HITRAN and HITEMP: Towards Molecular Spectroscopic Databases for any Possible Scenario

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The HITRAN2016 molecular spectroscopic database

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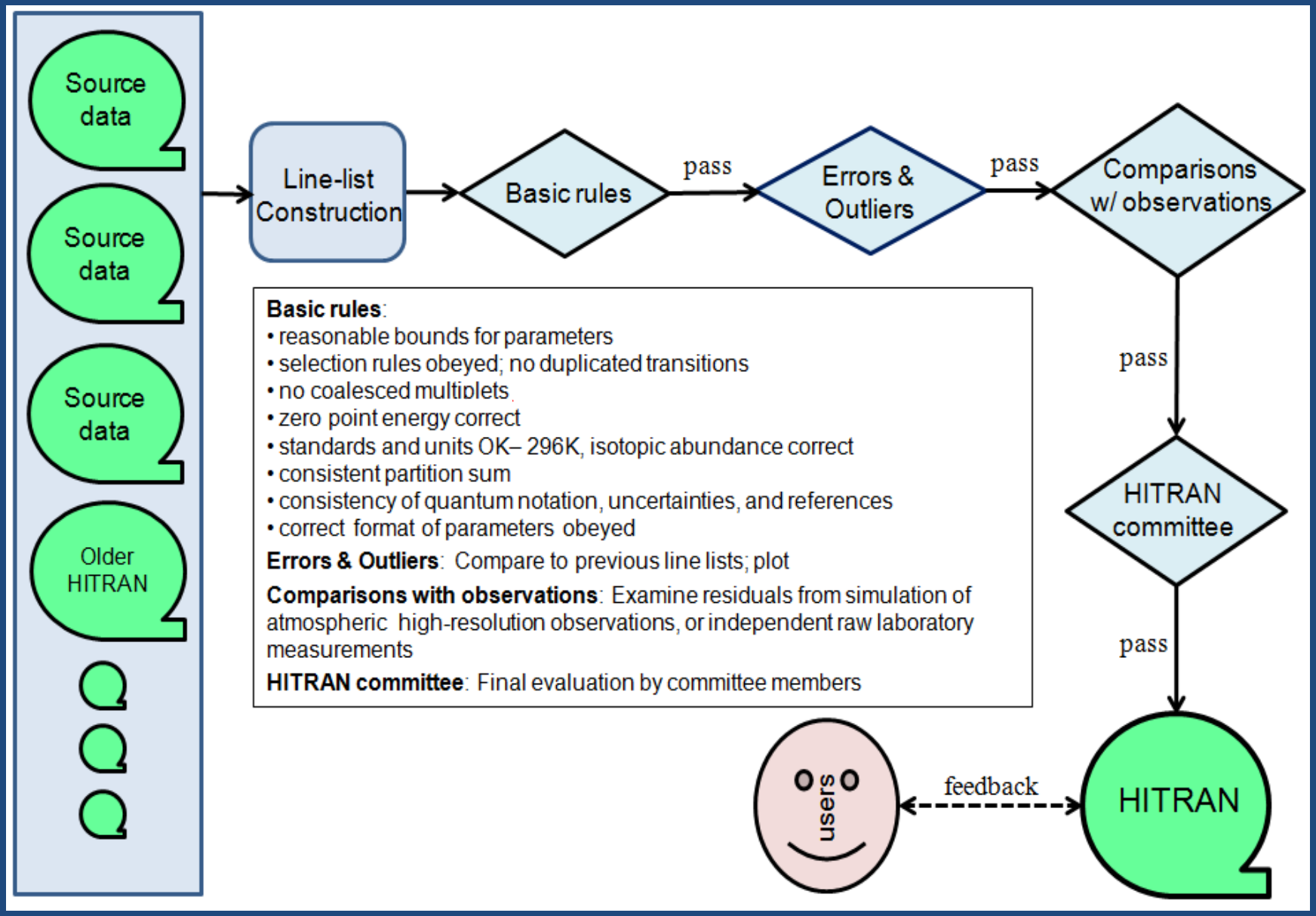
Scheme for Construction

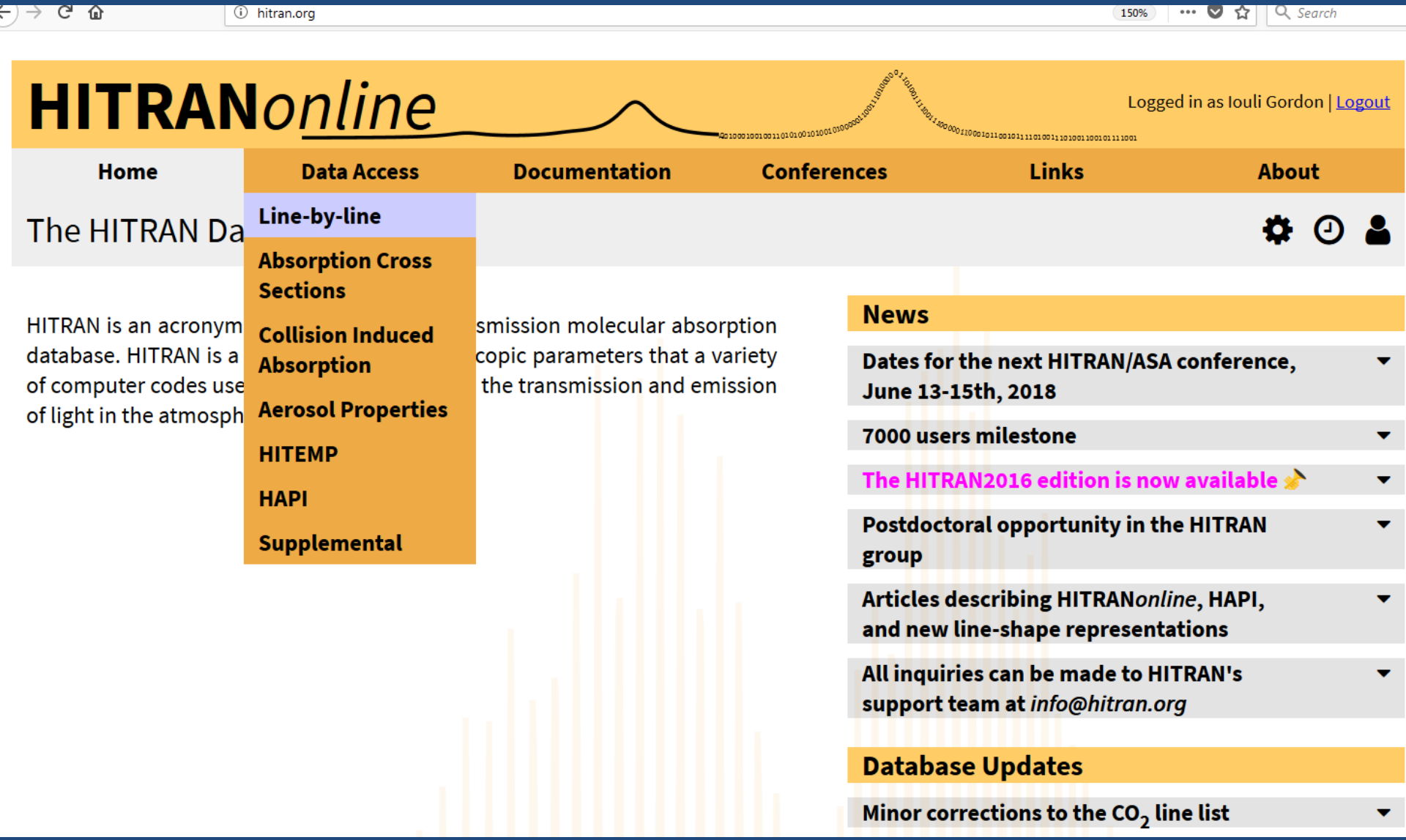


HITRAN2016 line-by-line section:

