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Atomic and Molecular databases

Peter van Hoof
Royal Observatory of Belgium

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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

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Introduction

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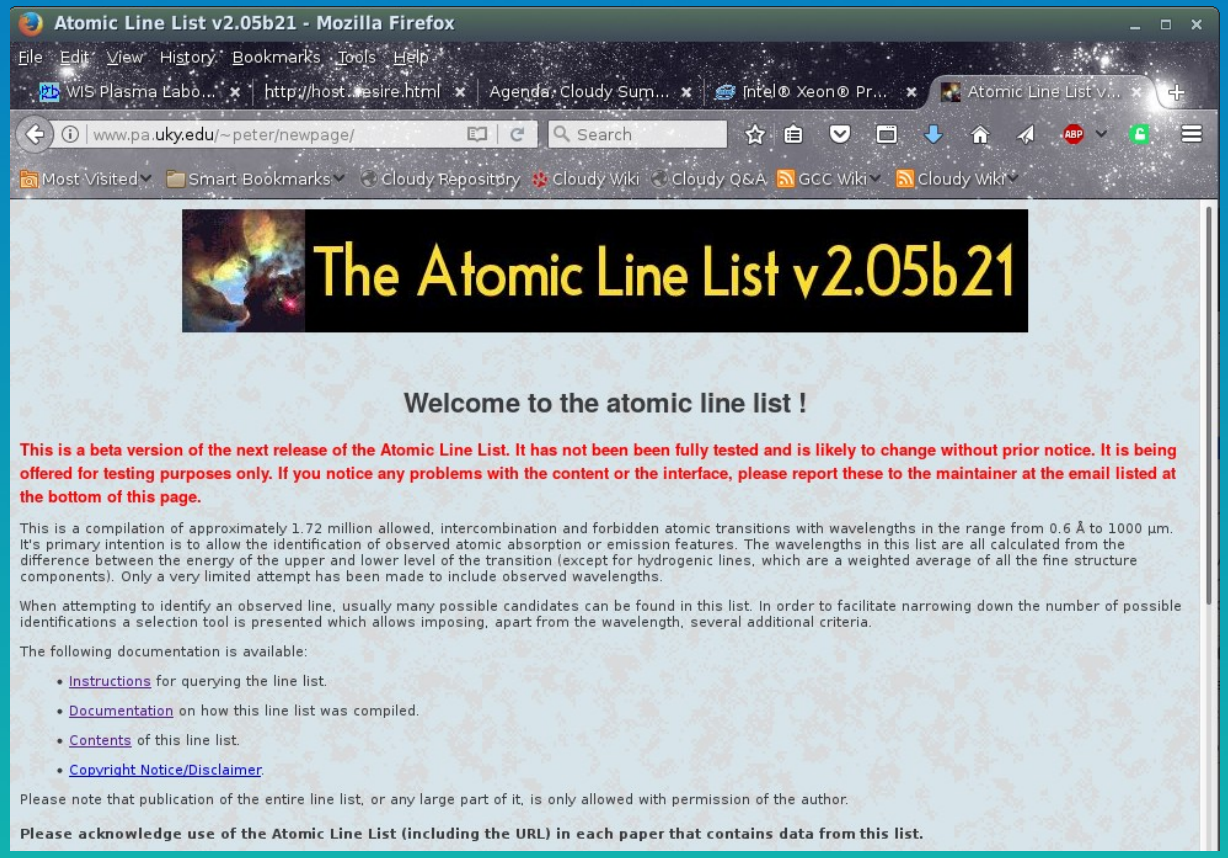
- Many on-line databases exist. This overview cannot be complete.
- ADS is a good resource! Many data sources are only available as a refereed paper, but not in a database.
- I try to present sites containing high quality data, at least as the primary source, but I cannot always verify that.
- Newer 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/



Line identification

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- 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)
  - $^2D2$ and $^2D1$ (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

