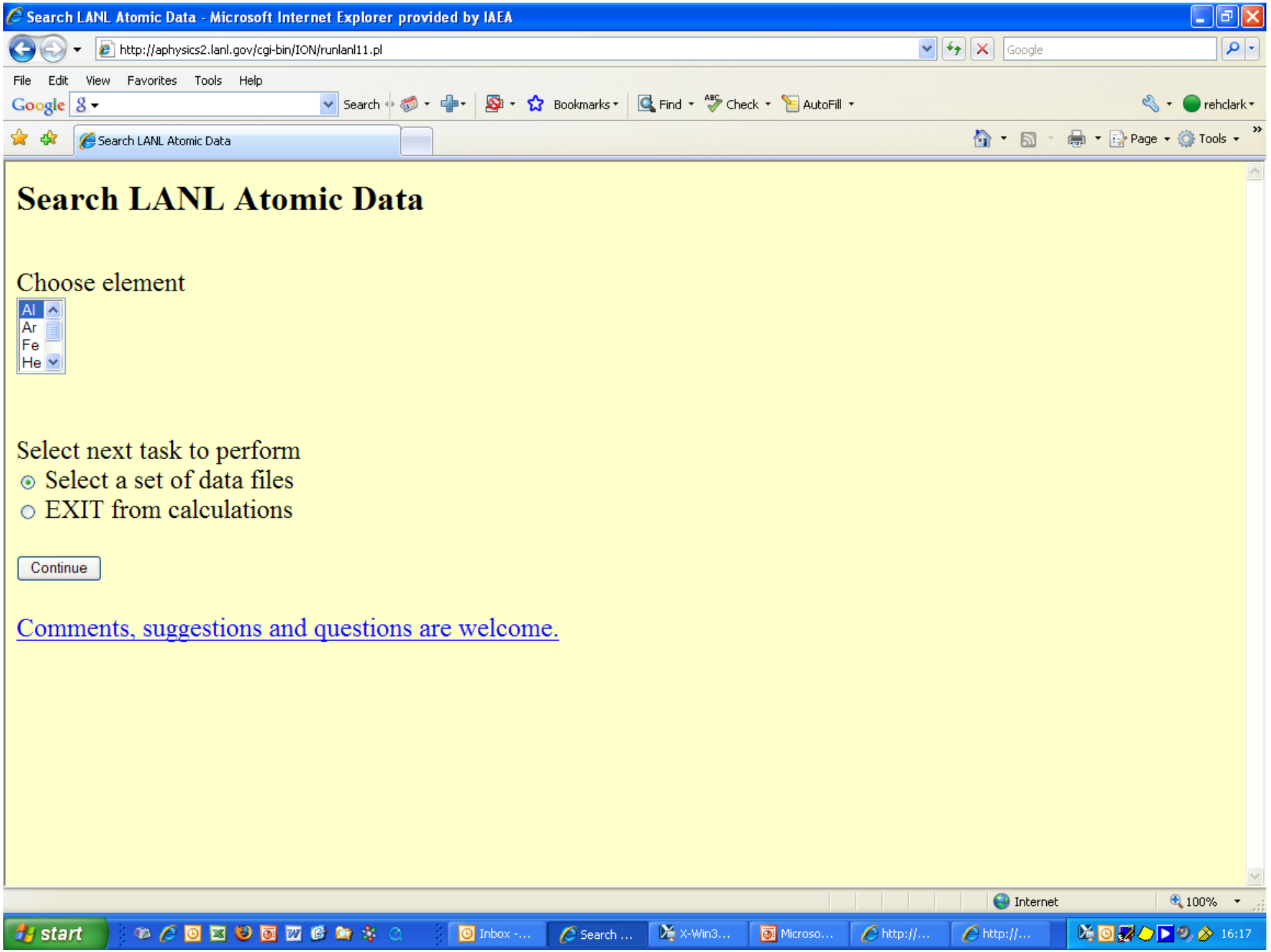
total number of gf is 22

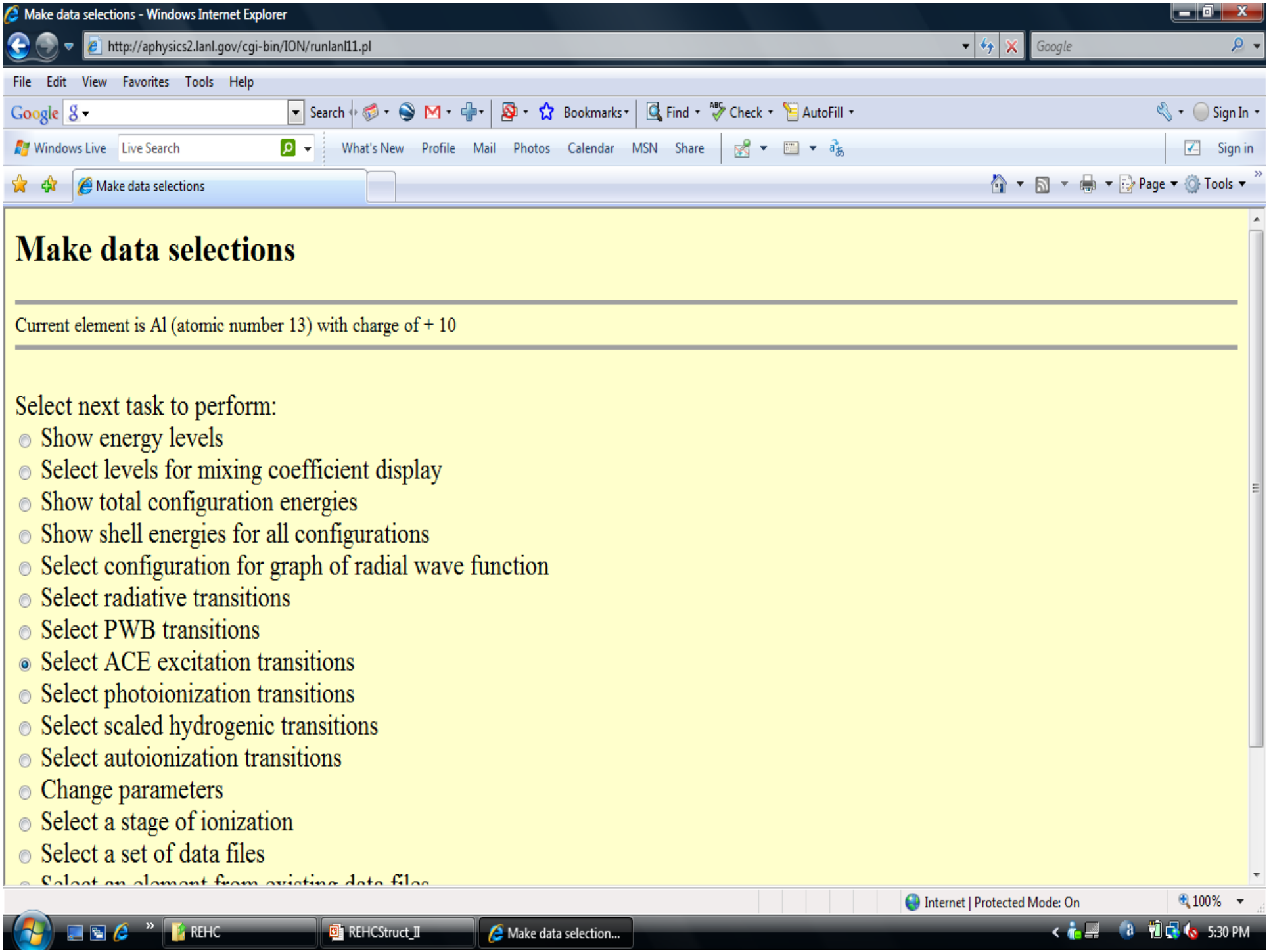
Wavelength in Å	Transition	gf
1.1607e+01	$(2s^1\,^2S)^2S\ (2p^1\,^2P)^3P_{1.0}$ -- $(2s^1\,^2S)^2S\ (3s^1\,^2S)^1S_{0.0}$	1.4087e-03
1.1664e+01	$(2s^1\,^2S)^2S\ (2p^1\,^2P)^3P_{0.0}$ -- $(2s^1\,^2S)^2S\ (3s^1\,^2S)^3S_{1.0}$	1.9983e-02
1.1708e+01	$(2s^1\,^2S)^2S\ (2p^1\,^2P)^3P_{1.0}$ -- $(2s^1\,^2S)^2S\ (3s^1\,^2S)^3S_{1.0}$	5.8123e-02
1.1838e+01	$(2s^1\,^2S)^2S\ (2p^1\,^2P)^3P_{2.0}$ -- $(2s^1\,^2S)^2S\ (3s^1\,^2S)^3S_{1.0}$	9.8450e-02
1.2123e+01	$(2s^1\,^2S)^2S\ (2p^1\,^2P)^1P_{1.0}$ -- $(2s^1\,^2S)^2S\ (3s^1\,^2S)^1S_{0.0}$	4.8603e-02
1.2233e+01	$(2s^1\,^2S)^2S\ (2p^1\,^2P)^1P_{1.0}$ -- $(2s^1\,^2S)^2S\ (3s^1\,^2S)^3S_{1.0}$	1.5319e-03
9.7030e+01	$(2s^1\,^2S)^2S\ (2p^1\,^2P)^3P_{1.0}$ -- $(2p^2\,^1S)^1S_{0.0}$	2.5474e-04
