HITRAN Application Programming Interface (HAPI): Extending HITRAN Capabilities

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(e) Ludwig-Maximilians-Universitat, Munich, and German Aerospace Center (DLR)

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The HITRAN database

- **HITRAN** is an acronym for high-resolution transmission molecular absorption database
- Compilation of spectroscopic parameters (line-by-line data, experimental cross-sections)
- Initially was used to predict and simulate the transmission and emission of light in the atmosphere
- Contains pure rotational as well as ro-vibrational (and even some transitions between different electronic states) transitions
- Applications: atmosphere modeling, troposphere pollutant tracing, planetary science, astrophysics, metrology, ...
- Many applications demand high accuracy for transition parameters
Latest HITRAN2012 edition

Features:
- 47 molecules with about 200 isotopologues in line-by-line section
- 50 molecules represented as experimental cross-sections at various pressures and temperatures (+ auxiliary info)
- Spectral range: from microwave to ultraviolet
- Applications: remote sensing, atmospheric absorption/radiance modeling, planetary science, astrophysics …
- Access using HITRANonline or HAPI: http://hitran.org

| Species (isotopologues) in line-by-line portion of HITRAN |
|---------------------------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|
| H₂O (6)                         | NO (3)       | HCl (4)      | N₂ (2)       | COF₂ (2)     | NO⁺ (1)      | C₄H₂ (1)     |
| CO₂ (10)                        | SO₂ (2)      | HBr (4)      | HCN (3)      | SF₆ (1)      | HOBr (2)     | HC₃N (1)     |
| O₃ (5)                          | NO₂ (1)      | HI (2)       | CH₃Cl (2)    | H₂S (3)      | C₂H₄ (2)     | H₂ (2)       |
| N₂O (5)                         | NH₃ (2)      | ClO (2)      | H₂O₂ (1)     | HCOOH (1)    | CH₃OH (1)    | CS (4)       |
| CO (6)                          | HNO₃ (2)     | OCS (5)      | C₂H₂ (3)     | HO₂ (1)      | CH₃Br (2)    | SO₃ (1)      |
| CH₄ (4)                         | OH (3)       | H₂CO (3)     | C₂H₆ (2)     | O (1)        | CH₃CN (1)    |
| O₂ (3)                          | HF (2)       | HOCl (2)     | PH₃ (1)      | ClONO₂ (2)   | CF₄ (1)      |
Astrophysics, planetary science => need for foreign broadeners & non-Voigt line-shapes

- Parameters for foreign broadenings are gathered and added in HITRAN
- HTP profile parameters for H$_2$ lines are obtained and added in HITRAN
Astrophysics, planetary science =>
need for foreign broadeners & non-Voigt line-shapes

✓ Parameters for foreign broadenings are gathered and added in HITRAN
✓ HTP profile parameters for H₂ lines are obtained and added in HITRAN

Large spectroscopic data volumes =>
efficient and flexible tools for data processing

✓ HITRANonline website was released
✓ HITRAN Application Programming Interface (HAPI)
Online interface for the HITRAN database

http://hitran.org => dedicated hardware server

- Line-by-line transition data on 47 molecules
- Absorption cross sections
- Collision-induced absorption
- Aerosols
- HITEMP
- HITRAN Application Programming Interface (HAPI)
- Customizable output format (+ “non-conventional” parameters)
- Auxiliary information (isotopes, band statistics etc...)
- Paper in JQSRT HighRus Special Issue (Hill et al., 10.1016/j.jqsrt.2015.12.012)
New HITRAN data on foreign broadening agents: H₂, He, and CO₂

Broadening, shifting, and temperature dependence parameters were gathered for 7 molecules of planetary science interest (~180,000 lines total)

Prepared datasets for half widths

<table>
<thead>
<tr>
<th></th>
<th>C₂H₂</th>
<th>SO₂</th>
<th>OCS</th>
<th>HCl</th>
<th>HF</th>
<th>CO</th>
<th>NH₃</th>
</tr>
</thead>
<tbody>
<tr>
<td>Perturbed by H₂</td>
<td>Y</td>
<td>Y</td>
<td>N</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>Perturbed by He</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>Perturbed by CO₂</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
</tbody>
</table>

Y = available; N = unavailable

H₂ in HITRAN
Model system for HTP tests

→ Strong Dicke narrowing
→ Strong speed dependence
→ Lines are well isolated

**H$_2$ in HITRAN**

Model system for HTP tests

- Strong Dicke narrowing
- Strong speed dependence
- Lines are well isolated

Yan Tan et al.
P1735: Cavity ring-down spectroscopy of hydrogen in the 784-852 nm region and corresponding line shape implementation into HITRAN.