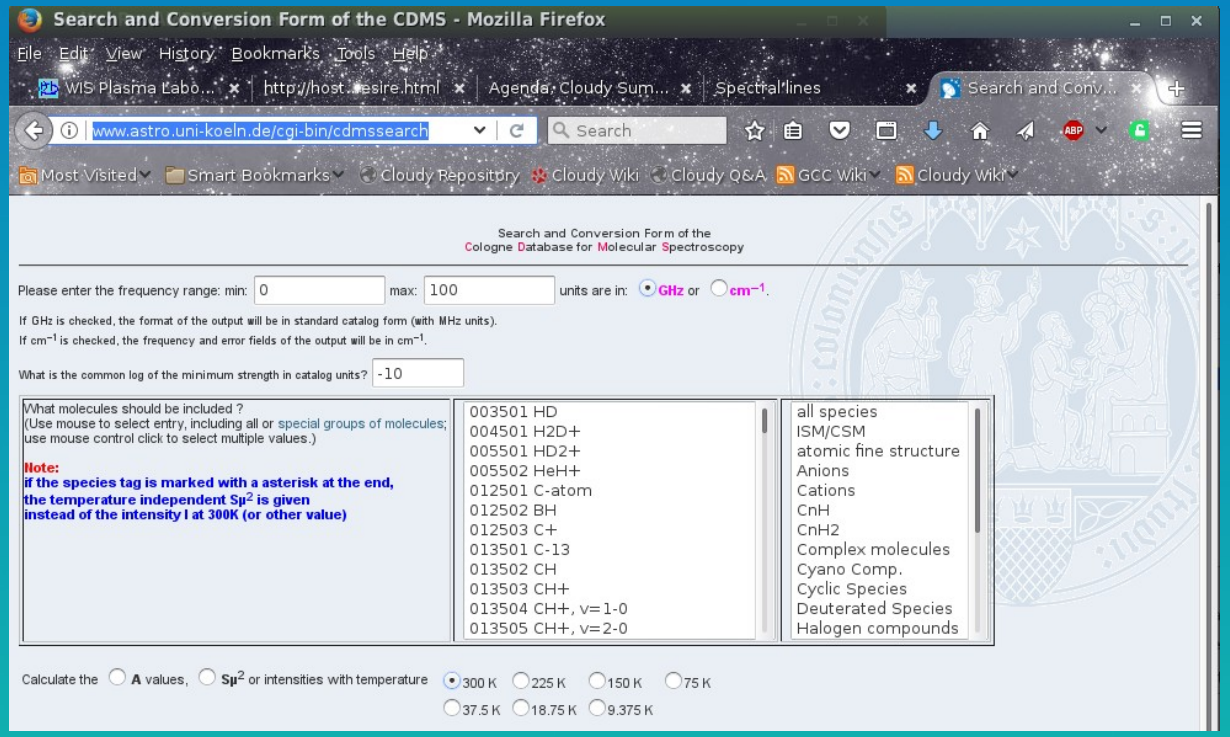
  are both the same.
- Especially with open d or f shells, configuration mixing can lead to strong deviations from LS coupling. One bad example:

  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



Line identification

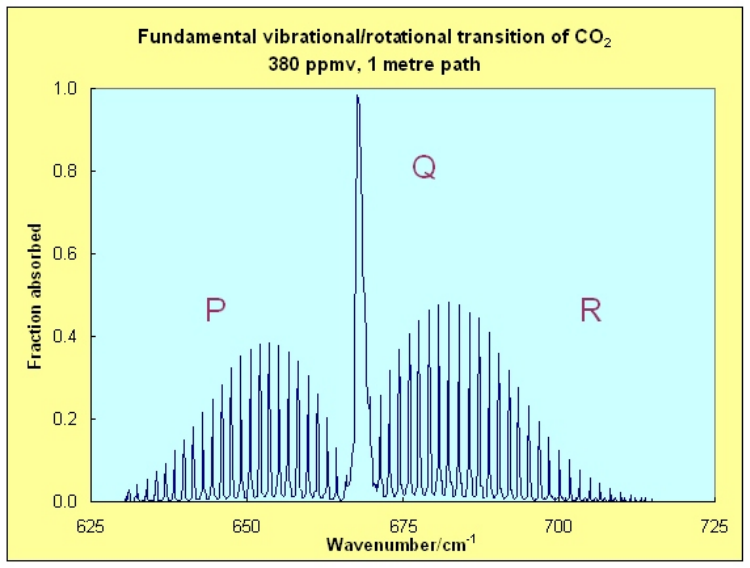
- Other sites are available:

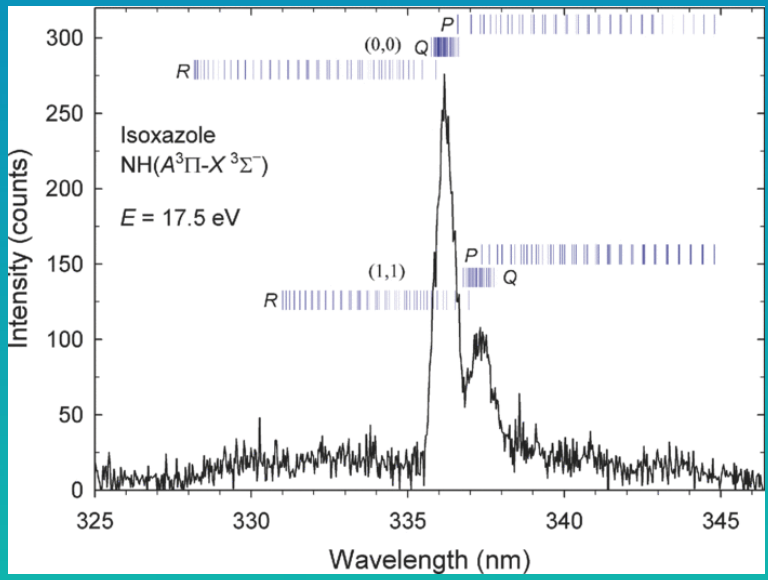
  https://spec.jpl.nasa.gov/ftp/pub/catalog/catform.html

  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. H_2O alone has >500 million lines.





Line identification

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- 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

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- 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

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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 5^{th} and 6^{th} row elements)

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

(links to papers, mainly s-process elements)

Collisional Data

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- 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 H_2 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

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- 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

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- 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

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- 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

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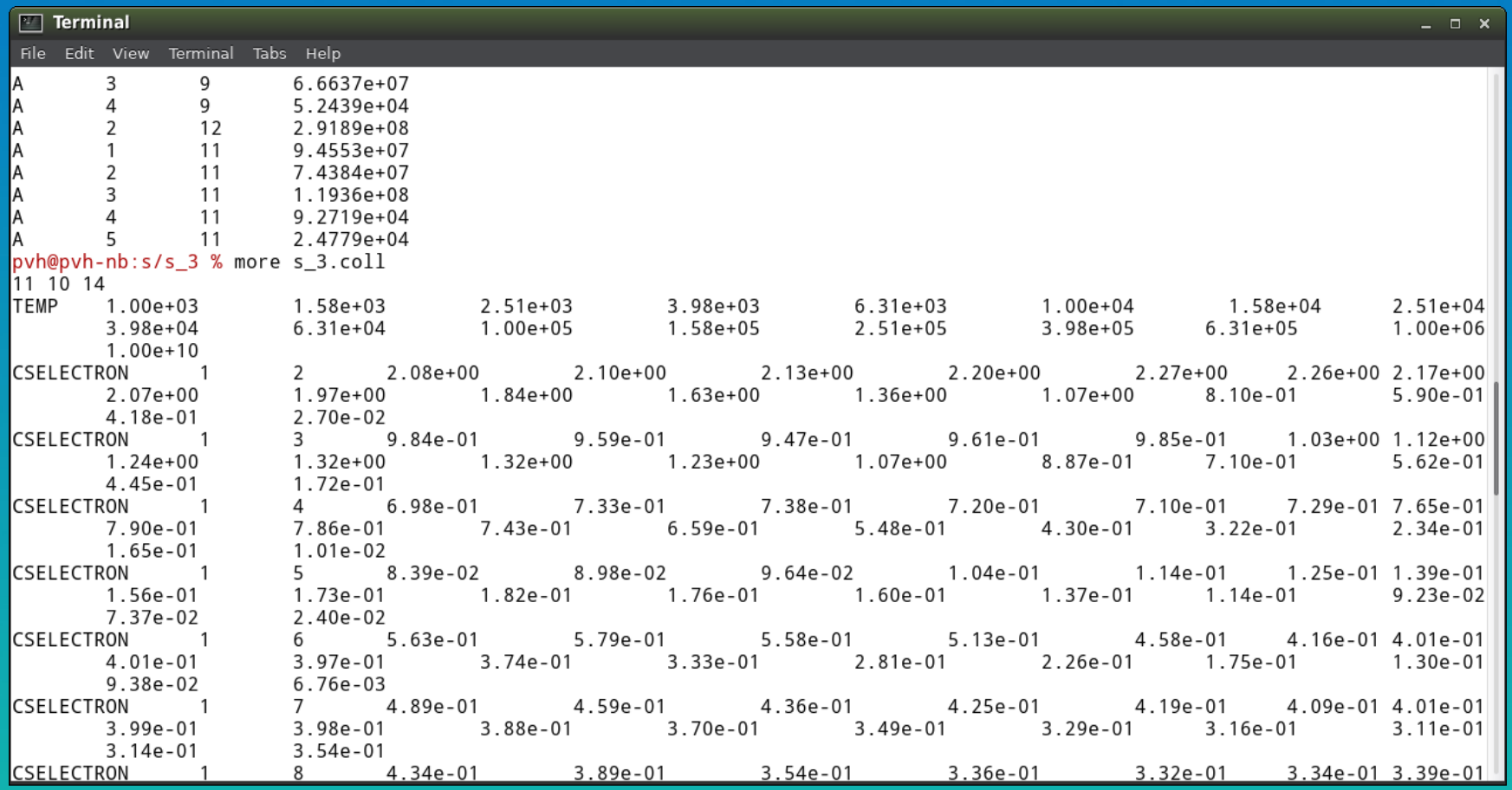
- The third data file defines the collision strengths or rate coefficients (s_3.coll)
- More details here: http://wiki.nublado.org/wiki/StoutData



Other Atomic Data

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- 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

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- 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).