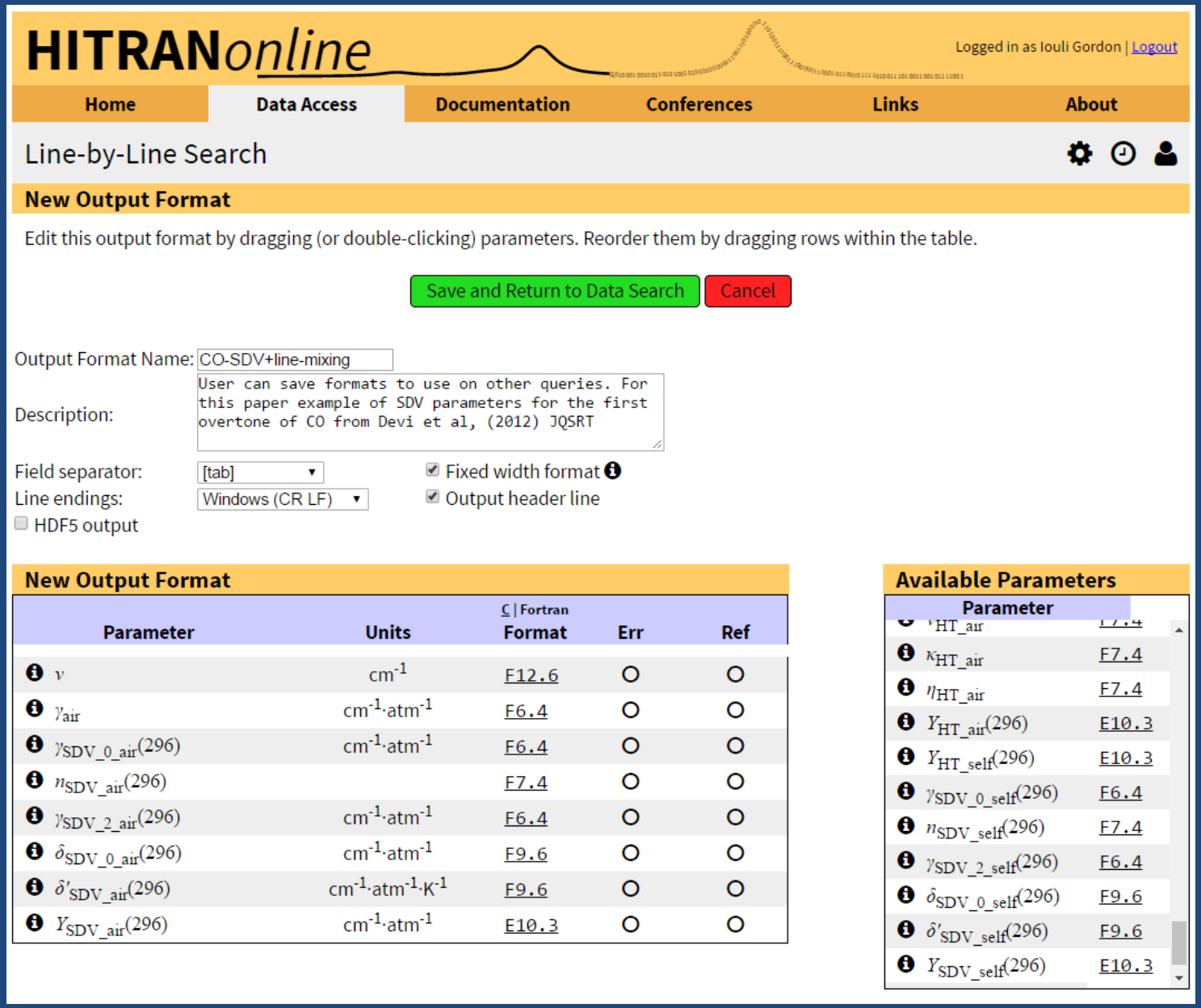
HITRAN2016 molecules (49)

Species (isotopologues) in line-by-line portion of HITRAN						
H_2O (7)	NO (3)	HCl (4)	N_2 (2)	COF2 (2)	NO^+ (1)	C_4H_2 (1)
CO_2 (12)	SO_2 (2)	HBr (4)	HCN (3)	SF_6 (1)	HOBr (2)	HC_3N (1)
O_3 (5)	NO_2 (1)	HI (2)	CH_3Cl (2)	H_2S (3)	C_2H_4 (2)	H_2 (2)
N_2O (5)	NH_3 (2)	ClO (2)	H_2O_2 (1)	HCOOH (1)	CH_3OH (1)	CS (4)
CO (6)	HNO_3 (2)	OCS (5)	C_2H_2 (3)	HO_2 (1)	CH_3Br (2)	SO_3 (1)
CH_4 (4)	OH (3)	H_2CO (3)	C_2H_6 (2)	O (1)	CH_3CN (1)	**C_2N_2 (1)**
O_2 (3)	HF (2)	HOCl (2)	PH_3 (1)	$ClONO_2$ (2)	CF_4 (1)	**$COCl_2$(2)**

New structure and interface at www.hitran.org



Example of creating custom output format



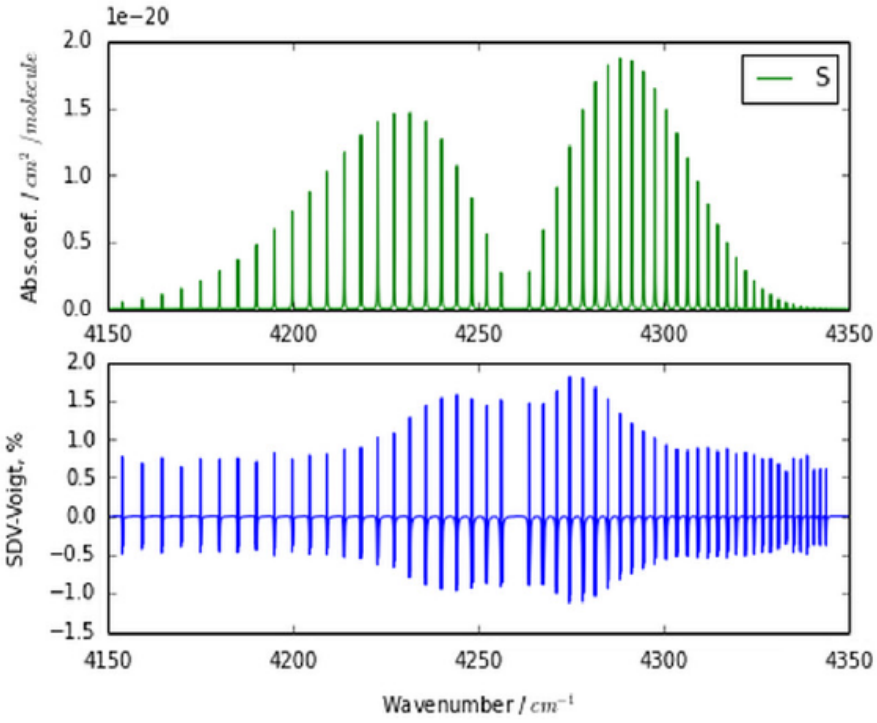
Retrieved parameters with custom output format