FA. Fundamental physics
Friday, 2016-06-24, 08:30 AM

doi:10.1016/j.jqsrt.2016.01.024.
**What is HITRAN API (HAPI)?**

- Python module (library of functions) to work with HITRAN data
- Main purpose: extending user's code by the data of HITRAN and functionality of HITRANonline
The macro-scale architecture of HAPI

- CUSTOM CODE
- EXTENSIONS
- USER’S LINELISTS
- Communication protocol
- Storage engine layer
- Logical data representation layer
- Spectroscopic code layer
- Interactive documentation layer
HITRAN Application Programming Interface (http://hitran.org/hapi)
- Python library for spectroscopic codes

What HAPI does?

- Retrieves and filters spectroscopic data, e.g. from HITRANonline (line-by-line data, cross sections, information on isotopic species etc...)

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(Python library code + Manual)

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Internal data representation:

Logical layer

Table: H2O
Table: O2
Table: CO

{ **parameter**: value, **parameter**: value, ... }
{ **nu**: 13010.452, **sw**: 1.982e-28, ... },
{ **nu**: 13010.600, **sw**: 1.029e-28, ... },
{ **nu**: 13010.812, **sw**: 2.263e-25, **beta_G_air**: 0.0183, ... },
{ **nu**: 13012.582, **sw**: 2.174e-25, **beta_G_air**: 0.0173, ... },
{ **nu**: 13013.024, **sw**: 2.970e-30, ... },
...

Database engine interface

Physical layer

Format conversion

Column fixed
160-char
Comma-separated
Binary
...
User DB
HITRAN Application Programming Interface ([http://hitran.org/hapi](http://hitran.org/hapi))

- Python library for spectroscopic codes

Data retrieval sample:

`fetch_by_ids('CO', [26,27,28], 3900, 4360, ParameterGroups=('160-char','SDVoigt'))`

BEGIN DOWNLOAD: CO
  65536 bytes written to ./CO.data
  65536 bytes written to ./CO.data
Header written to ./CO.header
END DOWNLOAD

Lines parsed: 644

PROCESSED
<table>
<thead>
<tr>
<th>Group ID</th>
<th>Parameters contained</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>par_line / 160-char / .par</td>
<td>par_line</td>
<td>Parameters from 160-character HITRAN line</td>
</tr>
<tr>
<td>ID</td>
<td>trans_id</td>
<td>Transition identifier</td>
</tr>
<tr>
<td>Standard</td>
<td>molec_id, local_iso_id, nu, sw, a, elower, gamma_air, delta_air, gamma_self, n_air, n_self, gp, gpp</td>
<td>Most commonly used HITRAN “standard” parameters (this intersects with par_line)</td>
</tr>
<tr>
<td>Labels</td>
<td>statep, statepp</td>
<td>Quantum state labels.</td>
</tr>
<tr>
<td>LineMixing</td>
<td>y_air, y_self</td>
<td>Parameters for line mixing</td>
</tr>
<tr>
<td>Voigt_Air</td>
<td>gamma_air, delta_air, deltap_air, n_air</td>
<td>Voigt profile coefficients for the air-broadening</td>
</tr>
<tr>
<td>Voigt_Self</td>
<td>gamma_self, delta_self, deltap_self, n_self</td>
<td>Voigt profile coefficients for the self-broadening</td>
</tr>
<tr>
<td>Voigt_H2</td>
<td>gamma_h2, delta_H2, deltap_h2, n_h2</td>
<td>Voigt profile coefficients for the H₂-broadening</td>
</tr>
<tr>
<td>Voigt_CO2</td>
<td>gamma_co2, delta_co2, n_co2</td>
<td>Voigt profile coefficients for the CO₂-broadening</td>
</tr>
<tr>
<td>Voigt_He</td>
<td>gamma_he, delta_he, n_he</td>
<td>Voigt profile coefficients for the He-broadening</td>
</tr>
<tr>
<td>Voigt</td>
<td>All Voigt parameters</td>
<td>This group contains all Voigt-related parameters</td>
</tr>
<tr>
<td>Group ID</td>
<td>Parameters contained</td>
<td>Description</td>
</tr>
<tr>
<td>-----------------</td>
<td>-----------------------------------------------------------</td>
<td>----------------------------------------------------------------------------</td>
</tr>
<tr>
<td>SDVoigt_Air</td>
<td>gamma_air, delta_air, deltap_air, n_air, sd_air</td>
<td>Speed-dependent Voigt profile coefficients for the air-broadening</td>
</tr>
<tr>
<td>SDVoigt_Self</td>
<td>gamma_self, delta_self, deltap_self, n_self, sd_self</td>
<td>Speed-dependent Voigt profile coefficients for the self-broadening</td>
</tr>
<tr>
<td>SDVoigt</td>
<td>All SDVoigt parameters</td>
<td>This group contains all Speed-dependent Voigt-related parameters</td>
</tr>
<tr>
<td>Galatry_Air</td>
<td>gamma_air, delta_air, deltap_air, n_air, beta_g_air</td>
<td>Galatry profile coefficients for the air-broadening</td>
</tr>
<tr>
<td>Galatry_Self</td>
<td>gamma_self, delta_self, deltap_self, n_self, beta_g_self</td>
<td>Galatry profile coefficients for the self-broadening</td>
</tr>
<tr>
<td>Galatry</td>
<td>All Galatry parameters</td>
<td>This group contains all Galatry-related parameters</td>
</tr>
<tr>
<td>All</td>
<td>All parameters at once</td>
<td></td>
</tr>
</tbody>
</table>
HITRAN Application Programming Interface (http://hitran.org/hapi)
- Python library for spectroscopic codes