1.2070e+02	$(2s^1\,^2S)^2S\ (2p^1\,^2P)^3P_{1.0}$ -- $(2p^2\,^1D)^1D_{2.0}$	5.1797e-03
1.3397e+02	$(2s^2\,^1S)^1S_{0.0}$ -- $(2s^1\,^2S)^2S\ (2p^1\,^2P)^1P_{1.0}$	1.5463e-01
1.3605e+02	$(2s^1\,^2S)^2S\ (2p^1\,^2P)^3P_{2.0}$ -- $(2p^2\,^1D)^1D_{2.0}$	6.9726e-02
1.4368e+02	$(2s^1\,^2S)^2S\ (2p^1\,^2P)^3P_{1.0}$ -- $(2p^2\,^3P)^3P_{2.0}$	8.4550e-02
1.4695e+02	$(2s^1\,^2S)^2S\ (2p^1\,^2P)^3P_{0.0}$ -- $(2p^2\,^3P)^3P_{1.0}$	6.4363e-02
1.5052e+02	$(2s^1\,^2S)^2S\ (2p^1\,^2P)^1P_{1.0}$ -- $(2p^2\,^1S)^1S_{0.0}$	1.0523e-01
1.5420e+02	$(2s^1\,^2S)^2S\ (2p^1\,^2P)^3P_{1.0}$ -- $(2p^2\,^3P)^3P_{1.0}$	4.4769e-02
1.6597e+02	$(2s^1\,^2S)^2S\ (2p^1\,^2P)^3P_{2.0}$ -- $(2p^2\,^3P)^3P_{2.0}$	1.5655e-01
1.7352e+02	$(2s^1\,^2S)^2S\ (2p^1\,^2P)^3P_{1.0}$ -- $(2p^2\,^3P)^3P_{0.0}$	5.6053e-02

