

HITRAN *online*: An online interface for the HITRAN database

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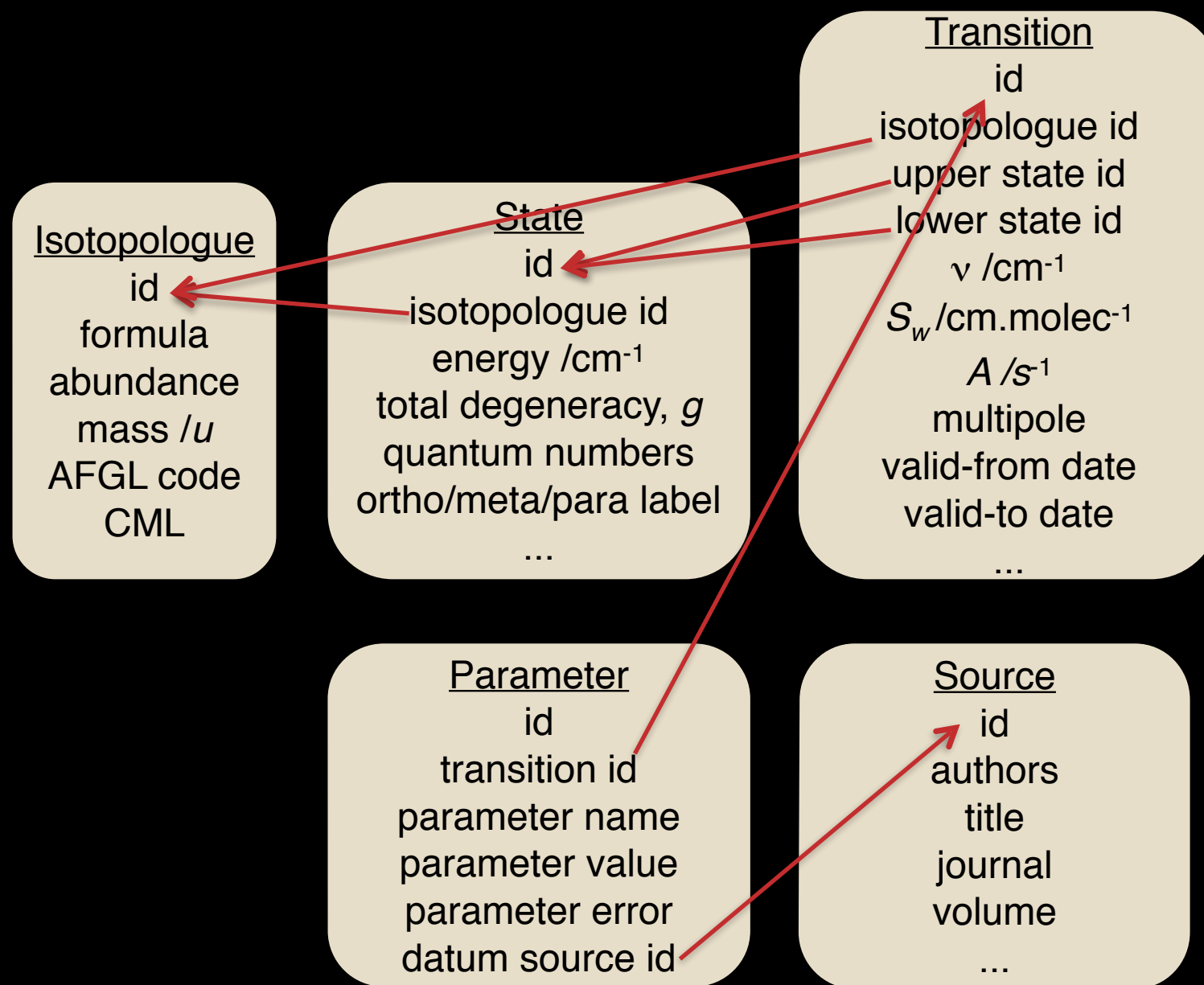
Harvard-Smithsonian Center for Astrophysics

