Using the CHIANTI routine new_burly_ups.pro

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This routine is used to fit effective collision strengths (upsilons) for inclusion in the CHIANTI database.

Requirements

Before using new_burly_ups you must have the following three CHIANTI data files in your working directory: a .elvlc file, a .upsdat file, and a .wgfa file.

Basic operation

At the most basic level, fitting upsilons with new_burly_ups is performed as follows.

First, start up new_burly_ups:

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IDL> new_burly_ups,'.',26,10
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(here we're working in the current working directory on Fe X).

The steps are:

1. Click on 'NEXT TRANSITION', which performs the fit to the first transition.
2. Check that fit is OK by inspection of the plot windows.
3. Repeat for every transition.
4. When message appears saying all transitions have been fitted, click 'EXIT'.

Fine-tuning the fit

For many transitions the initial fit performed by new_burly_ups will not be satisfactory and so some fine-tuning will be required. Note that the fundamental aim is that the fit reproduces the original data-points to a good accuracy. You can judge this by looking at the left-hand plot at the bottom of the widget. This shows the original upsilons (triangles) and the fit to these upsilons (stars). In addition a horizontal dashed line is shown together with a dotted line. The shape of the dotted line indicates the quality of the fit.

The dotted line graphically represents the difference between the fit and the original data in terms of a percentage. If the dotted line reaches to the top of the plot window, it implies the difference is +10%. If it reaches to the bottom it is -10%. If the dotted line lies exactly on the dashed line then it is a perfect fit.

A good fit should reproduce each individual point to within 1%, and so the complete dotted line should lie close to the dashed line. The user should thus always check the dotted line after each fit to make sure the points are fitted satisfactorily.

When you do fine-tuning of the fit, click on the 'RE-FIT TRANSITION' button to see the results. When you're happy click on 'NEXT TRANSITION'.

The following sections describe options for changing the fit.

Adjusting the number of spline points

This is changed using the button widget at the top-right of the GUI. Two options are available: 5 and 9 point splines. Generally if each transition has a large number of upsilons (say > 15) then the 9 point spline will be essential. A 5 point spline must be used if there are < 9 upsilons.

If the upsilon curve has very little structure then you may find that a 9 point spline introduces strange curves to the fit. In these cases it's worth trying a 5 point spline.

Adjusting the temperature range

Sometimes the upsilon curve shows so much structure that even a 9 point spline can not accurately fit the upsilons. In this case it is necessary to adjust the number of temperature points. The 'Temperature range' widget has sliders that allow to remove data points from the low and high temperature ends of the range.

By default, when moving to the next transition, the temperature range is reset back to the original full range. If you have decided to ignore some of the temperature points for all of the transitions, then go to 'Save range?' and click on 'Yes' and the routine will use your chosen temperature range for the next transition.

Extrapolating to 0 or 1

By default new_burly_ups performs no extrapolation and so the spline fit is free to choose to whatever values at 0 and 1 give the best fit to the data points. Sometimes this gives strange results and so the user has to constrain the values.

Clicking on '0 (auto)' tells the routine to perform a linear extrapolation of the first two data points to 0, and then use this value in the fit.

Clicking on '1 (auto)' tells the routine to perform a linear extrapolation of the last two data points to 1, and then use this value in the fit.

Clicking on '0 (user)' allows the user to manually specify the scaled upsilon value at 0.

Transition type

By default, new_burly_ups divides transitions into either Type 1 (allowed transitions), or Type 2 (forbidden transitions) depending on whether the transition has a gf-value or not.

If you're having trouble fitting a transition then you can try switching to Type 3 or Type 4. Do not use Type 5 or Type 6 which are reserved for dielectronic transitions and proton rates, respectively.

Adjusting the scaling parameter, C

new_burly_ups uses a minimization technique to work out which scaling parameter, C, gives the best fit. Sometimes this does not work, and so it's necessary to over-ride the C-value manually.

In the top-left of the GUI click on the 'C over-ride' button and then type in the number you'd like to try.

One of the main reasons for using C over-ride is when the C-value results in all the data points being bunched up towards either low or high temperatures.