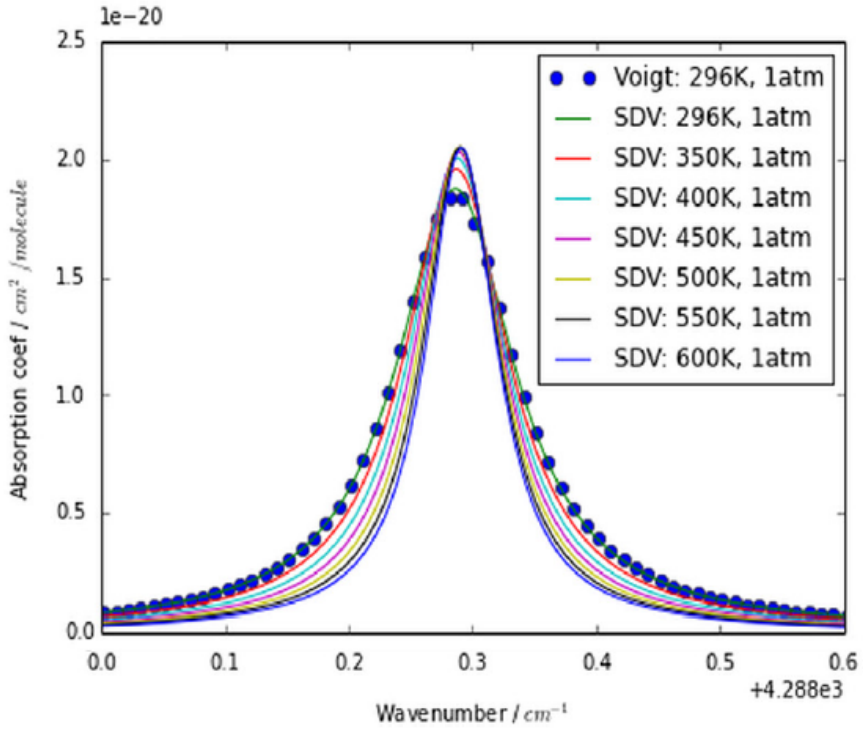
nu	gamma_air	gamma_SDV_0_air_296			n_SDV_air_296	gamma_SDV_2_air_296	delta_SDV_0_air_296	deltap_SDV_air_296	Y_SDV_air_296
4202.550466	0.0542	######	#######	######	#########	#########	##########		
4203.357916	0.0805	######	#######	######	#########	#########	##########		
4204.669501	0.0559	0.0551	0.7610	0.0036	-0.004730	0.000025	1.400e-03		
4205.187898	0.0535	######	#######	######	#########	#########	##########		
4207.752983	0.0526	######	#######	######	#########	#########	##########		
4209.343184	0.0566	0.0558	0.7702	0.0037	-0.004700	0.000025	1.400e-03		
4210.245573	0.0518	######	#######	######	#########	#########	##########		
4210.907967	0.0804	######	#######	######	#########	#########	##########		
4212.665523	0.0510	######	#######	######	#########	#########	##########		
4213.948622	0.0573	0.0564	0.7796	0.0040	-0.004620	0.000025	1.600e-03		
4214.577840	0.0753	######	#######	######	#########	#########	##########		
4215.012686	0.0502	######	#######	######	#########	#########	##########		
4217.286914	0.0495	######	#######	######	#########	#########	##########		
4218.177415	0.0713	######	#######	######	#########	#########	##########		
4218.485666	0.0579	0.0570	0.7833	0.0040	-0.004690	0.000025	1.400e-03		
4219.488062	0.0488	######	#######	######	#########	#########	##########		
4221.615983	0.0475	######	#######	######	#########	#########	##########		
4221.706546	0.0679	######	#######	######	#########	#########	##########		
4222.954171	0.0587	0.0578	0.7858	0.0045	-0.004590	0.000025	1.100e-03		
4223.670530	0.0466	######	#######	######	#########	#########	##########		
4225.165085	0.0648	######	#######	######	#########	#########	##########		
4225.651557	0.0469	######	#######	######	#########	#########	##########		
4227.353988	0.0596	0.0587	0.7847	0.0049	-0.004550	0.000024	8.000e-04		
4227.558918	0.0464	######	#######	######	#########	#########	##########		
4228.552886	0.0624	######	#######	######	#########	#########	##########		
4229.392465	0.0457	######	#######	######	#########	#########	##########		
4231.152052	0.0451	######	#######	######	#########	#########	##########		
4231.684972	0.0608	0.0598	0.7783	0.0055	-0.004410	0.000024	2.000e-04		
4231.869803	0.0607	######	#######	######	#########	#########	##########		
4235.115687	0.0595	######	#######	######	#########	#########	##########		
4235.946976	0.0625	0.0615	0.7664	0.0060	-0.004180	0.000024	-2.000e-04		
4238.290394	0.0585	######	#######	######	#########	#########	##########		
4240.139851	0.0649	0.0637	0.7618	0.0065	-0.004030	0.000023	-1.100e-03		
4241.393775	0.0578	######	#######	######	#########	#########	##########		
4244.263453	0.0679	0.0665	0.7591	0.0071	-0.003610	0.000021	-2.300e-03		
4244.425684	0.0571	######	#######	######	#########	#########	##########		
4247.385975	0.0564	######	#######	######	#########	#########	##########		
4248.317632	0.0713	0.0698	0.7689	0.0077	-0.003080	0.000017	-4.000e-03		

Cross-sections generated using HAPI

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

```
# Calculate absorptoin coefficient with Speed-dependent Voigt profile
nu,coef1 = absorptionCoefficient_SDVoigt(SourceTables='CO',OmegaStep=0.001,Environment={'p':1.,'T':296.})
# Calculate absorptoin coefficient with plain Voigt profile
nu,coef2 = absorptionCoefficient_Voigt(SourceTables='CO',OmegaStep=0.001,Environment={'p':1.,'T':296.})
```

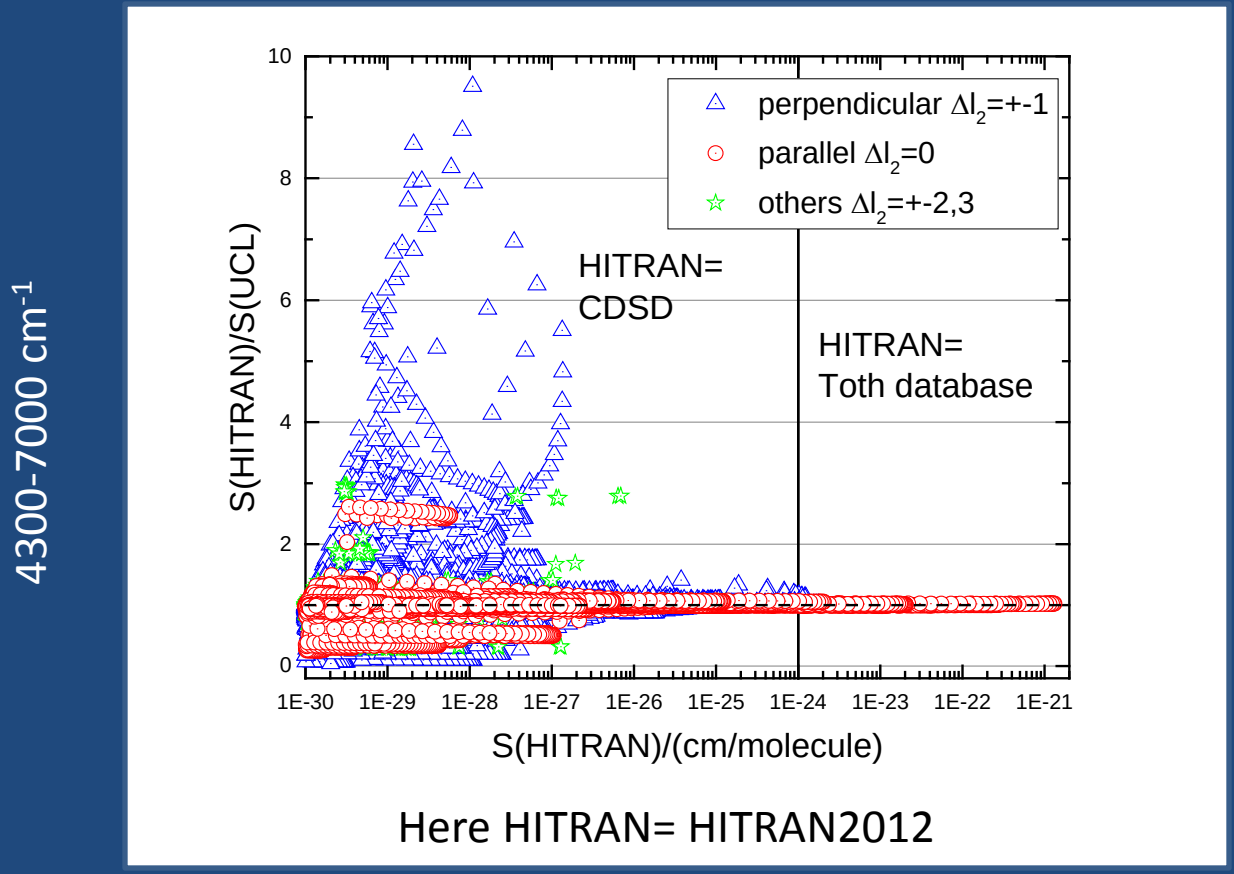




Kochanov et al, *J. Quant. Spectrosc. Radiat. Transfer* **177**, 15-30 (2016)