Current (HITRAN 2004+) 160-character .par format

```
...
21 2291.946330 4.940E-29 3.414E-02.06820.086 3595.59060.78-.007000      4 0 0 02      2 1 1 03      Q 32f      4455501221 1 1 1 4      65.0  65.0
21 2291.947360 1.660E-28 3.650E+02.06980.093 5204.94610.780.000400      0 4 4 21      0 4 4 11      R 24f      4455501221 1 1 1 4      51.0  49.0
21 2291.953028 4.614E-27 2.522E+00.06610.073 3633.90910.760.000000      0 4 4 11      0 4 4 01      Q 49f      454550 2 2 1 1 1 0*      99.0  99.0
23 2291.957370 6.450E-27 1.504E+02.08930.123 2501.49690.750.000000      2 0 0 13      2 0 0 03      R 1e      455550 2 2 1 1 1 0      5.0   3.0
21 2291.959750 4.980E-28 4.906E-01.06920.091 3634.14400.78-.007000      2 1 1 12      2 1 1 02      Q 27e      4455501221 1 1 1 4      55.0  55.0
22 2291.967650 4.920E-28 1.880E+02.06030.060 4140.44010.66-.007100      1 1 1 11      1 1 1 01      R 73e      4455501221 1 1 1 4      298.0 294.0
21 2291.974450 3.600E-29 1.790E+02.06660.075 5496.45810.77-.004490      0 7 7 11      0 7 7 01      R 45e      4455501221 1 1 1 4      93.0  91.0
21 2291.977720 5.480E-28 8.715E-04.06820.086 2345.92090.78-.007000      3 0 0 01      1 1 1 02      Q 32f      4455501221 1 1 1 4      65.0  65.0
21 2291.986760 1.620E-27 1.084E+00.07280.100 3473.12120.74-.007000      2 1 1 12      2 1 1 02      Q 18f      4455501221 1 1 1 4      37.0  37.0
27 2291.987280 4.040E-30 1.946E+02.06640.074 3386.79000.77-.004430      0 4 4 11      0 4 4 01      R 46e      4355501221 1 1 1 4      95.0  93.0
...
```

- ASCII text format: 160 bytes per transition
- Fixed-width formats for data fields (Fortran-friendly)
- Total database size (without supplementary data): 440 MB

