

Atomic and Molecular databases

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Outline

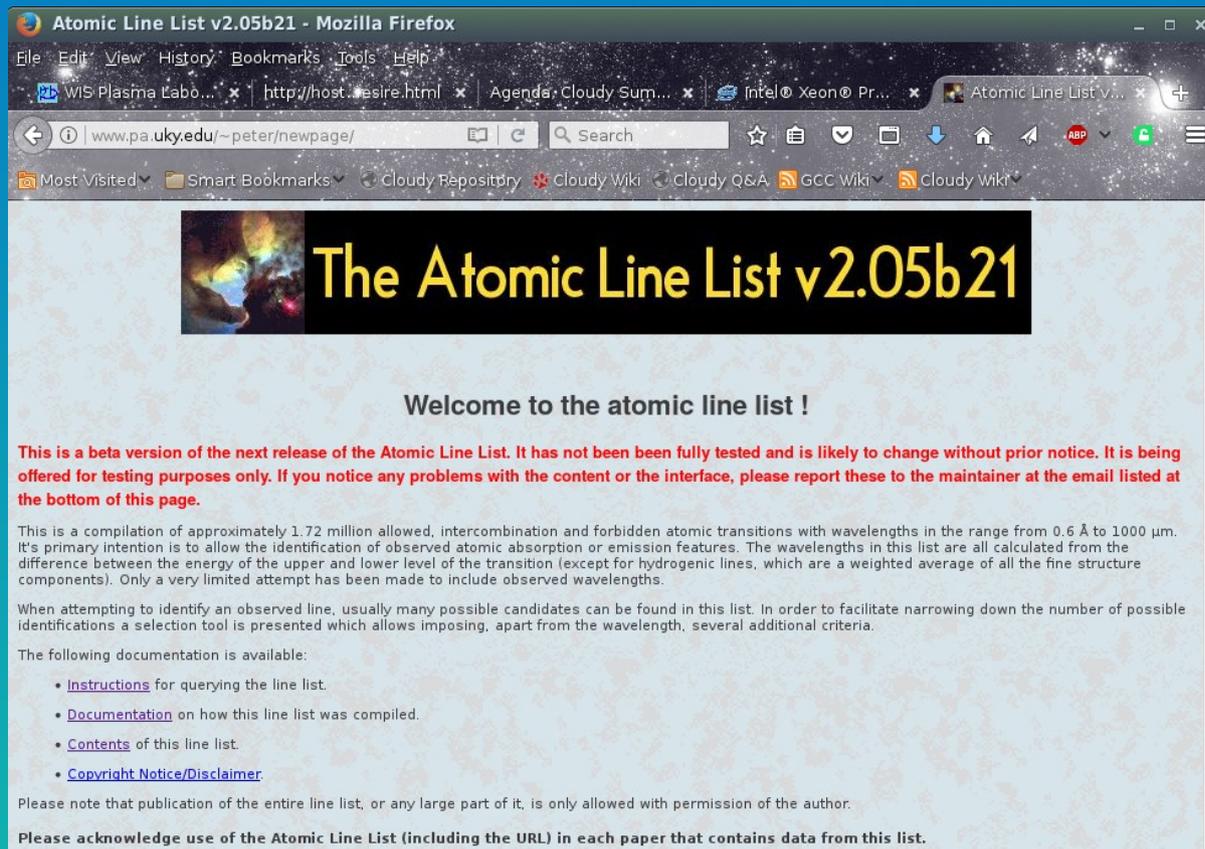
- Introduction
- Line identification
- Transition probabilities
- Collisional data
- Setting up a stout data module
- Other atomic data
- Miscellaneous data
- Chemical reactions
- Molecular data
- Atomic data codes
- The future

Introduction

- Many on-line databases exist. This overview cannot be complete.
- ADS is a good resource! Many data sources are only available as a refereed paper, but not in a database.
- I try to present sites containing high quality data, at least as the primary source, but I cannot always verify that.
- Newer calculations are not necessarily better than older ones!
- I will spend more time on data types that you need more likely.
- Data for reverse processes can be calculated using detailed balance (but remember that detailed balance doesn't hold for non-Maxwellian electron distributions).

Line identification

- One of the most basic tasks is identifying lines in a spectrum.
- For atomic lines multiple good sites are available:
<http://www.pa.uky.edu/~peter/newpage/>



Atomic Line List v2.05b21 - Mozilla Firefox

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www.pa.uky.edu/~peter/newpage/ Search

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The Atomic Line List v2.05b21

Welcome to the atomic line list !