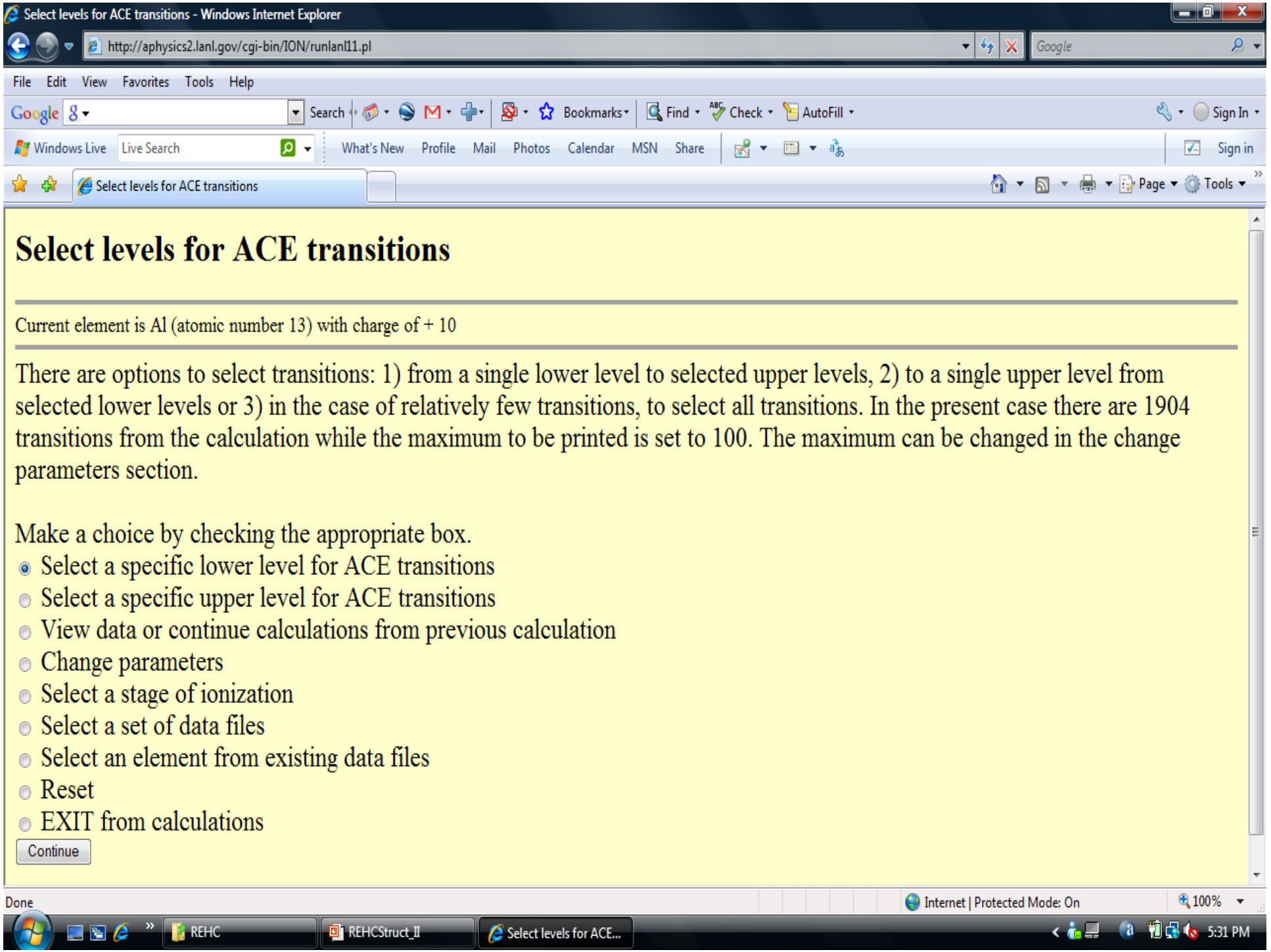
New index

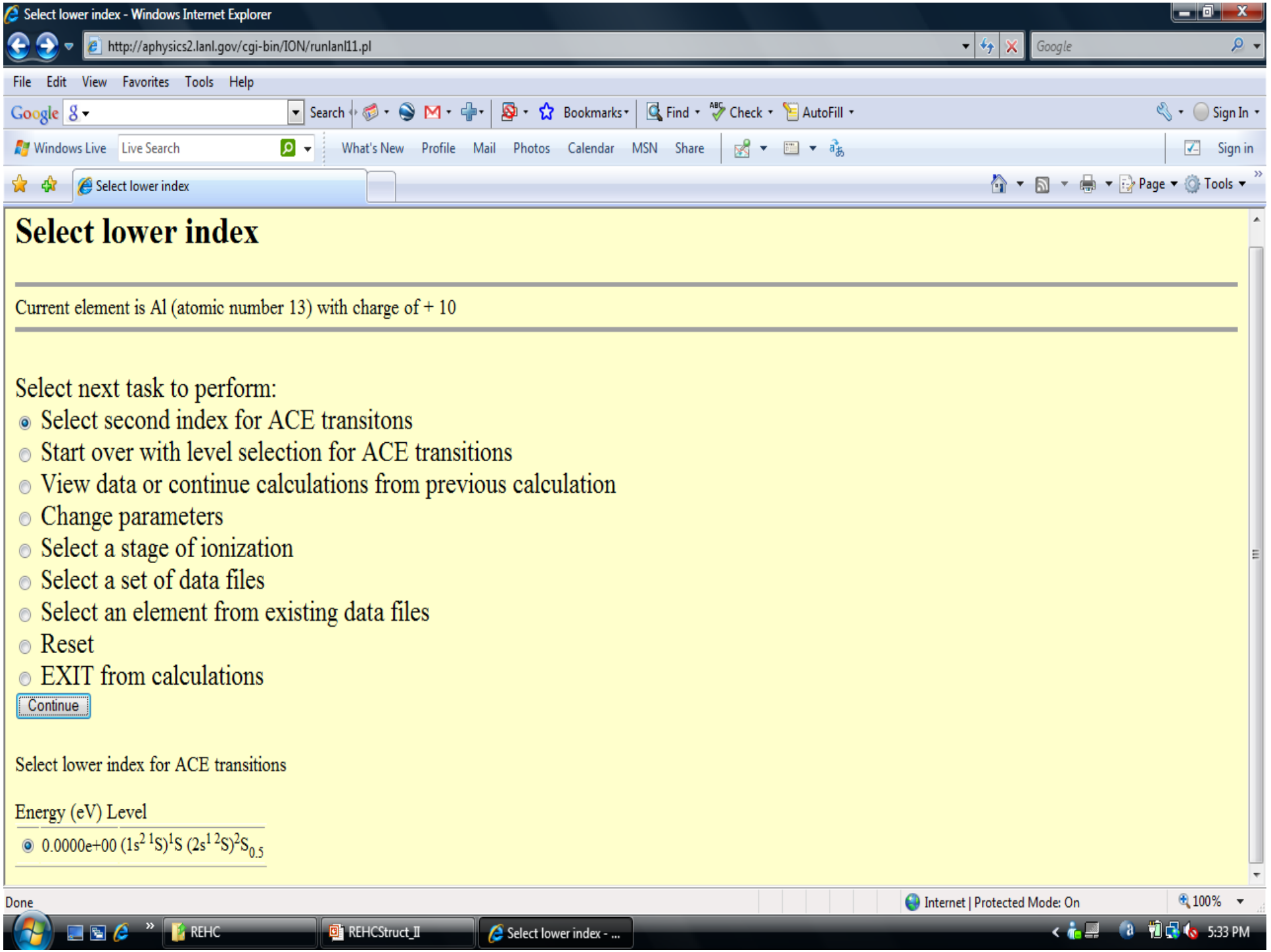
http://aphysics2.lanl.gov/tempweb/lanl/newindex.html