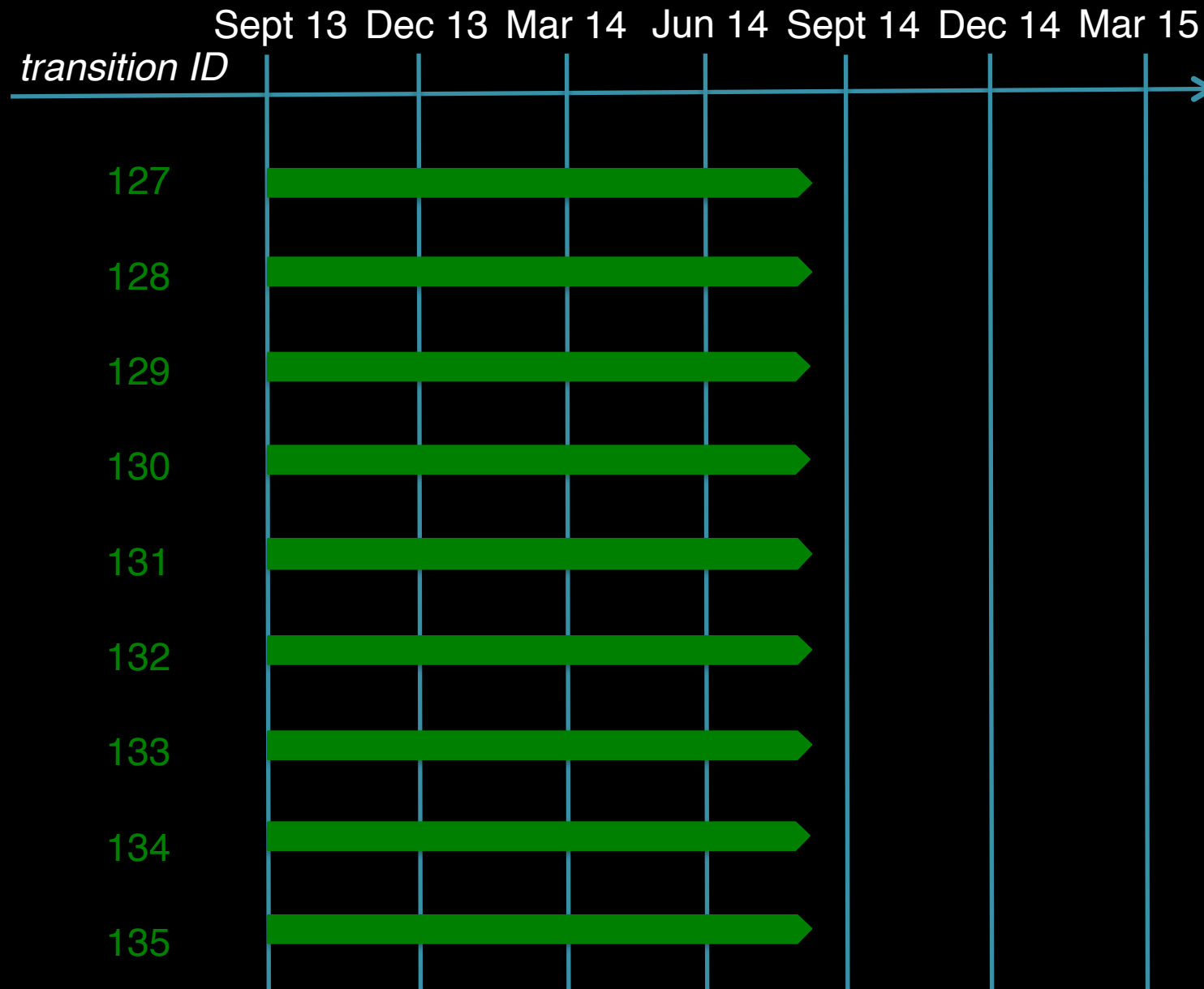
Relational Database: Table structure overview