This is a beta version of the next release of the Atomic Line List. It has not been fully tested and is likely to change without prior notice. It is being offered for testing purposes only. If you notice any problems with the content or the interface, please report these to the maintainer at the email listed at the bottom of this page.

This is a compilation of approximately 1.72 million allowed, intercombination and forbidden atomic transitions with wavelengths in the range from 0.6 Å to 1000 μm. It's primary intention is to allow the identification of observed atomic absorption or emission features. The wavelengths in this list are all calculated from the difference between the energy of the upper and lower level of the transition (except for hydrogenic lines, which are a weighted average of all the fine structure components). Only a very limited attempt has been made to include observed wavelengths.

When attempting to identify an observed line, usually many possible candidates can be found in this list. In order to facilitate narrowing down the number of possible identifications a selection tool is presented which allows imposing, apart from the wavelength, several additional criteria.

The following documentation is available:

- [Instructions](#) for querying the line list.
- [Documentation](#) on how this line list was compiled.
- [Contents](#) of this line list.
- [Copyright Notice/Disclaimer](#).

Please note that publication of the entire line list, or any large part of it, is only allowed with permission of the author.

Please acknowledge use of the Atomic Line List (including the URL) in each paper that contains data from this list.

Line identification

- Other sites that are available are

http://physics.nist.gov/PhysRefData/ASD/lines_form.html

<https://www.cfa.harvard.edu/ampcgi/kelly.pl>

<http://spectr-w3.snz.ru/splines.phtml>

- Using the NIST site you can also search for energy levels

http://physics.nist.gov/PhysRefData/ASD/levels_form.html

- Each site has its own advantages and disadvantages, e.g. the atomic line list contains many more infrared lines, but NIST contains elements beyond krypton.
- The Kelly site has a simplistic interface, but can have UV lines that are not found elsewhere.
- So it can be worthwhile looking on multiple sites!

Line identification

- Notation for levels can sometimes differ!
- 4 different coupling schemes

LS coupling: $L_c + l = L, S_c + s = S, L + S = J$

jj coupling: $L_c + S_c = J_c, l + s = j, J_c + j = J$

jK coupling: $L_c + S_c = J_c, J_c + l = K, K + s = J$

LK coupling: $L_c + l = L, L + S_c = K, K + s = J$

- Change can be due to different coupling scheme, e.g. LK vs. jK coupling

N I 2s2.2p2.(3P<1>).5f G[3]* 7/2 112868.73

N I 2s2.2p2.(3P<1>).5f 1[3]* 7/2 112868.73

- Different notation for LS terms of equivalent electrons. E.g. d^3 has two different 2D terms, which can be written as:
 - a^2D and b^2D (seniority index)
 - 2D_2 and 2D_1 (Nielson-Koster, preferred by NIST)
 - 2_3D and 2_1D (Racah seniority number)

Line identification

- The Racah seniority number is defined for all terms, but may be omitted when unique, e.g. $d^6 \ ^5D$ and $\ ^5_4D$ are the same.
- Intermediate term information may or may not be omitted when unambivalent, e.g.

Ni I 3d8.4s.(4F).5s 3F

Ni I 3d8.(3F).4s.(4F).5s 3F

are both the same.

- Especially with open d or f shells, configuration mixing can lead to strong deviations from LS coupling. One bad example:

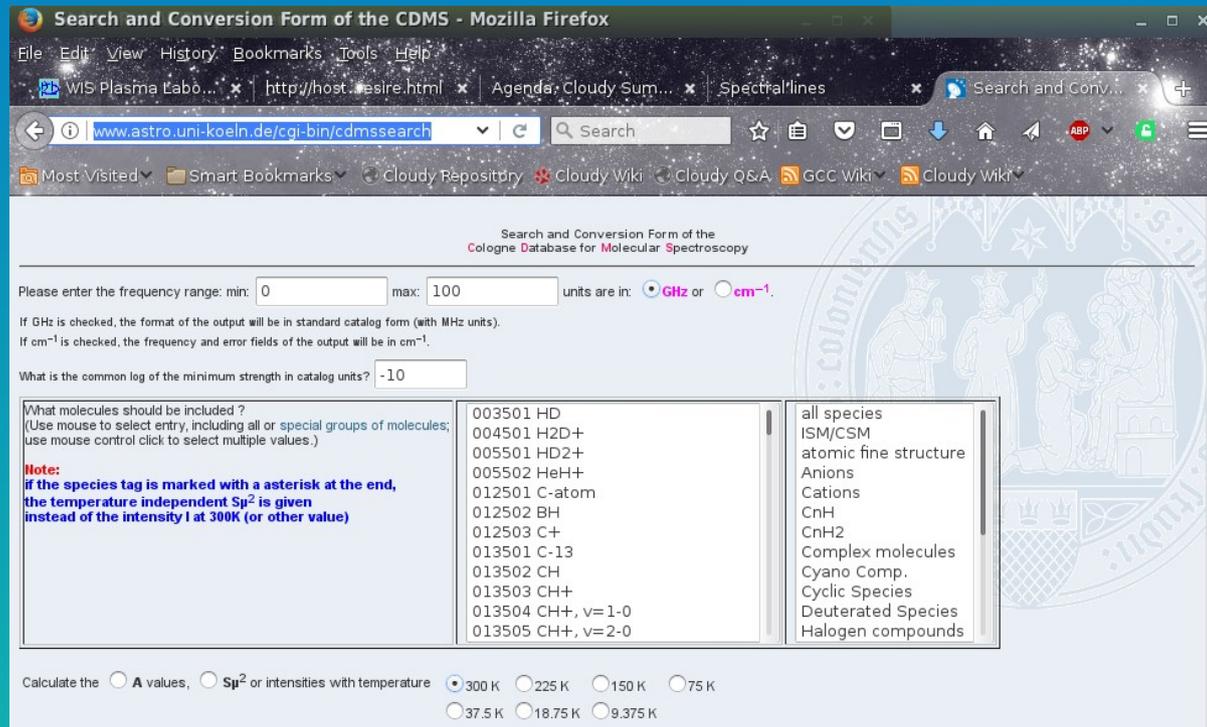
Fe II 104569.230 14% 4|3P4)2D + 13% 6|5D4)4F + 12% 4|3P4)4F + 9% 4|3P2)2D

- Usually the leading term is assigned, unless this would lead to duplicate assignments in which case the second (or even third!) term is chosen.
- NIST sometimes refuses to assign a term in these circumstances.
- Slight differences in the term analysis can cause the LS assignments to change!

Line identification

- For molecular lines the situation is more complex.
- For pure rotational lines (Herschel, ALMA, etc) you have quite a lot of resources.

<http://www.astro.uni-koeln.de/cgi-bin/cdmssearch>



Search and Conversion Form of the
Cologne Database for Molecular Spectroscopy

Please enter the frequency range: min: max: units are in: GHz or cm⁻¹.

If GHz is checked, the format of the output will be in standard catalog form (with MHz units).
If cm⁻¹ is checked, the frequency and error fields of the output will be in cm⁻¹.

What is the common log of the minimum strength in catalog units?

<p>What molecules should be included ? (Use mouse to select entry, including all or special groups of molecules; use mouse control click to select multiple values.)</p> <p>Note: if the species tag is marked with an asterisk at the end, the temperature independent Sp² is given instead of the intensity I at 300K (or other value)</p>	<p>003501 HD 004501 H2D+ 005501 HD2+ 005502 HeH+ 012501 C-atom 012502 BH 012503 C+ 013501 C-13 013502 CH 013503 CH+ 013504 CH+, v=1-0 013505 CH+, v=2-0</p>	<p>all species ISM/CSM atomic fine structure Anions Cations CnH CnH2 Complex molecules Cyano Comp. Cyclic Species Deuterated Species Halogen compounds</p>
--	---	--

Calculate the A values, Sp² or intensities with temperature 300 K 225 K 150 K 75 K
 37.5 K 18.75 K 9.375 K