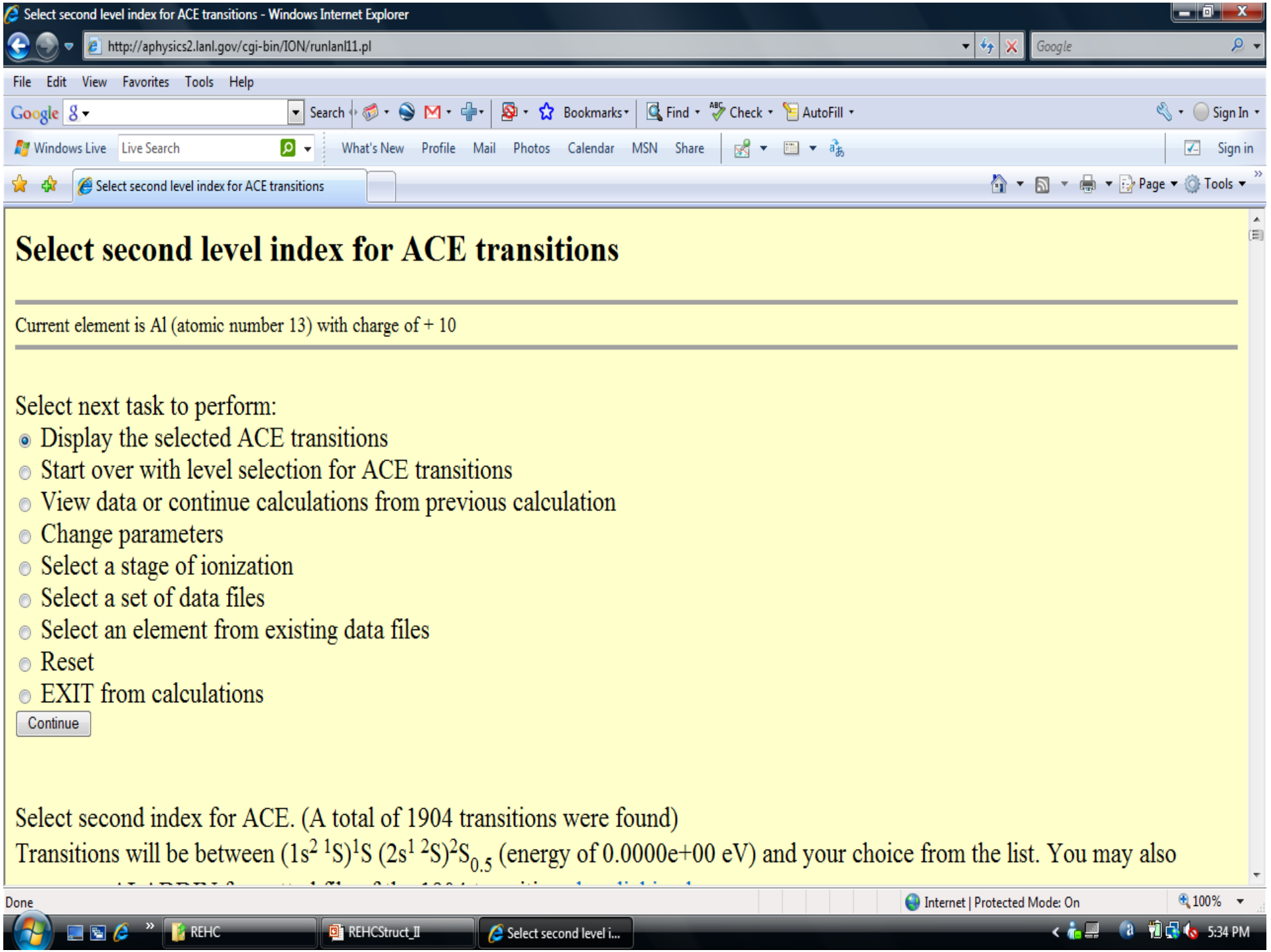

Select mode - Windows Internet Explorer
http://aphysics2.lanl.gov/cgi-bin/ION/runlanl11.pl
Google
File Edit View Favorites Tools Help
Google Search Bookmarks Find Check AutoFill Sign In
Windows Live Live Search What's New Profile Mail Photos Calendar MSN Share Sign in
Select mode
Page Tools
Select mode
What are the options
Calculate or view my own data
Select data from archives
Submit Query
Internet | Protected Mode: On
100%
REHC
REHCStruct_II
Select mode - Wind...
5:28 PM