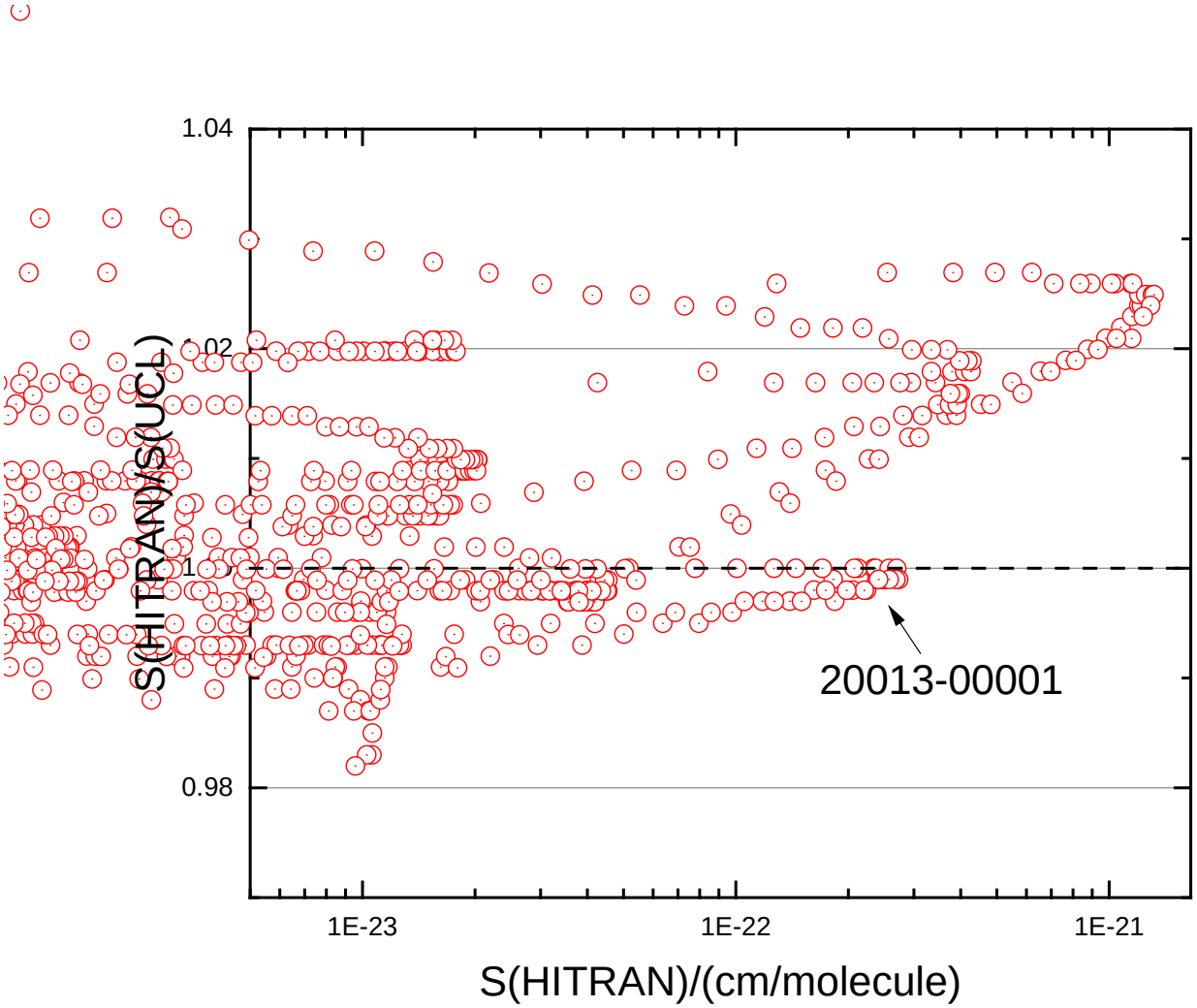
CO_2 update

General approach: UCL ab initio line intensities from Zak et al JQSRT(2016,2017) (except for resonance lines and unstable bands) with line positions derived from empirically determined energy levels (CDSD from IAO, Tomsk).



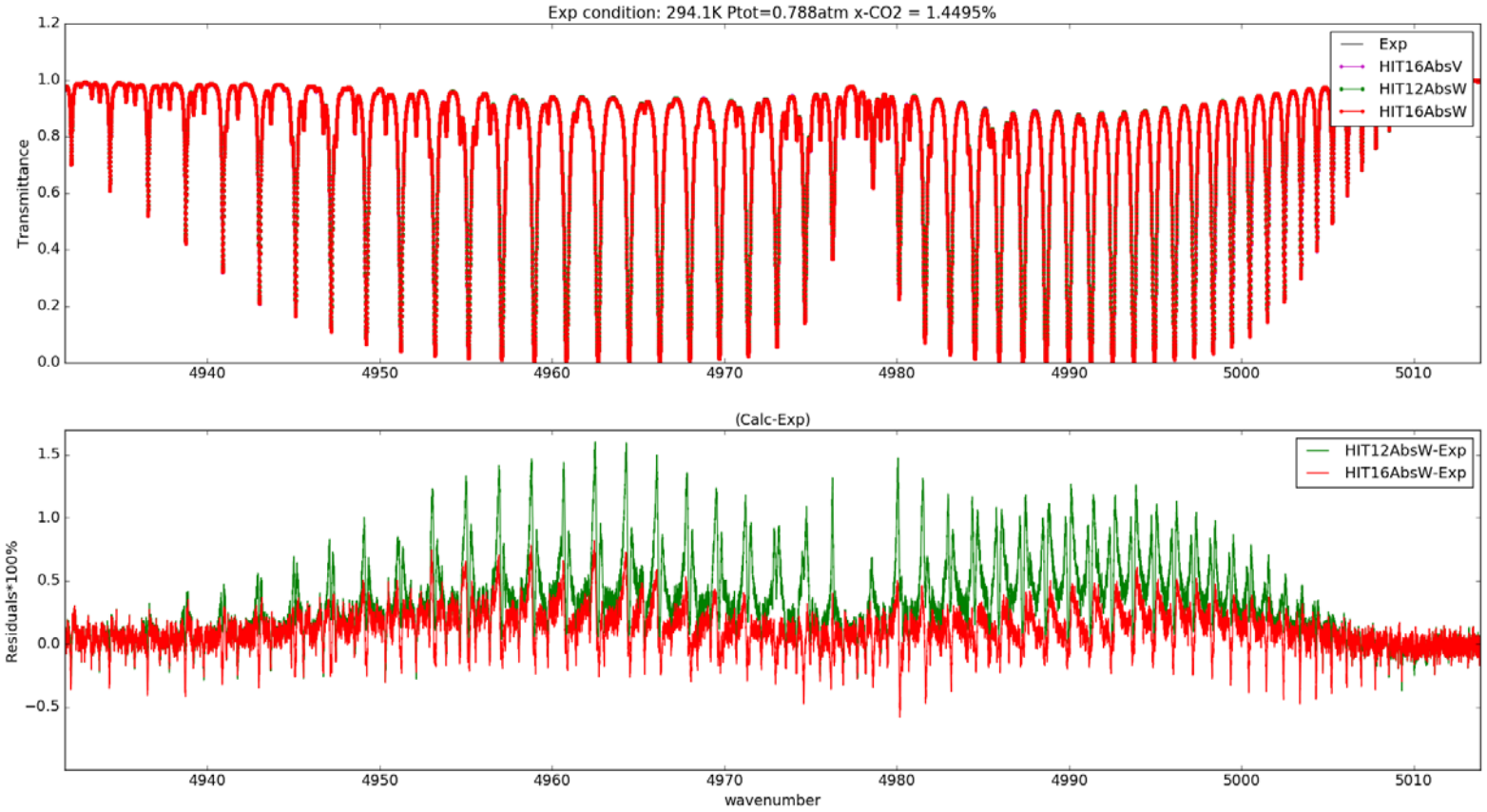
Here HITRAN= HITRAN2012

Zoom in to strong lines



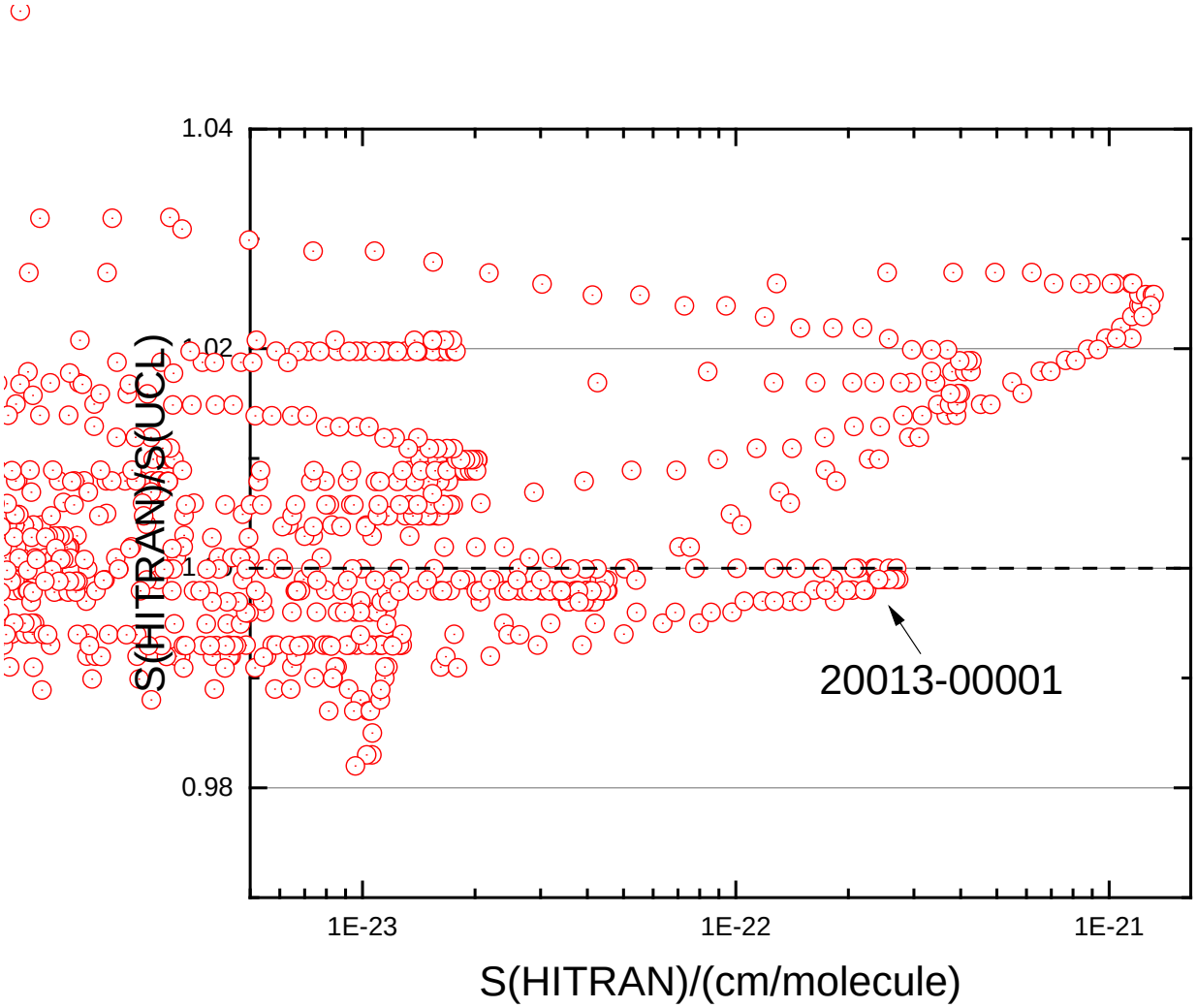
Laboratory validation of the 2-μm region

Laboratory spectra from Keeyoon Sung (JPL)

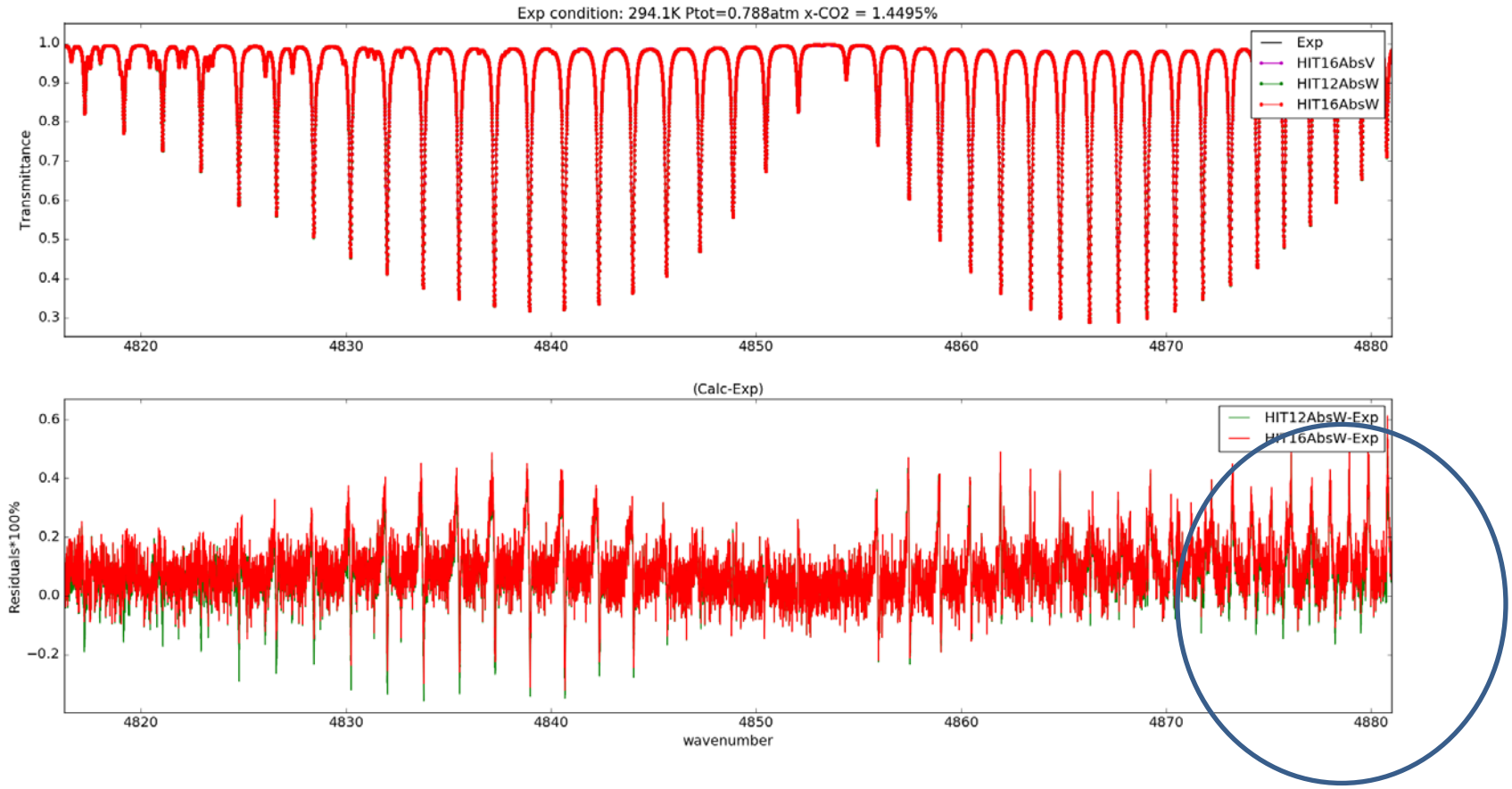


Note that linelist is supplemented with line shape parameters
from Gamache and Lamoroux (2013) and line mixing routine of Lamaroux et al (2015),
updated to be compatible with HITRAN2016

Zoom in to strong lines



Laboratory validation of the 2-µm region



Isotopologues

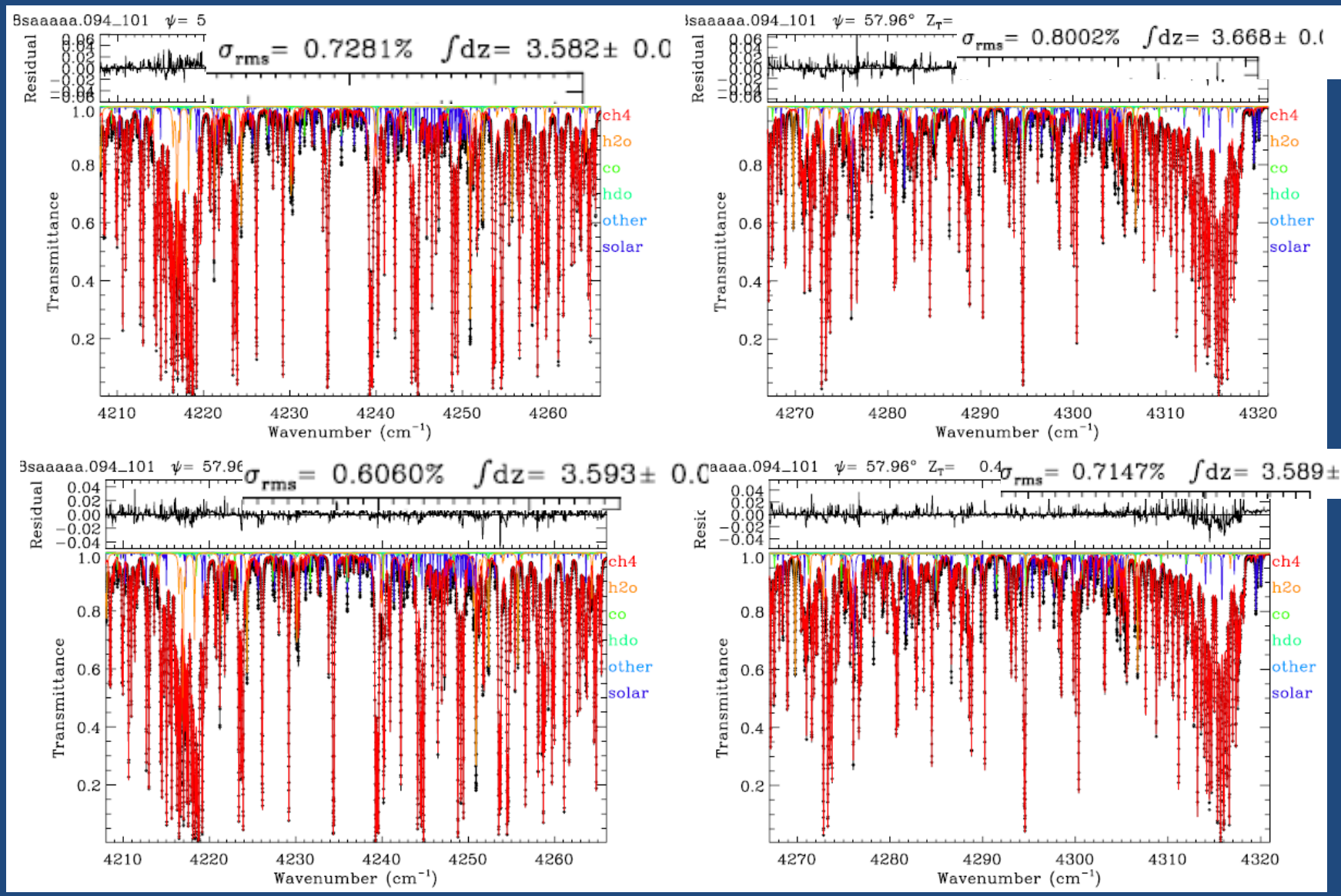
CH_4 update

Table 2.6.1. Scheme of HITRAN2016 update of $^{12}CH_4$ and $^{13}CH_4$. All regions not given in the table remain identical to the HITRAN2012 edition

Range (cm^{-1}):	Positions	Intensities	Line shapes
0-1370	HIT12, with many hot bands removed. P1–P0 (ν_4 band only), P1–P1, P2–P2, P3–P3, P2-P1 from MeCaSDa [13], $^{13}CH_4$ ν_2 band restored from HIT08	P1–P0 (ν_4 band only), P1–P1, P2–P2, P3–P3 from MeCaSDa [13], P2-P1 from HIT08	HIT12 when available or algorithm from Ref. [1]
1370-4000	HIT12 with many line positions fixed using HIT08, Tyuterev et al. [14] and empirical adjustments of HIT12 to properly fit KP spectra. Several missing lines restored from HIT08.	HIT12	HIT12
4000-4315	HIT08 with many lines improved using some of the preliminary results from DLR [15], and occasionally HIT12	HIT08 with many lines improved using some of the preliminary results from DLR	HIT08 and in some cases HIT12
4499-4630	HIT12 mixed with Devi et al [16]		HIT12 mixed with Devi et al [16]
4670-5300	Nikitin et al. [17] with 10^{-27} $cm^{-1}/(molecule \cdot cm^{-2})$ cutoff was applied in 4800-5000 cm^{-1} region		Nikitin et al. [17]
5300-5550	Nikitin et al. [18]		Nikitin et al. [18]
5550-5855	GOSAT list [19] for $^{12}CH_4$. Other isotopologues HIT12		GOSAT list [19] or algorithm from Ref. [1]
5855-6250	GOSAT list [19] with some lines from Nikitin et al [20], Devi et al and HIT12 based on validation for $^{12}CH_4$. For $^{13}CH_4$ Starikova et al. [21].		GOSAT list [19] or algorithm from Ref. [1]
7920-8250	CRDS measurements Béguier et al [22]		Algorithm from Ref. [1]
9028-10435	FTS measurements Béguier et al [23]		Algorithm from Ref. [1]

Note: HIT16 = new HITRAN edition, HIT08 = HITRAN2008 edition [24], HIT12 = HITRAN2012 edition [12], KP = Kitt Peak FTS lab spectra.

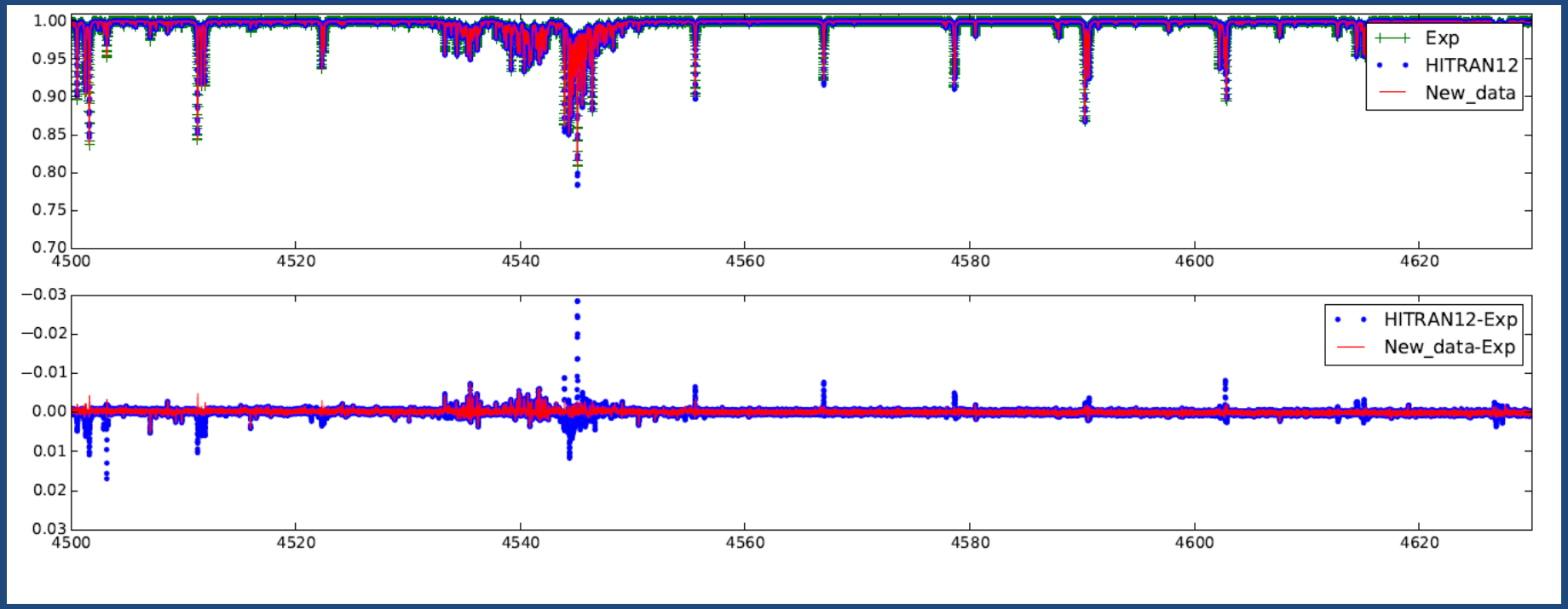
TCCON validation of the Octad band (prepared by Geoff Toon)



Top Panel: HITRAN2012; Bottom Panel: HITRAN2016

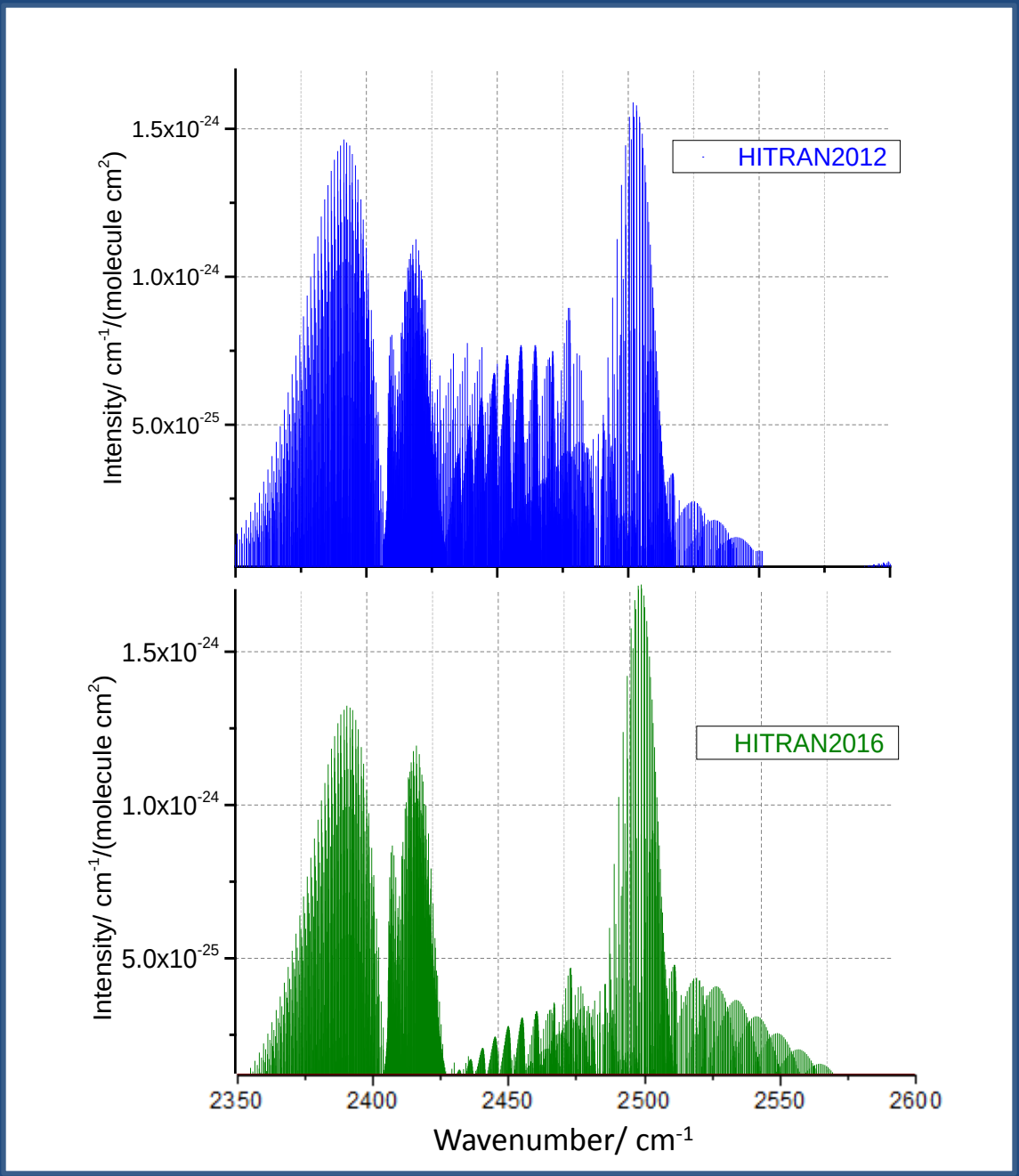
Laboratory validation of the Octad band

Laboratory spectra from Malathy Devi (College of William and Mary)



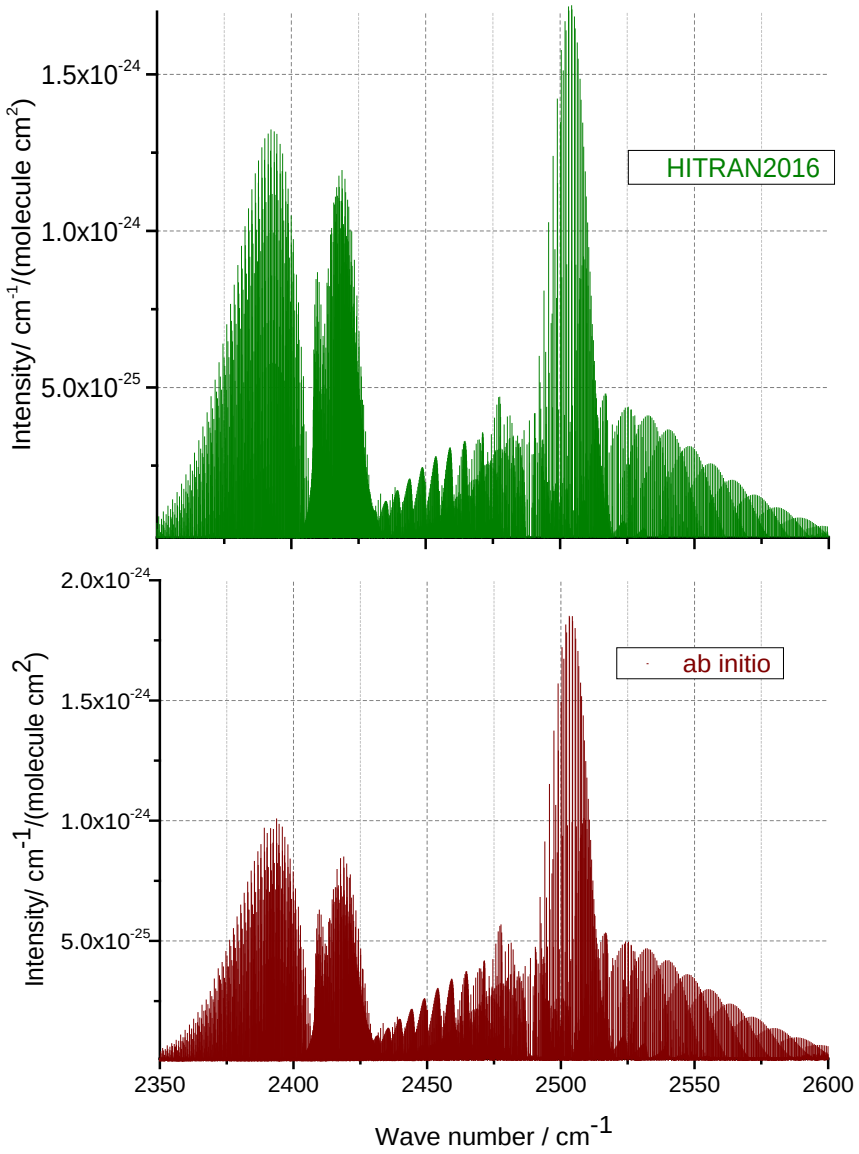
HITRAN2016 (in this region)= Strong lines from Devi et al, JQSRT (2015)+
weak lines from HITRAN2012)

Substantially improved ozone spectroscopy in the 5-µm region



Update made thanks to SMPO http://smpo.iao.ru/ Collaboration between Tomsk and Reims

Substantially improved ozone spectroscopy in the 5-µm region



From Vladimir Tyuterev (Reims)

Jupiter: H_2, He, CH_4, **C_2H_2**, C_2H_6, C_2H_4, H_2O, C_4H_2, C_6H_6, HD, C_3H_4, NH_3, PH_3, **CO**, GeH_4, AsH_3, CO_2, ...

Saturn: H_2, He, CH_4, **C_2H_2**, C_2H_6, C_3H_4, CH_3, H_2S, H_2O, C_3H_8, NH_3, SiH4, PH_3 , **CO**, GeH_4, AsH_3, $CO_{2,\ ...}$

Uranus: H_2, He, CH_4, C_3H_4, C_4H_2, C_2H_6, **C_2H_2**, **CO**, H_2S, ...

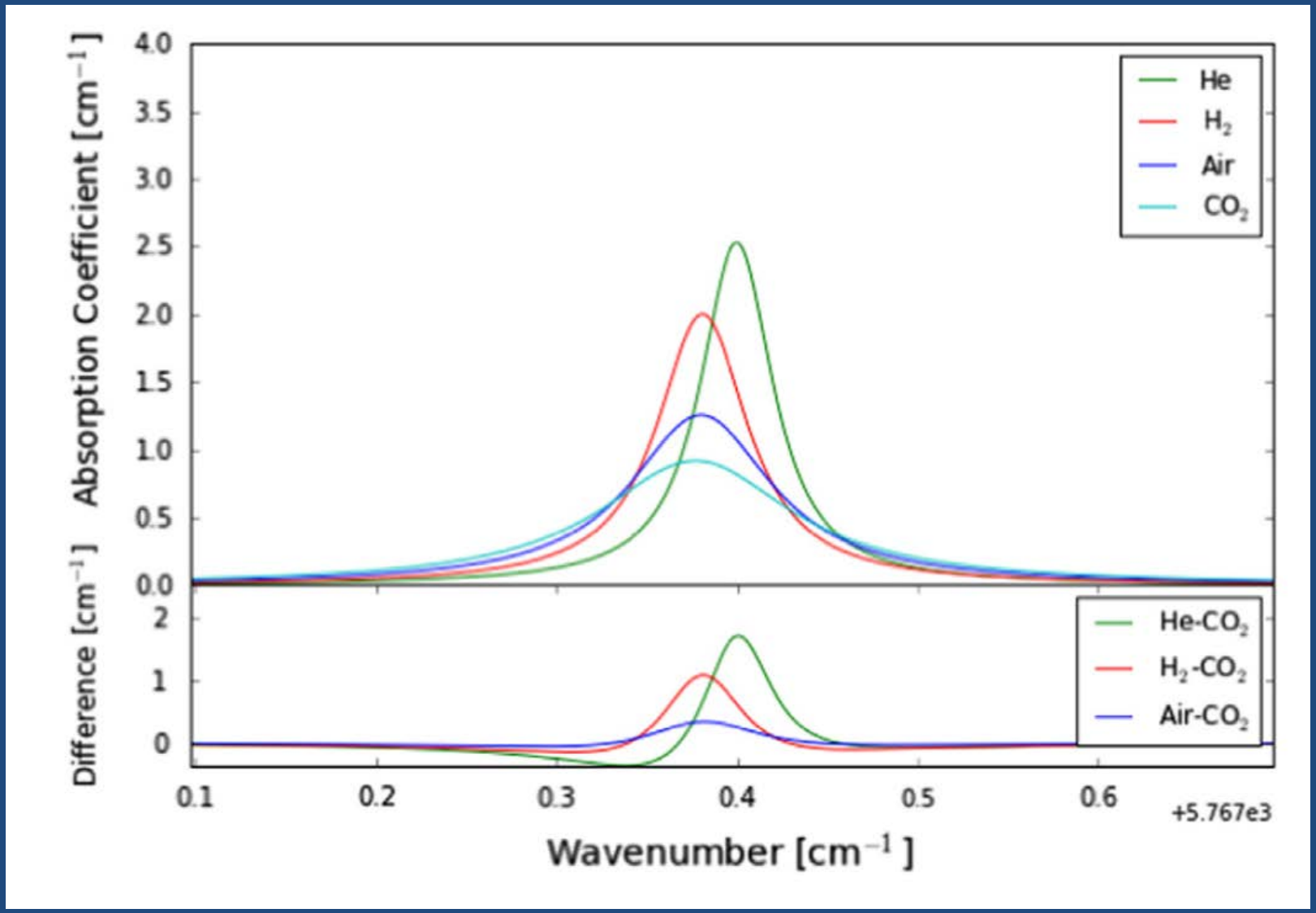
Neptune: H_2, He, CH_4, C_2H_4, **C_2H_2**, C_3H_4, CH_3, C_6H_6, ...