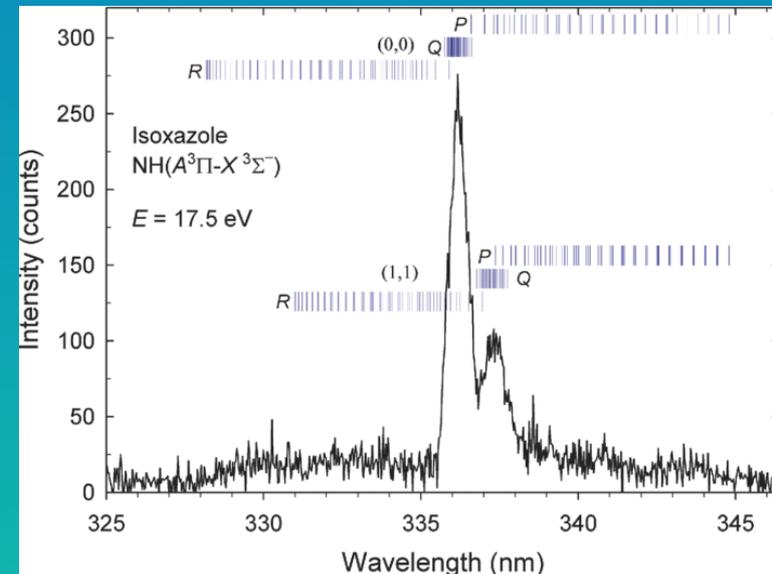
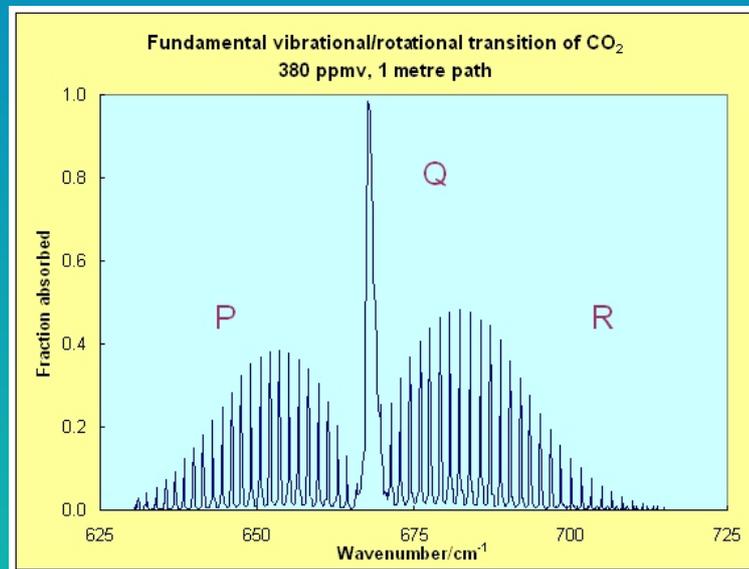
Line identification

- Other sites are available:

<https://spec.jpl.nasa.gov/ftp/pub/catalog/catform.html>

<http://www.cv.nrao.edu/php/splat/>

- Again, none of these sites are complete. So it can help to search multiple sites! Note that isotopologues will have lines at different frequencies!
- For ro-vibrational and electronic transitions the situation is more difficult! These spectra can be extremely complex, e.g. H₂O alone has >500 million lines.



Line identification

- Observed lines of this type usually are blends consisting of many individual components (band heads), especially in lower-resolution spectra.
- For the most important molecules (H_2 , CO, OH), there are links relevant for IR observers here:

<http://www.not.iac.es/instruments/notcam/ReferenceInfo/>

- Large compilations of molecular transitions exist, such as HITRAN and GEISA.

<https://www.cfa.harvard.edu/hitran/>

<http://www.pole-ether.fr/etherTypo/?id=950&L=0>

These are intended for modeling the Earth's atmosphere, so they only contain molecules relevant for that! HITRAN can be searched online:

<http://hitran.org/> (requires registration)

- Also GEISA can be searched online. HITRAN contains 47 molecules, GEISA 52.

Transition Probabilities

- For atomic lines, many databases exist that contain transition probabilities. All the line lists also have transition probabilities.

<http://www.pa.uky.edu/~peter/newpage/>

http://physics.nist.gov/PhysRefData/ASD/lines_form.html

<http://spectr-w3.snz.ru/index.phtml>

- Not all lines will have a transition probability attached.
- The data will have been chosen from various sources, implying some sort of quality assessment (or at least estimate).
- There are also sites dedicated to transition probabilities.