Data filtering:
- Similar to SQL (for single table queries)
- Parameters stored in tables
- Display and sort data (“select”, “sort”)

```python
1. select('CO', DestinationTableName='COFiltered', ParameterNames=(nu, sw), Conditions=('>', 'sw', 1.0e-25), File='co_linelist.out')
2.
```

- Filtering conditions include wide range of expressions on parameters, including regexps
- Adding/removing columns
- Group by parameter/expression value
HITRAN Application Programming Interface (http://hitran.org/hapi)

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What HAPI does?

- Retrieves and filters spectroscopic data, e.g. from HITRANonline (line-by-line data, cross sections, information on isotopic species etc...)

- Calculates absorption cross-sections in a flexible way accounting many parameters (air-, self-, and foreign broadenings and shifts, environment and instrument properties, custom line-shapes and partition sums ...)

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(Python library code + Manual)

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Absorption cross section calculation sample:

```python
from pylab import plot,show
nu,coef = absorptionCoefficient_Voigt(SourceTables='CO')
plot(nu,coef); show()
```
Cross-section simulation algorithm overview

PROFILE TYPE

LOCAL DATASET: HITRAN / CUSTOM

TEMPERATURE AND PRESSURE DEPENDENCES

INSTRUMENTAL FUNCTION

MIXTURE DEFINITION

ENVIRONMENT PARAMETERS: Pressure (p), temperature (T), path length (l)

CONTROL PARAMETERS: Wavenumber range, step size, line wing, intensity cutoff, output format

\[ \nu_0, S, \Gamma_D, \Gamma_0, \Gamma_2, \Delta_0, \Delta_2, \nu_{VC}, \eta, \ldots \]

\[ p, T \]

LINE PROFILE

Absorption coefficient

Transmittance spectrum

Absorption spectrum

Radiance spectrum

instrumental function

SIMULATED SPECTRUM
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- Provides basic routines for creating spectroscopic codes involving absorption cross-sections (atmosphere absorption modeling, direct and inverse spectroscopic problems etc...)

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Example: modeling of $\text{C}_2\text{H}_2 \nu_5$-band absorption in a He+H$_2$ atmosphere

```python
alphas = [0.1, 0.3, 0.5, 0.7, 0.9]
leg = []
for alpha in alphas:
    He_frac = alpha; H2_frac = 1-alpha
    nu, coef = absorptionCoefficient_Voigt(SourceTables='c2h2_v5', WavenumberRange=[727, 735],
                                             Diluent={'He':He_frac, 'H2':H2_frac}, HITRAN_units=False)
    plot(nu, coef)
    #leg.append('%1f%%' % alpha)
    leg.append('${\text{He}}$: %1f%; ${\text{H}_2}$: %1f%%' % (He_frac*100, H2_frac*100))
title('Absorption simulation of $\nu_5$-band of $\text{C}_2\text{H}_2$: variable atmospheric composition')
xlabel('Wavenumber / $\text{cm}^{-1}$'); ylabel('Absorption coefficient / $\text{cm}^{-1}$')
xlim(728, 734); grid(True); legend(leg)
```
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- Provides codes for profiles and partition sums rewritten in Python and tested

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Line profiles

- 7 line profiles (including **pCqSDHC**: *Partially Correlated Quadratic Speed dependent Hard Collision Profile*, Ngo et al. *JQSRT* 129 (2013) 89–100)