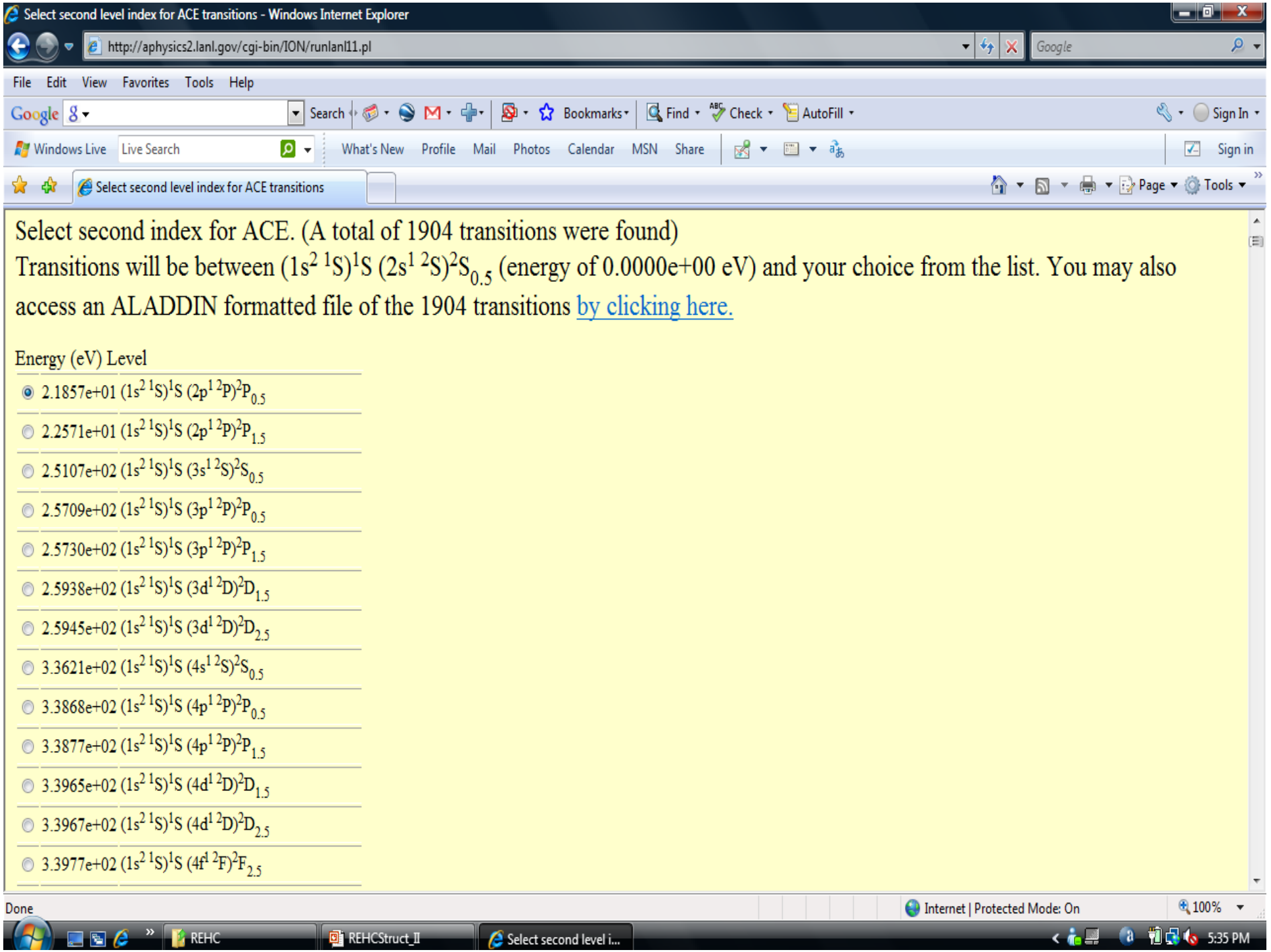

Search LANL Atomic Data - Microsoft Internet Explorer provided by IAEA
http://aphysics2.lanl.gov/cgi-bin/ION/runlanl11.pl
Google
File Edit View Favorites Tools Help
Search
Bookmarks
Find
Check
AutoFill
rehclark
Search LANL Atomic Data
Page
Tools
Search LANL Atomic Data
Choose element
Al
Ar
Fe
He
Select next task to perform
Select a set of data files
EXIT from calculations
Continue
Comments, suggestions and questions are welcome.
Internet
100%
start
Inbox -...
Search ...
X-Win3...
Microso...
http://...
http://...
16:17