<http://nlte.nist.gov/MCHF/>

(Froese-Fischer, high quality data, incl. IC and forbidden lines)

<http://cdsweb.u-strasbg.fr/topbase/topbase.html>

(Opacity Project/Iron Project, pure LS coupling, multiplet averaged)

Transition Probabilities

<http://norad.astronomy.ohio-state.edu/>

(Sultana Nahar, connected to the Iron Project, so same restrictions)

<http://kurucz.harvard.edu/atoms/>

(very comprehensive, but only lower ions, IC lines, but not forbidden)

<http://vald.astro.uu.se/>

(requires registration, well respected, email interface → VAMDC)

<http://open.adas.ac.uk/>

(data for inner-shell excitations)

<http://hosting.umons.ac.be/html/agif/databases/dream.html>

<http://hosting.umons.ac.be/html/agif/databases/desire.html>

(data for 5th and 6th row elements)

<http://www.as.utexas.edu/~chris/lab.html>

(links to papers, mainly s-process elements)

Collisional Data

- With the data we have gathered so far, you can only do LTE modeling.
- To create NLTE models you need data for impact excitation.
- Every particle can induce excitations upon impact (subject to selection rules), so in principle you need huge amounts of data.
 - For ions, electron impact will usually dominate.
 - For (near-) degenerate transitions, protons can be important.
 - For neutrals (e.g. [C I], [O I]), H can be important.
 - For molecules, typically H₂ and He are important, but electrons can be too (e.g. CN)...
- Only few sites exist that collect data for impact excitation.
- Most data only exists in the form of refereed journal publications that you need to search via ADS or some other bibliographical database.

Collisional Data

- Open ADAS has a large collection of collisional data for ions
<http://open.adas.ac.uk/adf04>
- NIST has a small database of collisional data (primarily ionization)
<https://www.nist.gov/pml/electron-impact-cross-sections-ionization-and-excitation-database>
- The IAEA ALADDIN database contains both atomic and molecular data (this site now hosts the Oak Ridge A&M data after it closed)
<https://www-amdis.iaea.org/ALADDIN/collision.html>
- Additional resources are here:
<http://dbshino.nifs.ac.jp/>
<http://www.camdb.ac.cn/e/collision/index.htm>
- For molecules the LAMDA database is helpful
<http://home.strw.leidenuniv.nl/~moldata/>

Setting up a data module

- With the data sources we have discussed so far, we can start defining our own stout modules.
- You need three data files. The first defines the energy levels (s_3.nrg).

```
Terminal
File Edit View Terminal Tabs Help
11 10 14
1      0.000      1.0      3s2.3p2(3P)
2     298.690     3.0      3s2.3p2(3P)
3     833.080     5.0      3s2.3p2(3P)
4    11322.700    5.0      3s2.3p2(1D)
5    27161.000    1.0      3s2.3p2(1S)
6    58671.920    5.0      3s.3p3(5S)
7    84019.300    3.0      3s.3p3(3D)
8    84046.700    5.0      3s.3p3(3D)
9    84099.400    7.0      3s.3p3(3D)
10   98745.300    5.0      3s.3p3(3P)
11   98765.900    3.0      3s.3p3(3P)
12   98772.200    1.0      3s.3p3(3P)
13  104159.700    5.0      3s2.3p.3d(1D)
14  122118.500    5.0      3s2.3p.3d(3F)
15  122404.000    7.0      3s2.3p.3d(3F)
16  122798.600    9.0      3s2.3p.3d(3F)
17  136843.780    3.0      3s.3p3(1P)
18  138066.600    3.0      3s.3p3(3S)
19  143097.080    1.0      3s2.3p.3d(3P)
20  143117.410    3.0      3s2.3p.3d(3P)
21  143125.280    5.0      3s2.3p.3d(3P)
22  146697.370    1.0      3s2.3p.4s(3P)
23  146737.550    3.0      3s2.3p.4s(3P)
24  147147.110    5.0      3s2.3p.4s(3P)
25  147551.600    3.0      3s2.3p.3d(3D)
26  147692.210    5.0      3s2.3p.3d(3D)
27  147745.700    7.0      3s2.3p.3d(3D)
28  148398.970    3.0      3s2.3p.4s(1P)
29  151978.540    5.0      3s.3p3(1D)
30  157610.310    7.0      3s2.3p.3d(1F)
--More--(55%)
```

