Dec18-05 **ADAS Bulletin**

Items:

1. ADAS release v2.10
2. Plans for ADAS release v3.0
3. OPEN-ADAS
4. Code and data updates in release v2.10.

1. ADAS release v2.10.

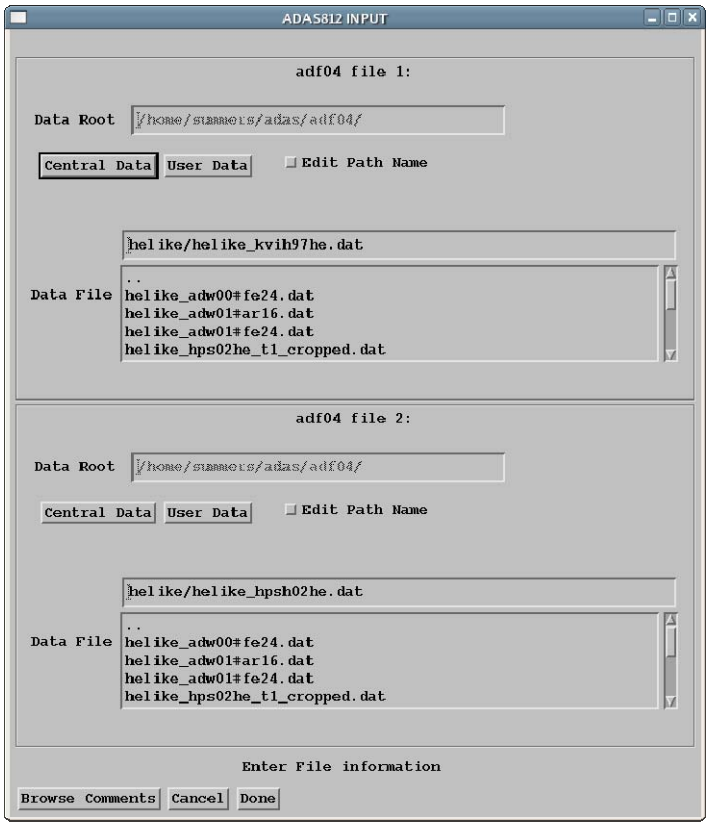
This release contains rather a lot of new data, but also some re-organisation of data, so I thought it useful to explain a little of what we are about. We have been mass producing high precision state selective dielectronic data, of format *adf09*, for some time. It is important as we work to heavier elements and to more complex iso-electronic sequences in fusion, but also in astrophysics. In fact most astrophysicists do not deal with dielectronic recombination in the full collisional-radiative complexity that we need for fusion, but they do worry about low temperature DR. Also in this case they also worry about radiative recombination at low temperature, so it seemed appropriate to produce state selective radiative recombination for very extended n-shells from AUTOSTRUCTURE in the same manner as for DR. Nigel has been giving a lot of attention to this. Also our current thinking is to move increasingly to scripts which run extended series of calculations automatically on parallel machines and to assemble the results properly and automatically in appropriately named ADAS data formats. Hence /*offline_adas* which at Strathclyde sits alongside the */fortran* , */idl* etc directories in */home/adas*. Recall that we only load /*offline_adas* up at sites which want to use the offline codes in collaboration with central ADAS staff since they need more guidance and tuning to local computational facilities. This mass production is progressing and we have decided to place all this compatible AUTOSTRUCTURE produced dielectronic, radiative, photo-excitation and photo-ionisation data in similar ADAS data formats (*adf09, adf38, adf39, adf48*) with all the drivers in sub-directories of *adf27* and *adf27*. We are rather pleased with this move to *offline_adas* and scripted running. We already have *adas8#1*, so we have now added *adas7#1* (DR) and adas8#3. The latter does extended R-matrix collision calculations, producing *adf04* files, along iso-electronic sequences at the top level of precision. We expect to add *adas8#2* for ionisation shortly – Stuart is driving this part.