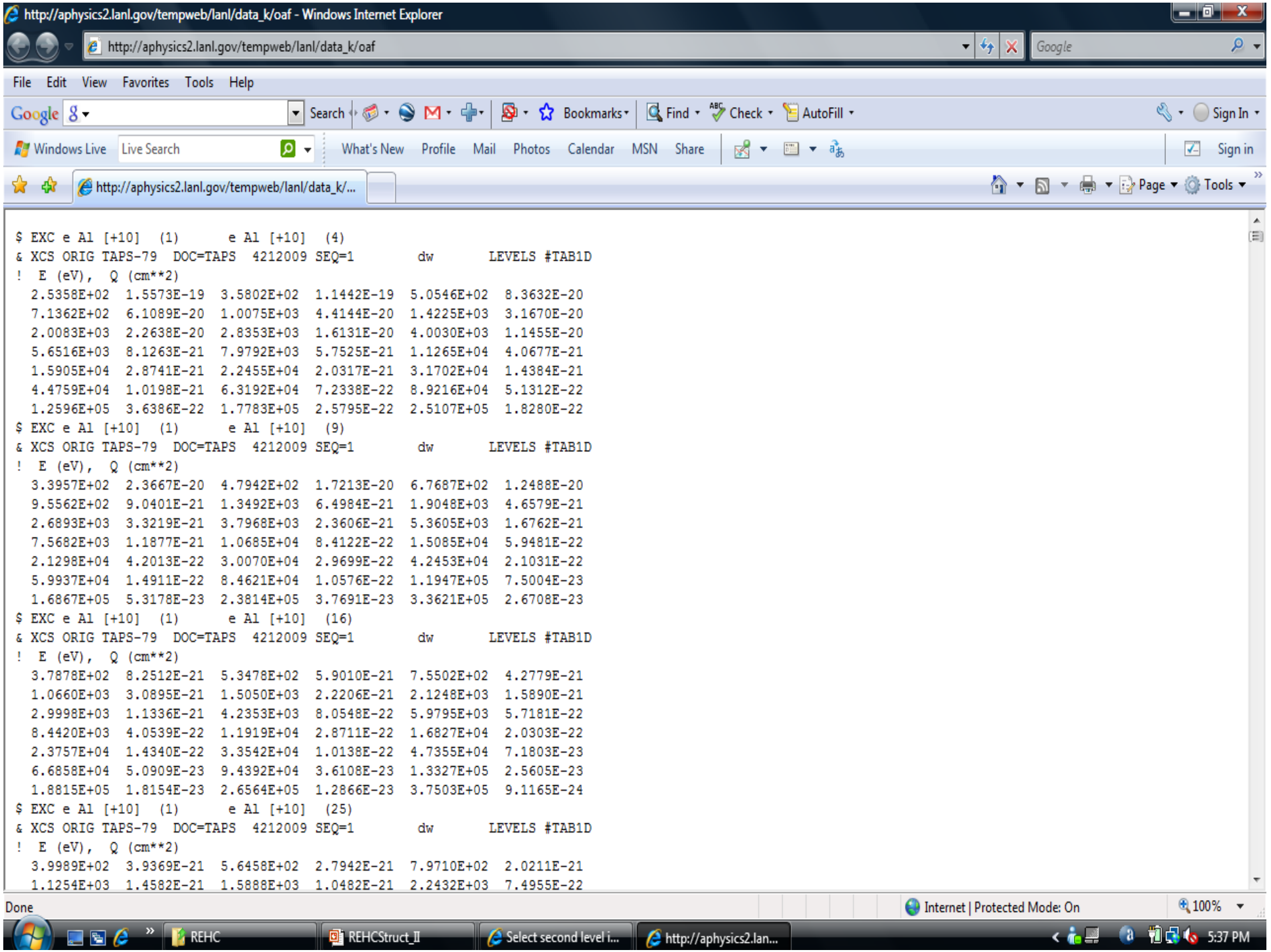

Make data selections - Windows Internet Explorer
http://aphysics2.lanl.gov/cgi-bin/ION/runlanl11.pl
Google
File Edit View Favorites Tools Help
Search
Bookmarks
Find
Check
AutoFill
Sign In
Windows Live
Live Search
What's New
Profile
Mail
Photos
Calendar
MSN
Share
Sign in
Make data selections
Page
Tools
Make data selections
Current element is Al (atomic number 13) with charge of + 10
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
100%
REHC
REHCStruct_II
Make data selection...
5:30 PM


Select levels for ACE transitions - 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
Select levels for ACE transitions
Page
Tools
Select levels for ACE transitions
Current element is Al (atomic number 13) with charge of + 10
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. In the present case there are 1904 transitions from the calculation while the maximum to be printed is set to 100. The maximum can be changed in the change parameters section.
Make a choice by checking the appropriate box.
Select a specific lower level for ACE transitions
Select a specific upper level for ACE 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
REHCStruct_II
Select levels for ACE...
5:31 PM


Select lower index - 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
Select lower index
Page Tools
Select lower index
Current element is Al (atomic number 13) with charge of + 10
Select next task to perform:
Select second index for ACE transitons
Start over with level selection for ACE 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
Select lower index for ACE transitions
Energy (eV) Level
0.0000e+00 (1s2 1S)1S (2s1 2S)2S0.5
Done
Internet | Protected Mode: On
100%
REHC
REHCStruct_II
Select lower index - ...
5:33 PM


Select second level index for ACE transitions - Windows Internet Explorer
http://aphysics2.lanl.gov/cgi-bin/ION/runlanl11.pl
Google
File Edit View Favorites Tools Help
Google Search Bookmarks Find Check AutoFill Sign In