Setting up a data module

- The second data file defines the transition probabilities for radiative transitions (s_3.tp)

```
Terminal
File Edit View Terminal Tabs Help
11 10 14
A 1 2 3.4178e-04
A 1 3 2.2766e-08
A 2 3 1.4298e-03
A 1 4 5.6376e-06
A 2 4 1.9534e-02
A 3 4 5.1568e-02
A 2 5 6.8755e-01
A 3 5 9.5322e-03
A 4 5 2.1885e+00
A 1 6 4.8634e-03
A 2 6 5.40e+03
A 3 6 1.54e+04
A 4 6 3.4499e+00
A 5 6 5.2712e-09
A 1 7 4.0237e+07
A 2 7 2.6619e+07
A 3 7 1.3751e+06
A 4 7 4.5668e+04
A 5 7 9.1951e+02
A 2 8 5.3797e+07
A 3 8 1.3883e+07
A 4 8 5.7067e+03
A 3 9 6.6637e+07
A 4 9 5.2439e+04
A 2 12 2.9189e+08
A 1 11 9.4553e+07
A 2 11 7.4384e+07
A 3 11 1.1936e+08
A 4 11 9.2719e+04
A 5 11 2.4779e+04
--More--(7%)
```

Setting up a data module

- The third data file defines the collision strengths or rate coefficients (s_3.coll)
- More details here: <http://wiki.nublado.org/wiki/StoutData>

```

Terminal
File Edit View Terminal Tabs Help
A 3 9 6.6637e+07
A 4 9 5.2439e+04
A 2 12 2.9189e+08
A 1 11 9.4553e+07
A 2 11 7.4384e+07
A 3 11 1.1936e+08
A 4 11 9.2719e+04
A 5 11 2.4779e+04
pvh@pvh-nb:s/s_3 % more s_3.coll
11 10 14
TEMP 1.00e+03 1.58e+03 2.51e+03 3.98e+03 6.31e+03 1.00e+04 1.58e+04 2.51e+04
3.98e+04 6.31e+04 1.00e+05 1.58e+05 2.51e+05 3.98e+05 6.31e+05 1.00e+06
1.00e+10
CSELECTRON 1 2 2.08e+00 2.10e+00 2.13e+00 2.20e+00 2.27e+00 2.26e+00 2.17e+00
2.07e+00 1.97e+00 1.84e+00 1.63e+00 1.36e+00 1.07e+00 8.10e-01 5.90e-01
4.18e-01 2.70e-02
CSELECTRON 1 3 9.84e-01 9.59e-01 9.47e-01 9.61e-01 9.85e-01 1.03e+00 1.12e+00
1.24e+00 1.32e+00 1.32e+00 1.23e+00 1.07e+00 8.87e-01 7.10e-01 5.62e-01
4.45e-01 1.72e-01
CSELECTRON 1 4 6.98e-01 7.33e-01 7.38e-01 7.20e-01 7.10e-01 7.29e-01 7.65e-01
7.90e-01 7.86e-01 7.43e-01 6.59e-01 5.48e-01 4.30e-01 3.22e-01 2.34e-01
1.65e-01 1.01e-02
CSELECTRON 1 5 8.39e-02 8.98e-02 9.64e-02 1.04e-01 1.14e-01 1.25e-01 1.39e-01
1.56e-01 1.73e-01 1.82e-01 1.76e-01 1.60e-01 1.37e-01 1.14e-01 9.23e-02
7.37e-02 2.40e-02
CSELECTRON 1 6 5.63e-01 5.79e-01 5.58e-01 5.13e-01 4.58e-01 4.16e-01 4.01e-01
4.01e-01 3.97e-01 3.74e-01 3.33e-01 2.81e-01 2.26e-01 1.75e-01 1.30e-01
9.38e-02 6.76e-03
CSELECTRON 1 7 4.89e-01 4.59e-01 4.36e-01 4.25e-01 4.19e-01 4.09e-01 4.01e-01
3.99e-01 3.98e-01 3.88e-01 3.70e-01 3.49e-01 3.29e-01 3.16e-01 3.11e-01
3.14e-01 3.54e-01
CSELECTRON 1 8 4.34e-01 3.89e-01 3.54e-01 3.36e-01 3.32e-01 3.34e-01 3.39e-01

```

Other Atomic Data

- Atomic Data for Astrophysics was compiled by Dima Verner. This site is no longer maintained, but still contains lots of useful data on photoionization, recombination, collisional ionization and autoionization, charge transfer, Auger processes, etc.:

<http://www.pa.uky.edu/~verner/atom.html>

- Open ADAS contains a collection of data on charge exchange, collisional excitation/ionization, radiative & dielectronic recombination, inner-shell excitation / autoionization, and photoionization:

<http://open.adas.ac.uk/>

- VAMDC gives central access to various databases and provides data support for the virtual observatory. Output is in XML format.

http://portal.vamdc.org/vamdc_portal/nodes.seam

<http://www.vamdc.org/activities/research/software/>

- AtomDB is an atomic database useful for X-ray plasma spectral modeling.