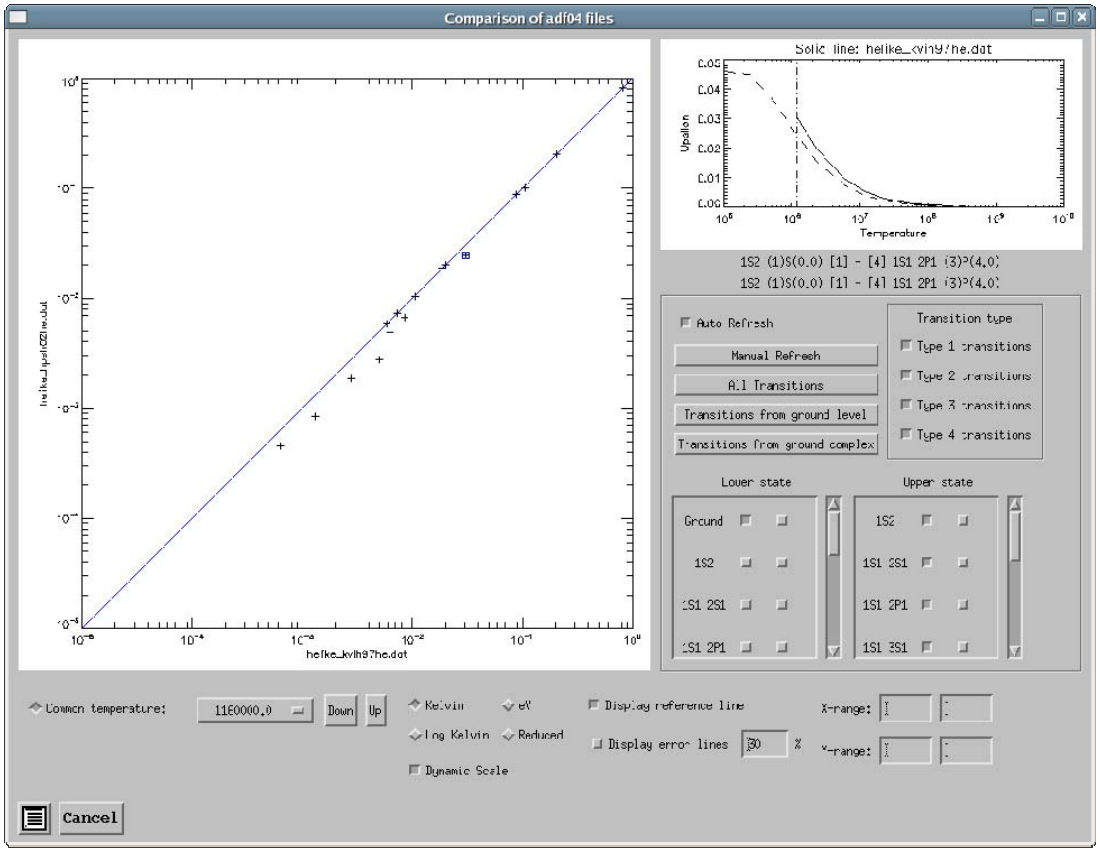
Given this increased automatic production of high grade fundamental data coordinated by Nigel and under the ADAS umbrella, it becomes important to set up display machinery to scrutinise data efficiently. For example, it is important to assess the differences in two R-matrix runs in which the configuration scope is different, with a view to drawing conclusions on precision and error bars. Thus it was felt that a dedicated pairwise *adf04* comparator was needed. Allan (with ideas from Mike) has written such a code for IDL-ADAS, called ADAS812. The input screen for the two files is shown below. A point of warning. ADAS812 is really oriented around comparison of *adf04* files which are automatically produced. That means that they have configurations and so on in standard notation, and the two files will be expected to find the same configuration formats in both files – so that it can match up levels properly. I guess the penalty of efficient mass handling of data is that what were previously free text areas become prescribed. If the two adf04 data sets can be matched, then we move on to the processing screen as shown next. This is quite a sophisticated interactive screen. The upsilon values at a selected common temperature are compared with each other for all transitions within transition categories chosen at the right of the screen. The scatter of points around the 45^{o} line is the issue. This allows us to decide if there is a problem in one of the calculations and if not then to use the scatter to assess precision and to decide the preferred data set. The crosses on the scatter diagram each correspond to a particular transition. Clicking on such a cross causes the transition to be selected and the complete set of upsilons for the transition, for both data sets, to be identified and displayed in a small graph at the top of the widget. I think this is a very helpful addition to the ADAS interactive code armoury. I shall put more details in the ADAS manual (see below). Mike of course, who is doing most scrutinising of R-matrix data, has other more complex comparators, some of which he showed in action at the ADAS workshop.

At this point, I should also draw attention to our big GCR-I publication

> 'Ionisation state, excited populations and emission of impurities in dynamic finite density plasmas.