<table>
<thead>
<tr>
<th>Profile</th>
<th>Function name</th>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hartmann-Tran</td>
<td>PROFILE_HT</td>
<td>$\Gamma_D, \Gamma_0, \Gamma_2, \Delta_0, \Delta_2, \nu_{VC}, \eta$</td>
</tr>
<tr>
<td>Speed-dependent</td>
<td>PROFILE_SDRAUTIAN</td>
<td>$\Gamma_D, \Gamma_0, \Gamma_2, \Delta_0, \Delta_2, \nu_{VC}$</td>
</tr>
<tr>
<td>Rautian</td>
<td>PROFILE_RAUTIAN</td>
<td>$\Gamma_D, \Gamma_0, \Delta_0, \nu_{VC}$</td>
</tr>
<tr>
<td>Speed-dependent</td>
<td>PROFILE_SDVOIGT</td>
<td>$\Gamma_D, \Gamma_0, \Gamma_2, \Delta_0, \Delta_2$</td>
</tr>
<tr>
<td>Voigt</td>
<td>PROFILE_VOIGT</td>
<td>$\Gamma_D, \Gamma_0, \Delta_0$</td>
</tr>
<tr>
<td>Lorentz</td>
<td>PROFILE_LORENTZ</td>
<td>$\Gamma_0, \Delta_0$</td>
</tr>
<tr>
<td>Doppler</td>
<td>PROFILE_DOPPLER</td>
<td>$\Gamma_D$</td>
</tr>
</tbody>
</table>
Partition sums

  - Included information about 51 molecules
  - 70-3000K temperature range
  - Very extensive update is underway

<table>
<thead>
<tr>
<th>Chemical formula</th>
<th>HITRAN molecule ID</th>
<th>HITRAN isotopologue ID</th>
<th>HITRANNonline global ID</th>
</tr>
</thead>
<tbody>
<tr>
<td>H$^{15}$N$^{16}$O$_3$</td>
<td>12</td>
<td>2</td>
<td>117</td>
</tr>
<tr>
<td>*D$^{19}$F</td>
<td>14</td>
<td>2</td>
<td>110</td>
</tr>
<tr>
<td>*D$^{35}$Cl</td>
<td>15</td>
<td>3</td>
<td>107</td>
</tr>
<tr>
<td>*D$^{37}$Cl</td>
<td>15</td>
<td>4</td>
<td>108</td>
</tr>
<tr>
<td>*D$^{79}$Br</td>
<td>16</td>
<td>3</td>
<td>111</td>
</tr>
<tr>
<td>*D$^{81}$Br</td>
<td>16</td>
<td>4</td>
<td>112</td>
</tr>
<tr>
<td>*D$^{127}$I</td>
<td>17</td>
<td>2</td>
<td>113</td>
</tr>
<tr>
<td>$^{14}$N$^{15}$N</td>
<td>22</td>
<td>2</td>
<td>118</td>
</tr>
<tr>
<td>$^{13}$C$^{16}$O$^{19}$F$_2$</td>
<td>29</td>
<td>2</td>
<td>119</td>
</tr>
<tr>
<td>♦$^{16}$O</td>
<td>34</td>
<td>1</td>
<td>86</td>
</tr>
<tr>
<td>♦$^{12}$CH$_3$$^{16}$OH</td>
<td>39</td>
<td>1</td>
<td>92</td>
</tr>
<tr>
<td>$^{32}$S$^{16}$O$_3$</td>
<td>47</td>
<td>1</td>
<td>114</td>
</tr>
</tbody>
</table>

List of the HITRAN isotopologues for which the partition sums are absent in TIPS-2011.

♦ Partition sums are given in HITRAN2008 (file “parsum.dat”).

* Partition sums for deuterated halogens are given in Ref. [Li G, Gordon IE et al Reference spectroscopic data for hydrogen halides, Part II: The line lists. JQSRT, 130, 284-295, 2013].
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- Provides codes for profiles and partition sums rewritten in Python and tested
- Provides an interactive help

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Embedded help system:

```python
In [8]: getHelp(select)
Help on function select in module hitranonline:

select(TableName, DestinationTableName='__BUFFER__', ParameterNames=None, Conditions=None,
INPUT PARAMETERS:
    TableName:        name of source table     (required)
    DestinationTableName: name of resulting table  (optional)
    ParameterNames:  list of parameters or expressions  (optional)
    Conditions:      list of logical expressions (optional)
    Output:         enable (True) or suppress (False) text output (optional)
    File:           enable (True) or suppress (False) file output (optional)
OUTPUT PARAMETERS:
    none
---
DESCRIPTION:
Select or filter the data in some table
either to standard output or to file (if specified)
---
EXAMPLE OF USAGE:
    select('samplertab',DestinationTableName='outtab',ParameterNames=(p1,p2),
    Conditions=((('and',('>','p1',1)),('<',('*','p1','p2'),20))))
    Conditions means (p1>=1 and p1*p2<20)
---
```
Performance optimization and benchmarks

The most computationally extensive part – absorption spectra calculation!