<http://www.atomdb.org/>

Other Atomic Data

- The universal atomic database aims to be a comprehensive repository of atomic physics quantities needed for astrophysics

<https://heasarc.gsfc.nasa.gov/uadb/>

- The GENIE search engine of the IAEA provides a convenient access point to multiple online databases for various types of data

<https://www-amdis.iaea.org/GENIE/>

- Various other databases

<http://www.camdb.ac.cn/e/>

<http://atom.kaeri.re.kr/>

- Various compilations of web sites

<https://www.cfa.harvard.edu/amp/ampdata/databases.html>

<http://plasma-gate.weizmann.ac.il/directories/databases/>

(on the latter site the links are mostly out of date).

Miscellaneous Data

- The Storey & Hummer Case A/B coefficients are here
<ftp://cdsarc.u-strasbg.fr/cats/VI/64/>
- Free-free Gaunt factors (both relativistic and non-relativistic)
<http://data.nublado.org/gauntff/>
- Periodic table
<http://www.ptable.com/>
- Atomic weights and isotopic composition
<https://www.nist.gov/pml/atomic-weights-and-isotopic-compositions-relative-atomic-masses>
- Nuclear properties of isotopes of elements
<http://www.nndc.bnl.gov/nudat2/>

Chemical Reactions

- There are several databases that define a network of chemical reactions that you can use to calculate molecular abundances.

- UMIST is available here

<http://udfa.ajmarkwick.net/>

Latest release is RATE12, available as an ascii file.

- KIDA is available here

<http://kida.obs.u-bordeaux1.fr/>

They provide a nice interactive interface!

- Quantemol is here (requires registration)

<https://quantemoldb.com/>

This is a commercial company, but they have open interface to reaction parameters. Redistribution of the data is not allowed.

Molecular Data

- The following sites give frequencies of rotational lines, as well as transition probabilities

<http://www.astro.uni-koeln.de/cdms/catalog>

<https://spec.jpl.nasa.gov/ftp/pub/catalog/catform.html>

<http://www.cv.nrao.edu/php/splat/>

http://newt.phys.unsw.edu.au/~jbailey/vstar_mol.html

- Collisional excitation data can be found here

<http://home.strw.leidenuniv.nl/~moldata/>

<http://basecol.obspm.fr/>

- These sites contain data needed for modeling the Earth's as well as exoplanet atmosphere

<https://www.cfa.harvard.edu/hitran/>

<http://www.pole-ether.fr/etherTypo/?id=950&L=0>

<http://spectra.iao.ru/> (largely based on HITRAN, GEISA)

Molecular Data

<http://exomol.com/>

http://satellite.mpic.de/spectral_atlas

<http://phys4entrydb.ba.imip.cnr.it/Phys4EntryDB/>

- The following site contains transition probability, photodissociation, and charge transfer data

<https://www.physast.uga.edu/ugamop/>

<https://www.physast.uga.edu/research/stancil-group/atomic-molecular-databases>

- Collections of various types of molecular data

<https://www-amdis.iaea.org/>

<http://webbook.nist.gov/chemistry/form-ser/>

<http://www.ucl.ac.uk/physics-astronomy/theory/moldata>

<https://molat.obspm.fr/index.php?page=pages/menuSpectreMol.php>

Atomic Data Codes

- If you feel up to the task, you could decide to calculate your own data. There are (more or less) open source codes available for this task.

- The well known Cowan codes for calculating atomic spectra and levels are now hosted in Ireland

<https://www.tcd.ie/Physics/people/Cormac.McGuinness/Cowan/>

- A similar code is FAC developed by M. F. Gu, available here

<https://www-amdis.iaea.org/FAC/>

- There is also an interface for calculating electron impact excitation and ionization cross sections from group T-4 at LANL here

<https://www-amdis.iaea.org/LANL/> (link currently broken)