Windows Live Live Search What's New Profile Mail Photos Calendar MSN Share Sign in
Select second level index for ACE transitions
Page Tools
Select second level index for ACE transitions
Current element is Al (atomic number 13) with charge of + 10
Select next task to perform:
Display the selected ACE transitions
Start over with level selection for ACE 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
Select second index for ACE. (A total of 1904 transitions were found)
Transitions will be between (1s2 1S)1S (2s1 2S)2S0.5 (energy of 0.0000e+00 eV) and your choice from the list. You may also
Done
Internet | Protected Mode: On
100%
REHC
REHCStruct_II
Select second level i...
5:34 PM


Select second level index for ACE transitions - Windows Internet Explorer
http://aphysics2.lanl.gov/cgi-bin/ION/runlanl11.pl
File Edit View Favorites Tools Help
Select second level index for ACE transitions
Select second index for ACE. (A total of 1904 transitions were found)
Transitions will be between $(1s^2\ ^1S)^1S\ (2s^1\ ^2S)^2S_{0.5}$ (energy of 0.0000e+00 eV) and your choice from the list. You may also access an ALADDIN formatted file of the 1904 transitions by clicking here.
Energy (eV) Level
2.1857e+01 $(1s^2\ ^1S)^1S\ (2p^1\ ^2P)^2P_{0.5}$
2.2571e+01 $(1s^2\ ^1S)^1S\ (2p^1\ ^2P)^2P_{1.5}$
2.5107e+02 $(1s^2\ ^1S)^1S\ (3s^1\ ^2S)^2S_{0.5}$
2.5709e+02 $(1s^2\ ^1S)^1S\ (3p^1\ ^2P)^2P_{0.5}$
2.5730e+02 $(1s^2\ ^1S)^1S\ (3p^1\ ^2P)^2P_{1.5}$
2.5938e+02 $(1s^2\ ^1S)^1S\ (3d^1\ ^2D)^2D_{1.5}$
2.5945e+02 $(1s^2\ ^1S)^1S\ (3d^1\ ^2D)^2D_{2.5}$
3.3621e+02 $(1s^2\ ^1S)^1S\ (4s^1\ ^2S)^2S_{0.5}$
3.3868e+02 $(1s^2\ ^1S)^1S\ (4p^1\ ^2P)^2P_{0.5}$
3.3877e+02 $(1s^2\ ^1S)^1S\ (4p^1\ ^2P)^2P_{1.5}$
3.3965e+02 $(1s^2\ ^1S)^1S\ (4d^1\ ^2D)^2D_{1.5}$
3.3967e+02 $(1s^2\ ^1S)^1S\ (4d^1\ ^2D)^2D_{2.5}$
3.3977e+02 $(1s^2\ ^1S)^1S\ (4f^1\ ^2F)^2F_{2.5}$
Done
Internet | Protected Mode: On
100%
REHC
REHCStruct_II
Select second level i...
5:35 PM