I The generalised collisional-radiative model for light elements' - H P Summers, William Dickson, Martin O'Mullane, N R Badnell, Allan Whiteford, David Brooks, J Lang, Stuart Loch and D C Griffin Plasma Physics & Control. Fusion (2006) ?? 1-31 – in press (also http://arxiv.org/archive/astro-ph/0511561)





2. Forward plans for ADAS release v3.0

We plan to issue the next release of ADAS in June. It will be all about heavy species and their handling and has been quite a long time in the gestation. I had originally planned it for towards the end of 2005, but two items, namely automatic configuration average ionisation calculations and the drivers for the Burgesss-Bethe General Program (BBGP) from AUTOSTRUCTURE, still require a little work. The release is going to incorporate substantial (hopefully transparent) changes to ADAS and warrants the step up to release 3.0. It will provide complete handling of superstages and partitions, which I have been talking of for some time and so will really set us up for interfacing with plasma models, transport, spectroscopy and quasi-continuum of arbitrary heavy species. Also it will mean a lot of heavy element data (*adf04, adf11, adf15, adf40*). All this effort on *offline_adas*, scripting and parallel machines will hopefully then prove justified to everyone.

3. OPEN-ADAS

I talked about a version of ADAS for the public domain (OPEN-ADAS) at the last Workshop and Steering Committee meeting and it follows on from ideas I presented about three years ago after a consultant visit to IAEA in Vienna. IAEA wishes to sponsor the ADAS Project to prepare an interface to selected ADAS data which can be made available from the IAEA website. There have been some issues to think out about in such a step, since there is a valuable and very valued cohesiveness of the participants in the ADAS Project. The connections with laboratories, the various objectives and the exclusiveness to those who really want to work together matters. Necessarily, the ADAS Project materials as a whole are not public domain. However, a lot of our data is already in the public domain and much of our (now very large) fundamental data production has to be in the public domain because of its funding sources. Although the latter originates from and is motivated by the ADAS Project, we do not always get full recognition for it. I have made up a plan for OPEN-ADAS which leaves our Project, its values and its raison d'etre intact, but which will make relevant data available to the general public. It will be through a search interface at IAEA, recognisably ADAS, which will enable identification and extraction of selected data and provision of necessary information on it. The ADAS members will also have this, but for Project members alone it will in addition provide a mechanism for selecting interactively the data for ADAS codes. Hopefully this will finally answer the criticism of knowing what ADAS data to use. I have attached the detailed planning for OPEN-ADAS (Schedule 2) along with this bulletin for ADAS members. Another consequence of all this is that I shall have the requirement to rewrite the ADAS manual – long overdue – and time to do it.

4. Code and data updates in v2.10.

Corrections and additions to codes (ADAS v2.9 to ADAS v2.10)

C.1 Correct failure of *read_adf14.pro* when given more than 24 input temperatures.

C.2 Addition of offline code *adas8#3* for automated R-matrix calculations.

C.3 *cxsqef.pro* did not close the *adf12* unit after use and IDL can get through units quickly.

C.4 *ADAS413* was not compiled for the last few releases. Fortunately it interrogates *adf23* ionisation data of which there are not very many examples. However this data format will become much more important soon as it is the primary storage of the Ionisation Project.

C.5 New IDL versions of *xxdata_01, xxdata_02* and *xxdata_12* to return all data in *adf01, adf02* and *adf12* files as f*ulldata* structures in the corresponding *read_adf01, read_adf02* and *read_adf12* routines.

The *adf01* data is accessed via an index generated from the quantum numbers. The *i4idfl.pro* is provided for this.

Obviously fortran *xxdata_01.for, xxdata_02.for* and *xxdata_12.for* are available and are in the *adaslib* library.

C.6 A command line version of *ADAS309*, *run_adas309.pro*, is now provided which can be used to speed up the generation of *adf12* data.

C.7 The incorrect scaling with Zeff of ion impact in CX emission (*ADAS306*, *ADAS307*, *ADAS308* and *ADAS309*) has been corrected.
See the data section for the effect on *adf12* emissivity data.

C.8 The dimensions in *read_adf04.pro* have been increased such that the *fulldata* structure can accommodate the amount of data in the high Z species *adf04* datasets.

C.9 Two new utility routines: *cast_value.pro* : function which forces input to the selected type and issue a warning if not possible. *adas_wait.pro* : routine to wait for fortran to finish have been added.

C.10 The IDL command version of *ADAS409* (GTN generation) failed if a recombination driver of iz1=10 was included. This was due to a poor format which was not picked up in testing.

C.11 An internal correction has been made in *ADAS305* which mostly affected SUN machines. There is no impact on other operating systems.

C.12 An IDL wrapper has been added to *xxerrd* routine which calculates energies relative to ground or ionisation potential (in Rydbergs) when given energies relative to ground in cm^{-1}.

C.13 Increased number of Te/Ne pairs which *read_adf11* can return without multiple calls (hidden from the user) to 2000.

C.14 Changes have been made to *h9int.pro*. Input values of dtype and dparam are explicilty cast to long and double respectively.

C.15 Added the interactive code for *adf04* scatter plot comparison - *ADAS812*.

C.16 Added command line version of *ADAS812* - *compare_adf04*.

C.17 Added *burgspace.pro* to take collision strengths or effective collision strengths and map them into Burgess-Tully space.

C.18 Added */noproc* keyword so that data is returned essentially unprocessed from *xxdata_04*. This is necessary for MC error propagation in IDL of the CR model.

C.19 3 digits are now given to upper and lower level specification in the *adf15* output of *ADAS208*.

C.20 *ADAS216* now uses *xxdata_04* to read in the specific ion files which allows larger datasets to be considered. A further change allows as many specific errors as transitions.

C.21 A J-resolved command line version of *ADAS307*, *run_adas307.pro*, has now been provided which complements the existing L-resolved *run_adas309.pro* routine.

C.22 An offline code, *adas7#1*, has been provided which contains scripts and source code used to produce all of the '05' RR, PE and PI data (*adf48*, *adf38* and *adf39* respectively). At the moment this is more a placeholder/historical record than a production code and contains a snapshot of what was used for this recent batch of data. Note also that recent DR data were also produced with these scripts/codes but most of the earlier data were processed manually. Guidance should be sought before attempting to use these codes.

C.23 Increased version number to 2.10

Corrections and updates to data (ADAS v2.9 to ADAS v2.10)

D.1 The *adf12* emissivity coefficients show incorrect behaviour at non-integer Zeff. They are flat and only change at each integer change which can introduce an error of up to 15% depending on element, transition, Zeff and plasma conditions selected.

The origin of the fault was in the routine which calculates the ion impact collisional rate coefficients which has also been corrected.

All the *adf12/qef*/qef** data in central adas is affected. ie in the *adf12* sub-directories *qef93#h/, qef93#he/, qef93#na/, qef97#h/, qef97#he/, qef97#li/* and *qef99#h/*. Some of the entries in the older *ionatom/* directory also have this fault.

The *qef** data has been replaced while leaving the ionatom collection as it is.

Usually we are reluctant to change data in central ADAS, preferring to add datasets with a later year designation. However in this case there is a fault so replacing it is the preferred action.

D.2 PEC data for Ni ionisation stages (Ni^{25+}, Ni^{24+}, Ni^{17+} and Ni^{16+}) have been added to the *adf15/transport/* directory. This collection is to support transport analysis. The input data is mostly from Sampson/Zhang and is outside the GCR framework.

D.3 One of the above ions, Mg-like Ni^{16+}, uses an *adf04* file generated from CHIANTI data. This can be found at *../adas/adf04/mglike/mglike_chianti#ni16.dat* with full references to the CHIANTI sources.

D.4 Added He-like *adf04* files for Ca, Fe and S from:Kimura et al (2000) J Phys B 33 3449
Files are:
adf04/helike/helike_adw00#ca18.dat
adf04/helike/helike_adw00#fe24.dat
adf04/helike/helike_adw00#s14.dat

D.5 Added He-like *adf04* file for O from: Delahaye and Pradhan (2002) J Phys B 35 3377
File is:
adf04/helike/helike_adw02#o6.dat

D.6 Replaced file *adf09/mb00#he/mb00#he_cu27ls12.dat* which was empty with a new version containing data.

D.7 Prepared new *adf09* files for he-like DR: *adf09/mb00#he* renamed to *adf09/nrbmb00#he*
Following files added:
nrb00#he_c4ic13.dat
nrb00#he_c4ls13.dat
nrb00#he_fe24ic13.dat
nrb00#he_fe24ls13.dat
nrb00#he_xe52icr13.dat

D.8 Added driver files for above *adf09* files in: *adf27/helike/nrb00#*he and *adf28/helike/nrb00#he*

D.9 Added new preferred Ne-like DR datasets in: *adf09/nrb00#ne* with corresponding drivers in: *adf27/nelike/nrb00#ne* and *adf28/nelike/nrb00#ne*

The previous data (*oiz00#ne*) were flawed because i) they only went up to l=3, just good enough for totals, particularly as (ii) the structure overestimated the core dipole radiative rates, and Ne-like only has the 2-3 contribution. The *oiz* calculations have been retained but the *nrb* data should now be seen as the preferred datasets.