- Some other well known codes

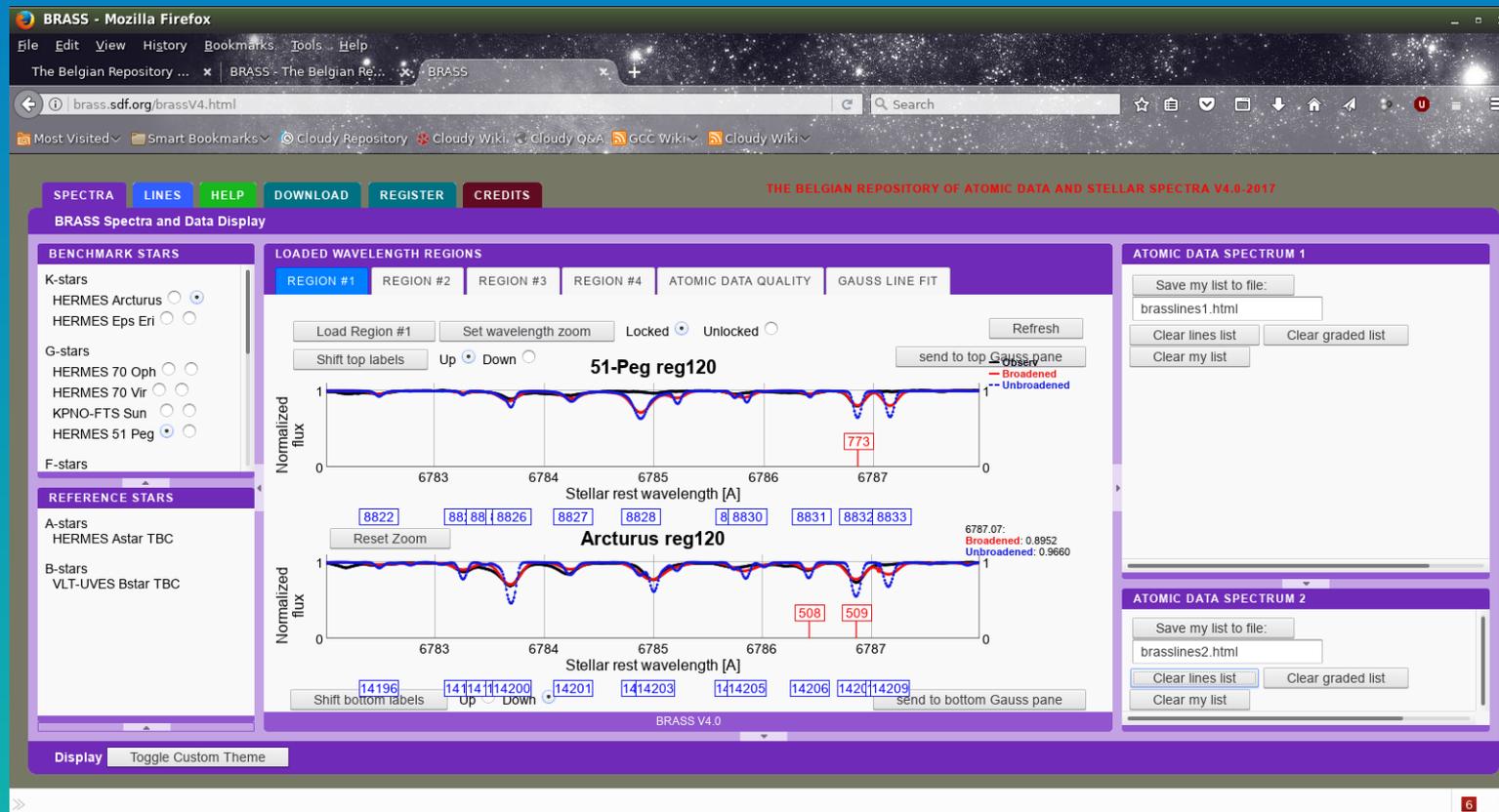
<https://www-amdis.iaea.org/GRASP2K/> (MCHDF)

http://amdpp.phys.strath.ac.uk/UK_RmaX/codes.html (R-matrix, etc)

<http://plasma-gate.weizmann.ac.il/directories/free-software/> (various)

The Future

- BRASS = The Belgian Repository of Atomic Data and Stellar Spectra
<http://brass.sdf.org/>
- This site is still under development!



The Future

- The atomic data collection is not complete
- Efforts for generating atomic data are under pressure (both theoretical and lab experiments).
- Groups are disappearing (e.g. ORNL), or people are retiring.
- Some institutions like NIST and IAEA can provide continuity. Also VAMDC?
- Nuclear fusion still attracts money, so atomic data production will tend to focus on nuclear fusion needs.
- The molecular data collection is far less complete, and their needs are significantly more complex.
- Astrochemistry is an emerging field, so I expect this situation to improve quickly.
- A lot of emphasis will be on modeling atmospheres of exoplanets as well as chemistry leading to prebiotic molecules.