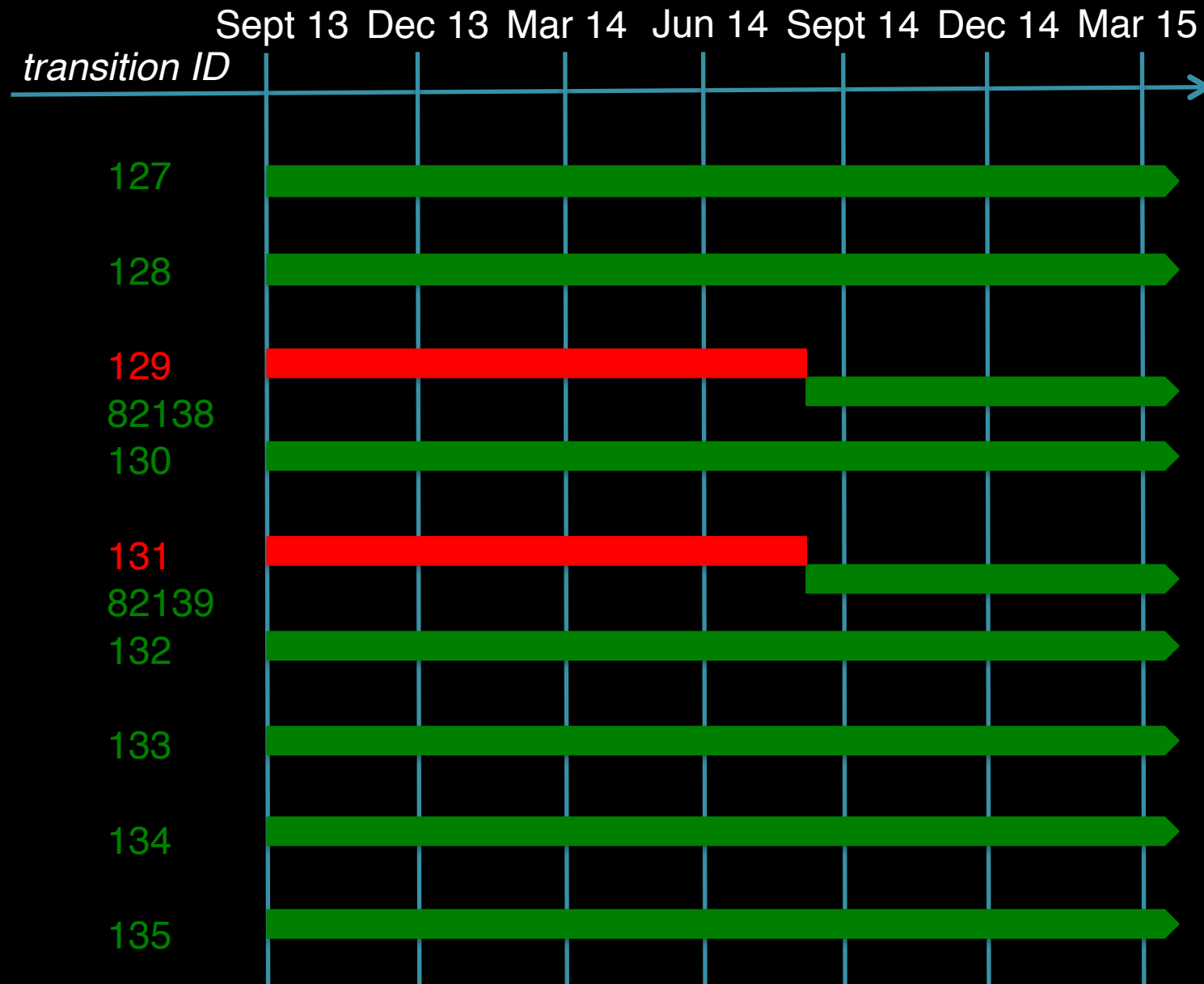
Relational Database: Advantages

- Unlimited transition parameters (e.g. other line shapes such as “HTP”, broadening by species other than air and “self”)
- > 9 isotopologues per molecule (e.g. CO₂)
- Greater precision for transition wave numbers (c.f. F12.6 in .par format)
- More flexibility and less ambiguity in specifying quantum numbers / labels
- Data provenance:
 - Timestamping
 - Direct link between data and original sources

Timestamping



Timestamping



HITRAN *online* interface

- Under development at <http://hitranazure.cloudapp.net/>
- Easy-to-use interface for making queries of the HITRAN database and returning data in a variety of formats:
 - “Native” 160-character .par format
 - Text output with user-specified:
 - fields chosen from available parameters,
 - field separators and formats,
 - line endings (Windows vs. Mac)
 - HDF5 output
 - XSAMS output for VAMDC compatibility

HITRAN *online* interface

- *Optional* User profile (login required) to customise and store units preferences, pre-defined output formats, etc.
- Data visualization: overview spectra, interactive HTML tables (for smaller queries) for examination in browser
- Bibliography (HTML and BibTeX) customized to returned data
- API: see talk by Roman Kochanov

HITRAN *online* interface

<http://hitranazure.cloudapp.net>

- Software Stack:
 - Virtual Machine running Apache 2 on Ubuntu 14.04 LTS Linux as a Microsoft Azure service:
 - Initially: 1 core, 1.75 GB RAM
 - Easily scalable
 - MySQL
 - Python 2.7, NumPy, Matplotlib, Django
 - HTML, CSS, Javascript, JQuery
 - Version control with git




HITRANonline interface

HITRANonline

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Line-by-Line Search

1. Select Molecules

This is the pre-release, beta version of HITRANonline. Use at your own risk!