CPF (complex probability function)

- HUMLICEK (modified):
  Ngo NH, Lisak D, Tran H, Hartmann J-M.
  An isolated line-shape model to go beyond the Voigt profile in spectroscopic databases and radiative transfer codes.

- SCHREIER (2011)
  Schreier F.
  Optimized implementations of rational approximations for the Voigt and complex error function.

VARIABLES[‘CPF’] = hcpf
VARIABLES[‘CPF’] = hum1_wei
Performance optimization and benchmarks

<table>
<thead>
<tr>
<th></th>
<th>Methane_I</th>
<th>Methane_II</th>
<th>Methane_III</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Dataset properties</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Number of lines</td>
<td>3804</td>
<td>59805</td>
<td>468013</td>
</tr>
<tr>
<td>Wavenumber range, cm⁻¹</td>
<td>1000-1100</td>
<td>1000-1500</td>
<td>0.001-11505</td>
</tr>
<tr>
<td><strong>Data filtering time, s</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Filtering using condition (24)</td>
<td>0.275</td>
<td>4.176</td>
<td>34.535</td>
</tr>
<tr>
<td><strong>Absorption coefficient calculation time, s</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SCPF, 50 HWHMs</td>
<td>1.756</td>
<td>27.331</td>
<td>317.371</td>
</tr>
<tr>
<td>SCPF, 200 HWHMs</td>
<td>2.897</td>
<td>44.101</td>
<td>437.317</td>
</tr>
<tr>
<td>SCPF, 500 HWHMs</td>
<td>4.948</td>
<td>79.493</td>
<td>710.458</td>
</tr>
<tr>
<td>HCPF, 50 HWHMs</td>
<td>6.895</td>
<td>109.530</td>
<td>869.950</td>
</tr>
<tr>
<td>HCPF, 200 HWHMs</td>
<td>9.855</td>
<td>154.834</td>
<td>1202.387</td>
</tr>
<tr>
<td>HCPF, 500 HWHMs</td>
<td>15.447</td>
<td>249.162</td>
<td>1930.663</td>
</tr>
<tr>
<td><strong>Instrumental function convolution time, s</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Step = 0.01 cm⁻¹</td>
<td>0.007</td>
<td>0.032</td>
<td>0.740</td>
</tr>
<tr>
<td>Step = 0.001 cm⁻¹</td>
<td>0.953</td>
<td>3.820</td>
<td>94.058</td>
</tr>
<tr>
<td>Step = 0.0001 cm⁻¹</td>
<td>102.58</td>
<td>661.858</td>
<td>12456.012</td>
</tr>
</tbody>
</table>
Plans

- More sophisticated line mixing schemes
- Including new profiles and parameters
- Working with “raw” cross-sections
- Graphical user interface (GUI), IPython notebook integration
- Integration of HAPI into the Python Package Index
- Github repository

Questions / bug reports:

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HITRAN Application Programming Interface (HAPI)

Recent Uploads

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Kochanov Roman; Iouli Gordon; Laurence Rothman; Christian Hill; et al.
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HITRAN Application Programming Interface (HAPI) - V.1.0.0
Kochanov Roman; Iouli Gordon; Laurence Rothman; Christian Hill; et al.
HAPI is a tool providing a possibility to work with spectroscopic data in HITRAN format. It gives fast and easy access to HITRANonline data. In addition, HAPI provides flexible functions to calculate absorption cross-sections from line-by-line spectral data.

HAPI means HITRAN Application Programming Interface.
Current beta version of HAPI is a library written in Python and requires NumPy to be installed.

https://zenodo.org/collection/user-hapi
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Active HAPI users (out of ~300):
Dr Anand K. Ramanathan (NASA, USA), Dr. Teofil Minea (FOM DIFFER, Netherlands), Dr. Mike Georgiadis (Thermo Fisher Scientific, USA)

Colleagues from:
- Laboratory of Quantum Mechanics of Molecules and Radiative Processes, Tomsk State University (esp. Yuri Babikov)
- Laboratory of Theoretical Spectroscopy, Institute of Atmospheric Optics (esp. Semen Mikhailenko)
- Groupe de Spectrométrie Moléculaire et Atmosphérique, Université de Reims Champagne-Ardenne.

... for advises, comments and discussions

NASA: PATM, PDART, AURA

TSU: International Competitiveness Improvement Program
The HITRAN team: