**The problem of matching up energy levels from various sources**

Energy levels from various sources have different conventions for the labeling of the levels. IN many cases, these formats were chosen to give a compact description of the term that could be used in a specific program. However, the use of these formats makes it hard to match the levels and thus line identifications from different programs. For example:

1. ASD format: The levels downloaded as an ASCII text file from the NIST Atomic Spectra Database are of the following format for the ground term of Fe II:

3d6.(5D).4s | a 6D | 9/2 | 0.0000 | 0.0000 | 1.58 | **100** | [L18349](javascript:void(0)),[L18361c138](javascript:void(0))

| | 7/2 | 384.7872 | 0.0003 | 1.58 | **100** | [L18349](javascript:void(0)),[L18361c138](javascript:void(0))

| | 5/2 | 667.6829 | 0.0003 | 1.655 | **100** | [L18349](javascript:void(0)),[L18361c138](javascript:void(0))

| | 3/2 | 862.6118 | 0.0004 | 1.862 | **100** | [L18349](javascript:void(0)),[L18361c138](javascript:void(0))

| | 1/2 | 977.0498 | 0.0004 | 3.31 | **100** | [L18349](javascript:void(0)),[L18361c138](javascript:void(0))

Note that the first two columns are empty, causing a problem for programs. This has been fixed in the .csv tables (something I had to pester Sasha for a few years ago), but then the output is not as human readable:

"=""3d6.(5D).4s""","=""a 6D""","=""9/2""","="" 0.0000""","=""0.0000""","=""1.58""","="" 100 ""","=""L18349,L18361c138"""

"=""3d6.(5D).4s""","=""a 6D""","=""7/2""","="" 384.7872""","=""0.0003""","=""1.58""","="" 100 ""","=""L18349,L18361c138"""

"=""3d6.(5D).4s""","=""a 6D""","=""5/2""","="" 667.6829""","=""0.0003""","=""1.655""","="" 100 ""","=""L18349,L18361c138"""

"=""3d6.(5D).4s""","=""a 6D""","=""3/2""","="" 862.6118""","=""0.0004""","=""1.862""","="" 100 ""","=""L18349,L18361c138"""

"=""3d6.(5D).4s""","=""a 6D""","=""1/2""","="" 977.0498""","=""0.0004""","=""3.31""","="" 100 ""","=""L18349,L18361c138"""

1. For the past three decades I have used a compressed version of this in my programs, in order to keep the output of my programs to a single page width, making it easier to read:

5D4s a6D4 4.5 0.0000 0.0000 1

5D4s a6D3 3.5 384.7872 0.0003 1

5D4s a6D2 2.5 667.6829 0.0004 1

5D4s a6D1 1.5 862.6118 0.0004 1

5D4s a6D0 0.5 977.0498 0.0005 1

In this case, the energy levels match because ASD was based on my analysis. However, this is not generally the case and differences of 0.1 cm-1 or more would not be unusual.

1. Kurucz uses the following format for energy levels that have been matched to experimental values:

26.01EVE 1 0.000 4.5 (5D)4s a6D 1.580 0.00E+00

26.01EVE 1 384.790 3.5 (5D)4s a6D 1.580 2.14E-03

26.01EVE 1 667.683 2.5 (5D)4s a6D 1.655 1.58E-03

26.01EVE 1 862.613 1.5 (5D)4s a6D 1.862 7.22E-04

26.01EVE 1 977.053 0.5 (5D)4s a6D 3.310 1.89E-04

Here, the energy levels do not match exactly, so it is not possible to match up the three sets of data using just the energy level.

1. Raassen and Uylings use the following format (some spaces have been deleted):

.000 -6.620 6.620 100% 2|5D4)6D + 0% 2|3F4)4F + 0% 8|6S5)6D + 0% 2|3F2)4F

384.790 380.448 4.342 100% 2|5D4)6D + 0% 8|6S5)6D + 0% 2|3F4)4F + 0% 2|5D4)4D

667.683 665.659 2.024 100% 2|5D4)6D + 0% 8|6S5)6D + 0% 2|3P2)4P + 0% 2|3P4)4P

862.613 862.478 .135 100% 2|5D4)6D + 0% 2|3P2)4P + 0% 8|6S5)6D + 0% 2|3P4)4P

977.053 978.138 -1.085 100% 2|5D4)6D + 0% 2|3P2)4P + 0% 8|6S5)6D + 0% 2|3P4)4P

This was taken from their older calculations and the energy levels may have been updated since this file was downloaded, but I think the configuration and term assignments are similar. In their energy level file, the levels are sorted according to J value and hence this does not appear on each line corresponding to a level. Their list of E1 transitions looks like this:

2599.396 .38419 4.5 .00\* 2|5D4)6D 4.5 38458.98\* 1|5D4)6D

2404.887 .17790 2.5 667.68\* 2|5D4)6D 3.5 42237.03\* 1|5D4)6F

2395.626 .39182 3.5 384.79\* 2|5D4)6D 4.5 42114.82\* 1|5D4)6F

2382.039 .53613 4.5 .00\* 2|5D4)6D 5.5 41968.05\* 1|5D4)6F

2343.496 .09769 4.5 .00\* 2|5D4)6D 3.5 42658.22\* 1|5D4)6P

1144.938 .03695 4.5 .00\* 2|5D4)6D 5.5 87340.98\* 2|4G5G,6F

The question is, how do we tell a program that all of these formats for the energy level refer to the same thing. An initial idea to match the levels based on the level value and the J value works fine for the lower levels, but for higher levels can fail if the levels get too close together. Consider the following (5D)6h levels with J=11/2 in Fe II, in my short format:

5D6h3\_65 5.5 118889.5458 0.0055 0

5D6h3\_55 5.5 118890.2101 0.0054 0

5D6h2\_55 5.5 119196.4443 0.0054 0

5D6h2\_65 5.5 119196.4530 0.0049 0

5D6h1\_65 5.5 119385.5300 0.1401 0

They have the following values in Kurucz’s calculations:

26.01ODD 70 118889.500 5.5 5D)6h 3[6] 1.079 2.92E-03

26.01ODD 71 118890.158 5.5 5D)6h 3[5] 1.181 2.91E-03

26.01ODD 74 119196.405 5.5 5D)6h 2[5] 1.043 1.83E-03

26.01ODD 75 119196.410 5.5 5D)6h 2[6] 1.139 1.83E-03

26.01ODD 76 119385.482 5.5 5D)6h 1[6] 1.005 6.77E-04

The two levels near 119196 cm-1 cannot be matched on energy and J-value alone. They also cannot be reliably matched by requiring the same order for the experimental and calculated levels as the atomic structure calculations are not sufficiently reliable to even get the order correct. Some knowledge of the expected transitions from these levels is required to be able to make a reliable match of the experimental and calculated levels, and this is not easy to transmit to a new student starting the analysis. Kurucz has in fact made this match based on his experience for many elements using recent analyses based on FTS, but as soon as new analyses are published or he revises his calculations, these matches need to be made again.

My solution to this problem in the past has been to construct a look-up table for the levels, with a single key representing the energy level and different columns in the table denoting the notation used in the various programs. This has also been useful to format a table for publication, where a format similar to ASD is required for a machine-readable table and a similar one formatted in LaTeX using the conventional superscripts and subscripts is needed for the short table stub in the main body of the paper. However, this table is not always easy to construct and not easy to get right.

Maybe there is a better solution to this problem, which is common to almost all types of analysis that we do. Perhaps just making a table in a nice user interface with an initial match of levels between the different sources that can be edited as required would help. This could then be used to construct the lookup table that is used by other programs.