Select individual molecules below or [Select all](#) [Select first 7](#)

ID	Formula	Name	—	Line count	$\nu_{\min}/\text{cm}^{-1}$	$\nu_{\max}/\text{cm}^{-1}$	$S_{\min}/\text{cm}^{-1}/(\text{molec}\cdot\text{cm}^{-2})$ ⓘ	$S_{\max}/\text{cm}^{-1}/(\text{molec}\cdot\text{cm}^{-2})$ ⓘ	Overview spectrum
<input type="checkbox"/> 1	H ₂ O	Water		224515	0.007	25710.825	1.393×10^{-37}	2.651×10^{-18}	
<input type="checkbox"/> 2	CO ₂	Carbon Dioxide		471847	0.736	12784.056	3.934×10^{-35}	3.543×10^{-18}	
<input type="checkbox"/> 3	O ₃	Ozone		422116	0.026	6996.681	1.498×10^{-31}	4.059×10^{-20}	
<input type="checkbox"/> 4	N ₂ O	Nitrous Oxide		47843	0.838	7796.633	1.229×10^{-28}	1.004×10^{-18}	
<input type="checkbox"/> 5	CO	Carbon Monoxide		4606	3.462	8464.882	1.378×10^{-56}	4.461×10^{-19}	
<input type="checkbox"/> 8	NO	Nitric Oxide		105079	1.000×10^{-6}	9273.214	1.451×10^{-95}	2.322×10^{-20}	
<input type="checkbox"/> 9	SO ₂	Sulfur Dioxide		95121	0.017	4092.948	3.101×10^{-30}	4.851×10^{-20}	
<input type="checkbox"/> 10	NO ₂	Nitrogen Dioxide		104223	0.498	3074.153	4.240×10^{-28}	1.302×10^{-19}	
<input type="checkbox"/> 12	HNO ₃	Nitric Acid		961962	0.007	1769.982	3.246×10^{-29}	3.130×10^{-20}	
<input type="checkbox"/> 13	OH	Hydroxyl Radical		31979	0.003	19267.804	8.504×10^{-84}	1.894×10^{-18}	
<input type="checkbox"/> 14	HF	Hydrogen Fluoride		34376	13.620	47364.678	1.000×10^{-99}	1.460×10^{-17}	




HITRANonline interface

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Line-by-Line Search

4. Select Output Format

Select an output format, then [5. Start Data Search](#)

Available Output Formats

- .par (160 chars)** 
- Xn's test  
- HCl test   
- Xn's test   
- Xn's test (HDF5)   

Output Format Description

.par (160 chars)

The 160-byte fixed-width format used since HITRAN 2004 - see Table 1 in [Rothman et al., JQSRT 96, 139 \(2005\)](#).

Field separator: [no separator], Line endings: Windows (CR LF)
This output format has variable-width fields and no header line.

Parameter	Units	C Fortran Format	Err	Ref
i Molecule ID		I2		
i Isotopologue ID		I1		
i ν	cm^{-1}	F12.6	✓	
i S	$\text{cm}^{-1}/(\text{molec}\cdot\text{cm}^{-2})$	E10.3	✓	
i A	s^{-1}	E10.3		
i γ_{air}	$\text{cm}^{-1}\cdot\text{atm}^{-1}$	F5.4	✓	
i γ_{self}	$\text{cm}^{-1}\cdot\text{atm}^{-1}$	F5.3	✓	

HITRANonline interface



Search Results

699 transitions written in 2.81 secs (query time: 1.48 secs).

Downloads

6 output files were generated using the output format Xn's test.

[54491d7b.sigma.png](#) [27.7 KB] Cross section as a stick-plot

[54491d7b.s.png](#) [20.7 KB] Graphical overview of intensities

[54491d7b.bib.html](#) [1.9 KB] List of sources (html format)

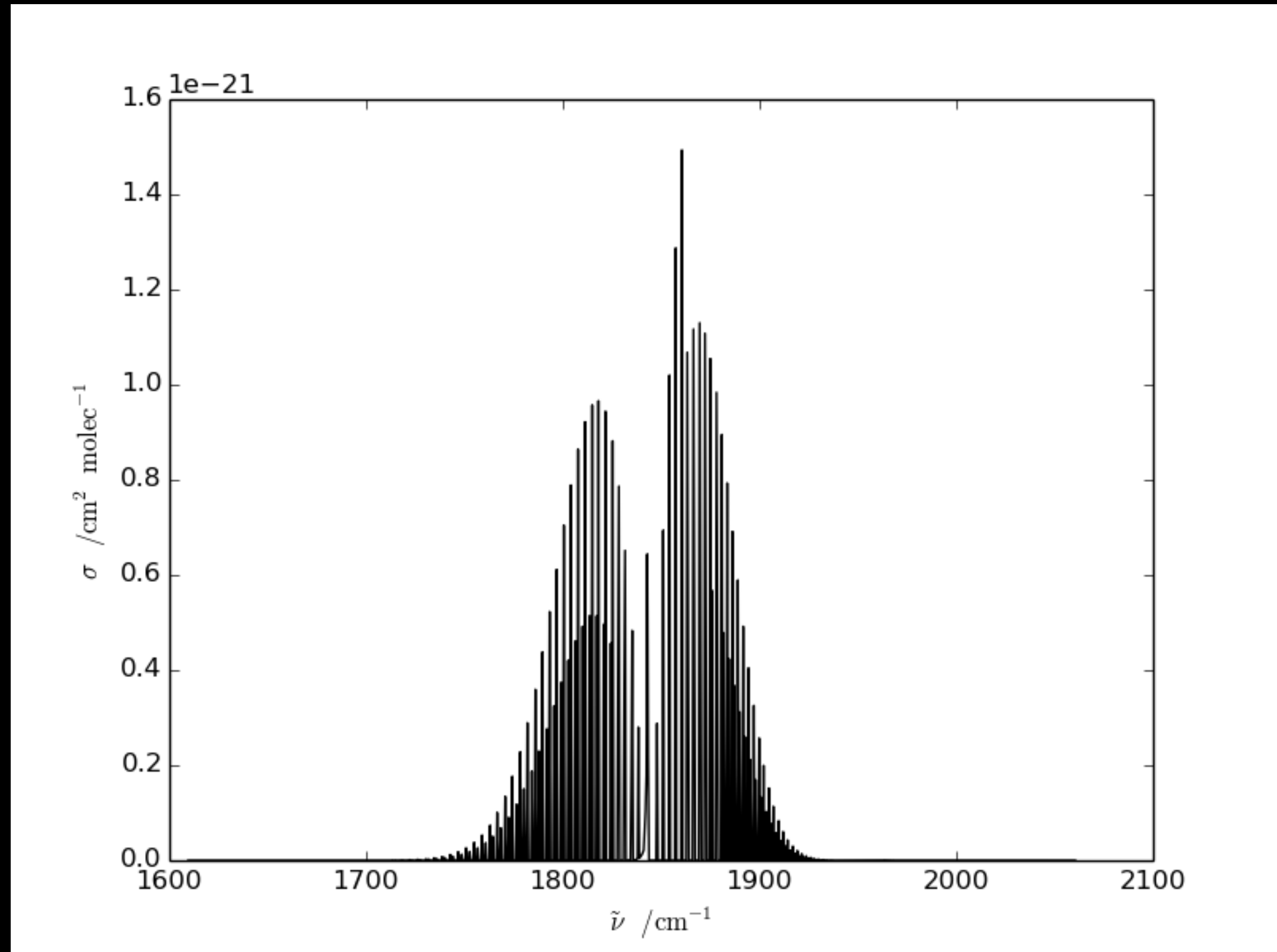
[54491d7b.bib](#) [1.4 KB] List of sources (BibTeX format)

[54491d7b.out](#) [43.1 KB] Output transitions data

[readme-15.txt](#) [1.0 KB] Explanation of output format

Note that the search will only appear as an interactive table on this page if there are 10000 transitions or fewer matching your query. Spectrum images are only produced for queries yielding 1000000 transitions or fewer.

HITRAN *online* interface



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