D.10 Fixed the formatting of files in *adas/arch602*. These had been corrupted by CVS.

D.11 Replaced configuration labels in two older He^0 datasets with a more standard version.
adf04/helike/helike_hpsl91he.dat
adf04/helike/helike_hpsh91he.dat

D.12 Moved the position of the ionisation error block in *adf04/helike/helike_hps02he.dat* in order to accommodate *ADAS216*. This code is due an update and the error descriptions will be held in an additional .err file in future.

D.13 Charge exchange cross section data (*adf01*) from neutral lithium donor (2s, 2p, 3s, 3p and 3d levels) to fully stripped carbon and helium receivers has been added. The data were assembled by Elisabeth Wolfrum of IPP-Garching from CTMC and CCAO calculations.

D.14 Moved directories:
adf09/za00#b to *adf09/nrbza00#b*
adf09/oiz00#o to *adf09/nrboiz00#o*
adf09/dmm00#n to *adf09/nrbdmm00#n*
to allow for the addition of *nrb* files to them.

D.15 The following DR files were added:
adf09/nrbza00#b/nrb00#b_c1ic222.dat
adf09/nrbza00#b/nrb00#b_c1ls222.dat
adf09/nrbza00#b/nrb00#b_c1ls22.dat
adf09/nrbza00#b/nrb00#b_c1ic22.dat
with corresponding drivers:
adf27/blike/nrb00#b/c1ic22-2.dat
adf27/blike/nrb00#b/c1ic22-n.dat
adf27/blike/nrb00#b/c1ic22_str.dat
adf28/blike/nrb00#b/c1ic222.dat
adf28/blike/nrb00#b/c1ic22.dat
adf28/blike/nrb00#b/c1ls222.dat
adf28/blike/nrb00#b/c1ls22.dat
The files contain data for 2s->2p core excitations with capture to n=2 which had not previously been calculated and also replacements for the *za00#b_c1[ls,ic]22.dat* files (i.e. 2s-2p capture to n (>2)) which used poor target structure.

D.16 The following DR files were added:
adf09/nrboiz00#o/nrb00#o_f1ic222.dat
adf09/nrboiz00#o/nrb00#o_f1ls222.dat
with corresponding drivers:
adf27/olike/nrb00#o/f1ic22-2.dat
adf28/olike/nrb00#o/f1ic222.dat
adf28/olike/nrb00#o/f1ls222.dat
for 2s->2p core excitations with capture to n=2. These data had not previously been calculated.

D.17 The following DR files were added:
adf09/nrboiz00#c/nrb00#c_n1ic222.dat
adf09/nrboiz00#c/nrb00#c_n1ls222.dat
with corresponding drivers:
adf27/clike/nrb00#c/n1ic22-2.dat
adf28/clike/nrb00#c/n1ic222.dat
adf28/clike/nrb00#c/n1ls222.dat
for 2s->2p core excitations with capture to n=2. These data had not previously been calculated.

D.18 The following DR files were added:
adf09/nrbdmm00#n/nrb00#n_o1ic223.dat
adf09/nrbdmm00#n/nrb00#n_o1ls223.dat
with corresponding drivers:
adf27/nlike/nrb00#n/o1ic22-3.dat
adf28/nlike/nrb00#n/o1ic223.dat

adf28/nlike/nrb00#n/o1ls223.dat

for 2s-2p core excitations with capture to n=3. These data had not previously been calculated.

D.19 The *adf27* and *adf28* directory structure was altered, there is now an additional layer such that we have:

adf27/dr
adf27/rr
adf27/pe
adf27/pi
adf28/dr
adf28/rr
adf28/pe
adf28/pi

The "dr" directories contain what used to sit at the top level (i.e. directories like "blike", "clike" etc.). *adf27/28* are now used for RR, PI and PE driver files (see below)