http://aphysics2.lanl.gov/tempweb/lanl/data_k/oaf - Windows Internet Explorer
http://aphysics2.lanl.gov/tempweb/lanl/data_k/oaf
File Edit View Favorites Tools Help
Windows Live
Live Search
What's New Profile Mail Photos Calendar MSN Share
Sign in
http://aphysics2.lanl.gov/tempweb/lanl/data_k/...
Page Tools
$ EXC e Al [+10] (1) e Al [+10] (4)
& XCS ORIG TAPS-79 DOC=TAPS 4212009 SEQ=1 dw LEVELS #TAB1D
! E (eV), Q (cm**2)
2.5358E+02 1.5573E-19 3.5802E+02 1.1442E-19 5.0546E+02 8.3632E-20
7.1362E+02 6.1089E-20 1.0075E+03 4.4144E-20 1.4225E+03 3.1670E-20
2.0083E+03 2.2638E-20 2.8353E+03 1.6131E-20 4.0030E+03 1.1455E-20
5.6516E+03 8.1263E-21 7.9792E+03 5.7525E-21 1.1265E+04 4.0677E-21
1.5905E+04 2.8741E-21 2.2455E+04 2.0317E-21 3.1702E+04 1.4384E-21
4.4759E+04 1.0198E-21 6.3192E+04 7.2338E-22 8.9216E+04 5.1312E-22
1.2596E+05 3.6386E-22 1.7783E+05 2.5795E-22 2.5107E+05 1.8280E-22
$ EXC e Al [+10] (1) e Al [+10] (9)
& XCS ORIG TAPS-79 DOC=TAPS 4212009 SEQ=1 dw LEVELS #TAB1D
! E (eV), Q (cm**2)
3.3957E+02 2.3667E-20 4.7942E+02 1.7213E-20 6.7687E+02 1.2488E-20
9.5562E+02 9.0401E-21 1.3492E+03 6.4984E-21 1.9048E+03 4.6579E-21
2.6893E+03 3.3219E-21 3.7968E+03 2.3606E-21 5.3605E+03 1.6762E-21
7.5682E+03 1.1877E-21 1.0685E+04 8.4122E-22 1.5085E+04 5.9481E-22
2.1298E+04 4.2013E-22 3.0070E+04 2.9699E-22 4.2453E+04 2.1031E-22
5.9937E+04 1.4911E-22 8.4621E+04 1.0576E-22 1.1947E+05 7.5004E-23
1.6867E+05 5.3178E-23 2.3814E+05 3.7691E-23 3.3621E+05 2.6708E-23
$ EXC e Al [+10] (1) e Al [+10] (16)
& XCS ORIG TAPS-79 DOC=TAPS 4212009 SEQ=1 dw LEVELS #TAB1D
! E (eV), Q (cm**2)
3.7878E+02 8.2512E-21 5.3478E+02 5.9010E-21 7.5502E+02 4.2779E-21
1.0660E+03 3.0895E-21 1.5050E+03 2.2206E-21 2.1248E+03 1.5890E-21
2.9998E+03 1.1336E-21 4.2353E+03 8.0548E-22 5.9795E+03 5.7181E-22
8.4420E+03 4.0539E-22 1.1919E+04 2.8711E-22 1.6827E+04 2.0303E-22
2.3757E+04 1.4340E-22 3.3542E+04 1.0138E-22 4.7355E+04 7.1803E-23
6.6858E+04 5.0909E-23 9.4392E+04 3.6108E-23 1.3327E+05 2.5605E-23
1.8815E+05 1.8154E-23 2.6564E+05 1.2866E-23 3.7503E+05 9.1165E-24
$ EXC e Al [+10] (1) e Al [+10] (25)
& XCS ORIG TAPS-79 DOC=TAPS 4212009 SEQ=1 dw LEVELS #TAB1D
! E (eV), Q (cm**2)
3.9989E+02 3.9369E-21 5.6458E+02 2.7942E-21 7.9710E+02 2.0211E-21
1.1254E+03 1.4582E-21 1.5888E+03 1.0482E-21 2.2432E+03 7.4955E-22
Done
Internet | Protected Mode: On
100%
REHC
REHCStruct_II
Select second level i...
http://aphysics2.lan...
5:37 PM

Summary

- Interface allows calculation of atomic structure: radial wave functions, energy levels, oscillator strengths, mixing coefficients, plane wave Born cross sections for arbitrary ion
- Interface gives access to archived sets of data at LANL