Miscelleneous Data

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- 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

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- 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

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Atomic Data Codes

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- 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

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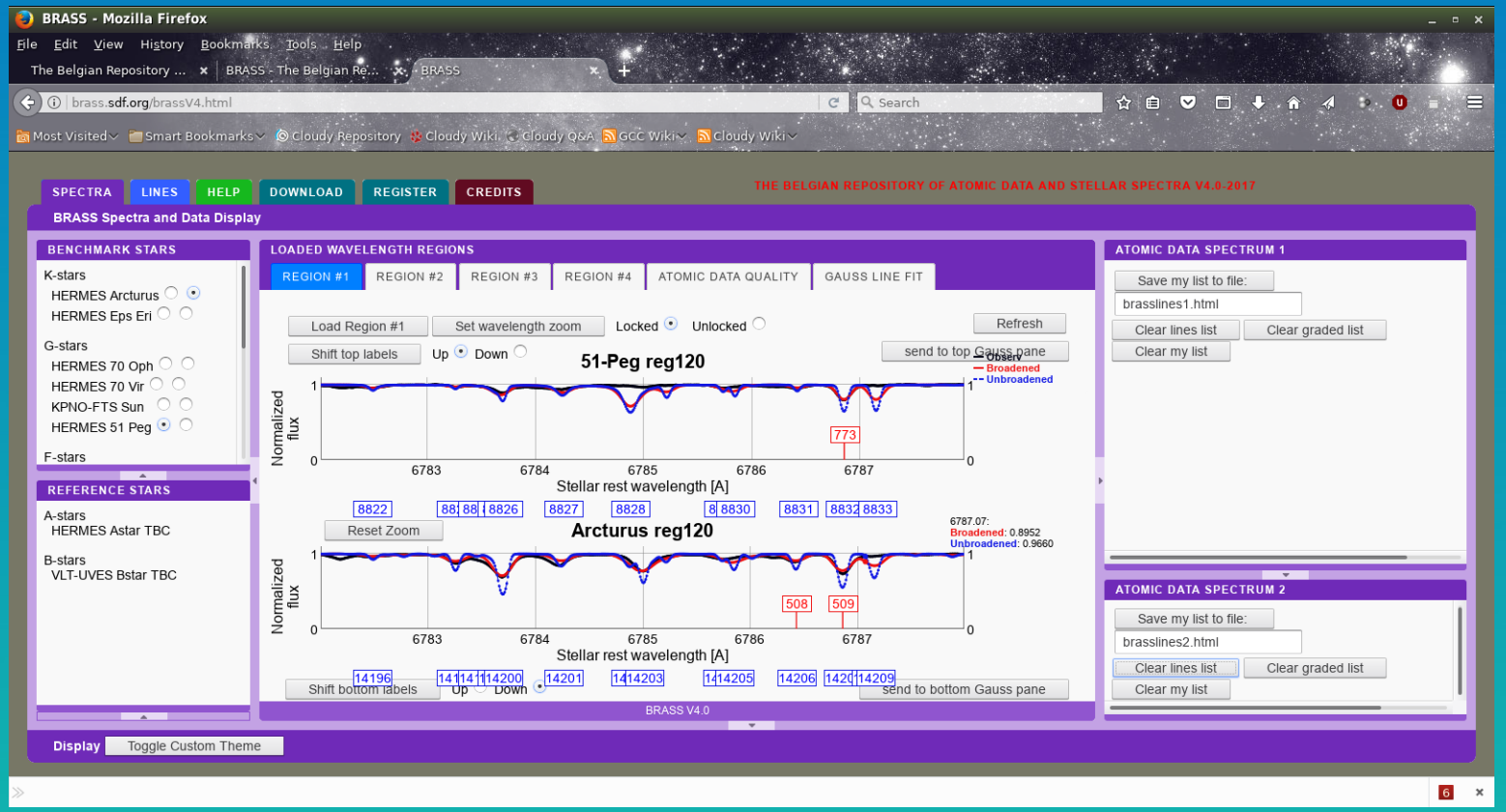
- BRASS = The Belgian Repository of Atomic Data ans Stellar Spectra

  http://brass.sdf.org/
- This site is still under development!



The Future

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- 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.