D.20 Added radiative-recombination data in a new ADAS data format as:

adf48/nrb05##/
adf48/nrb05#b/
adf48/nrb05#be/
adf48/nrb05#c/
adf48/nrb05#f/
adf48/nrb05#h/
adf48/nrb05#he/
adf48/nrb05#li/
adf48/nrb05#n/
adf48/nrb05#na/
adf48/nrb05#ne/
adf48/nrb05#o/

with drivers in:

adf27/rr/belike/nrb05#be/
adf27/rr/blike/nrb05#b/
adf27/rr/clike/nrb05#c/
adf27/rr/flike/nrb05#f/
adf27/rr/helike/nrb05#he/
adf27/rr/hlike/nrb05#h/
adf27/rr/#like/nrb05##/
adf27/rr/lilike/nrb05#li/
adf27/rr/nalike/nrb05#na/
adf27/rr/nelike/nrb05#ne/
adf27/rr/nlike/nrb05#n/
adf27/rr/olike/nrb05#o/
adf28/rr/blike/nrb05#b/
adf28/rr/clike/nrb05#c/
adf28/rr/flike/nrb05#f/
adf28/rr/helike/nrb05#he/
adf28/rr/hlike/nrb05#h/
adf28/rr/#like/nrb05##/
adf28/rr/lilike/nrb05#li/
adf28/rr/nalike/nrb05#na/
adf28/rr/nelike/nrb05#ne/
adf28/rr/nlike/nrb05#n/
adf28/rr/olike/nrb05#o/

D.21 Added photo-excitation data in:

adf38/nrb05##/
adf38/nrb05#b/
adf38/nrb05#be/
adf38/nrb05#c/

adf38/nrb05#f/
adf38/nrb05#h/
adf38/nrb05#he/
adf38/nrb05#li/
adf38/nrb05#n/
adf38/nrb05#na/
adf38/nrb05#ne/
adf38/nrb05#o/

with drivers in:

adf27/pe/belike/nrb05#be/
adf27/pe/blike/nrb05#b/
adf27/pe/clike/nrb05#c/
adf27/pe/flike/nrb05#f/
adf27/pe/helike/nrb05#he/
adf27/pe/lilike/nrb05#li/
adf27/pe/nalike/nrb05#na/
adf27/pe/nelike/nrb05#ne/
adf27/pe/nlike/nrb05#n/
adf27/pe/olike/nrb05#o/
adf28/pe/belike/nrb05#be/
adf28/pe/blike/nrb05#b/
adf28/pe/clike/nrb05#c/
adf28/pe/flike/nrb05#f/
adf28/pe/helike/nrb05#he/
adf28/pe/hlike/nrb05#h/
adf28/pe/lilike/nrb05#li/
adf28/pe/nalike/nrb05#na/
adf28/pe/nelike/nrb05#ne/
adf28/pe/nlike/nrb05#n/
adf28/pe/olike/nrb05#o/
adf28/pe/urlike/nrb05##/

Note that these are '05' data, produced with relaxed orbitals and only for transitions from the ground state. Transitions between all excited states are archived as '04' data (but relaxed orbitals were not used) and are not routinely released with ADAS due to the volume of the data.

D.22 Added photo-ionisation data in:

adf39/nrb05##/
adf39/nrb05#b/
adf39/nrb05#be/
adf39/nrb05#c/
adf39/nrb05#f/
adf39/nrb05#h/
adf39/nrb05#he/
adf39/nrb05#li/
adf39/nrb05#n/
adf39/nrb05#na/
adf39/nrb05#ne/
adf39/nrb05#o/

with drivers in:

adf27/pi/belike/nrb05#be/
adf27/pi/blike/nrb05#b/
adf27/pi/clike/nrb05#c/
adf27/pi/flike/nrb05#f/
adf27/pi/helike/nrb05#he/
adf27/pi/hlike/nrb05#h/
adf27/pi/#like/nrb05##/
adf27/pi/lilike/nrb05#li/
adf27/pi/nalike/nrb05#na/
adf27/pi/nelike/nrb05#ne/

adf27/pi/nlike/nrb05#n/
adf27/pi/olike/nrb05#o/
adf28/pi/blike/nrb05#b/
adf28/pi/clike/nrb05#c/
adf28/pi/flike/nrb05#f/
adf28/pi/helike/nrb05#he/
adf28/pi/hlike/nrb05#h/
adf28/pi/#like/nrb05##/
adf28/pi/lilike/nrb05#li/
adf28/pi/nalike/nrb05#na/
adf28/pi/nelike/nrb05#ne/
adf28/pi/nlike/nrb05#n/
adf28/pi/olike/nrb05#o/

Note that these are '05' data, produced with relaxed orbitals and only for transitions from the ground state. Transitions from all excited states are archived as '04' data (but relaxed orbitals were not used) and are not routinely released with ADAS due to the volume of the data.

HPS
06 Jan. 2006