Venus: CO_2 , N_2, **SO_2**, H_2SO_4, **CO**, O, N_2, O_3, **HCl**, **HF**, Ne, H_2S, **OCS**, H, H_2, He, H_2O, O_2, Cl, ClO, ClO_2, COCl , ...

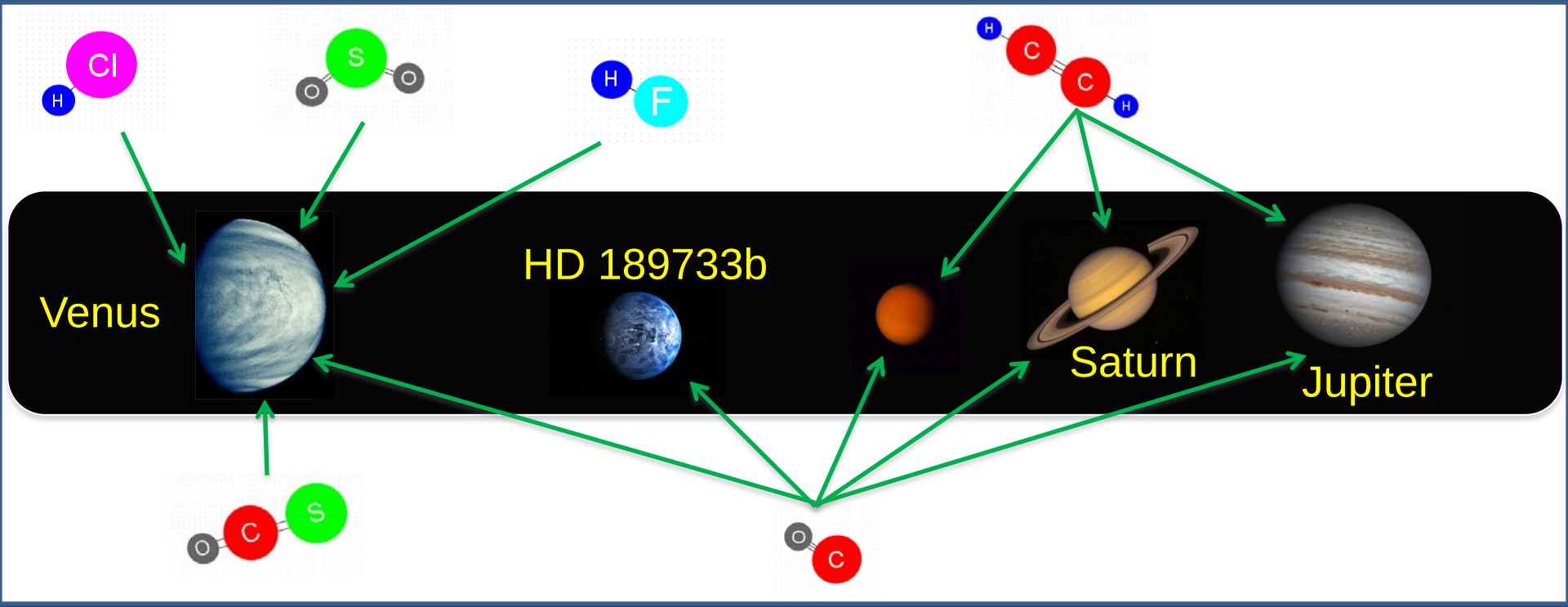
Titan: N_2, CH_4, Ar, C_2H_6, C_3H_8, H_2O, **CO**, CO_2, CH_3D, CH_3, C_2H_4, NH_3, HCN, C_2N_2, HC_3N, CH_3CN, C_4H_2, **C_2H_2**...

HD 189733b: H_2, H_2O, O, CH_4, **CO**, ...

Example of broadening and shifting by different gases: $H^{35}Cl$ 2-0 R(5)



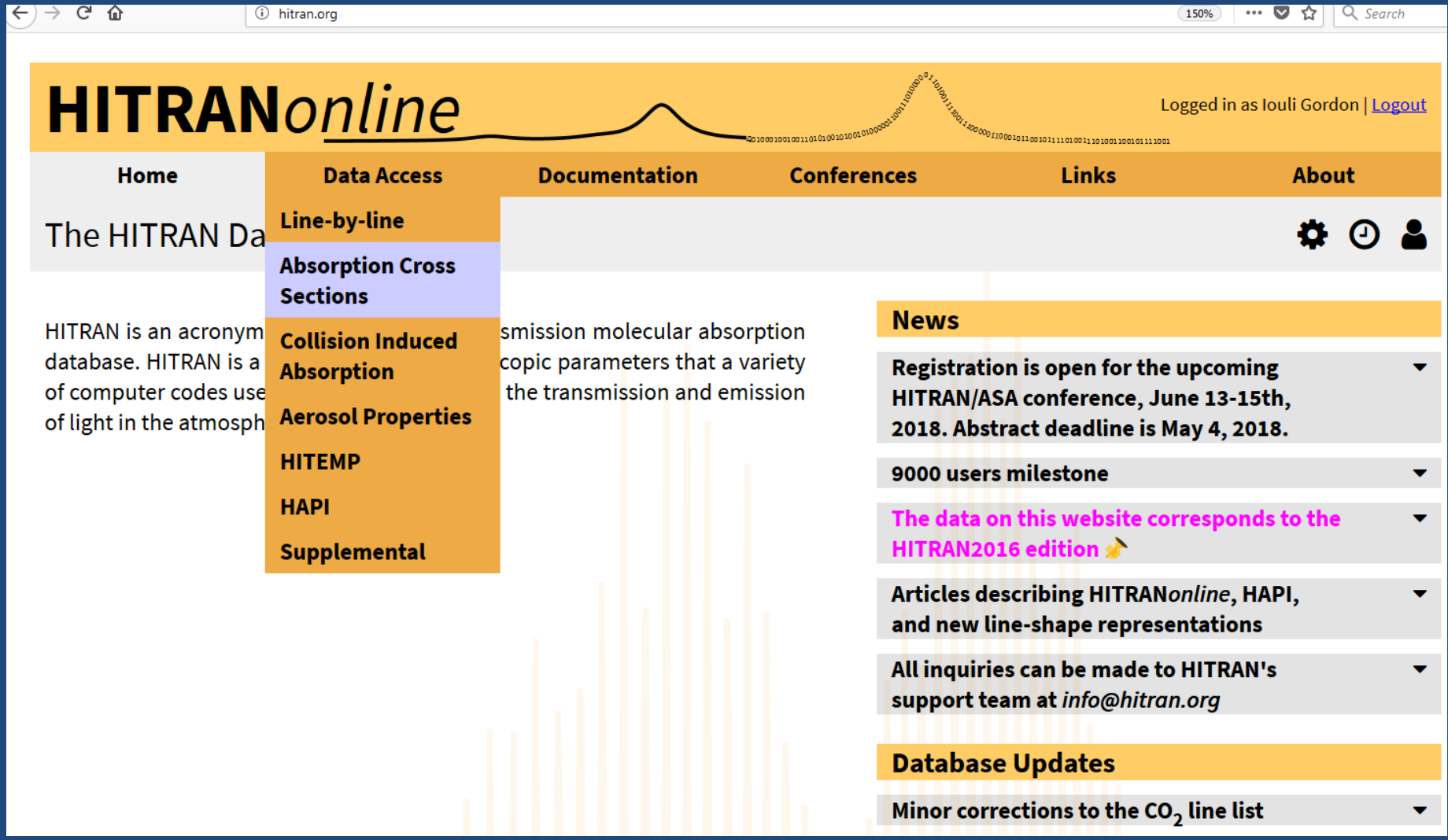
Broadening and shifting by gases dominant in planetary atmospheres



Wilzewski et al, "H_2, He, and CO_2 line-broadening coefficients, pressure shifts and temperature-dependence exponents for the HITRAN database. Part 1: SO_2, NH_3, HF, HCl, OCS and C_2H_2," JQSRT 168 (2016) 193–206.

Li et al, "Rovibrational Line Lists for Nine Isotopologues of the CO Molecule in the $X^1\Sigma^+$ Ground Electronic State," ApJ. Suppl. Ser. 216 (2015) 15.

Absorption cross-sections

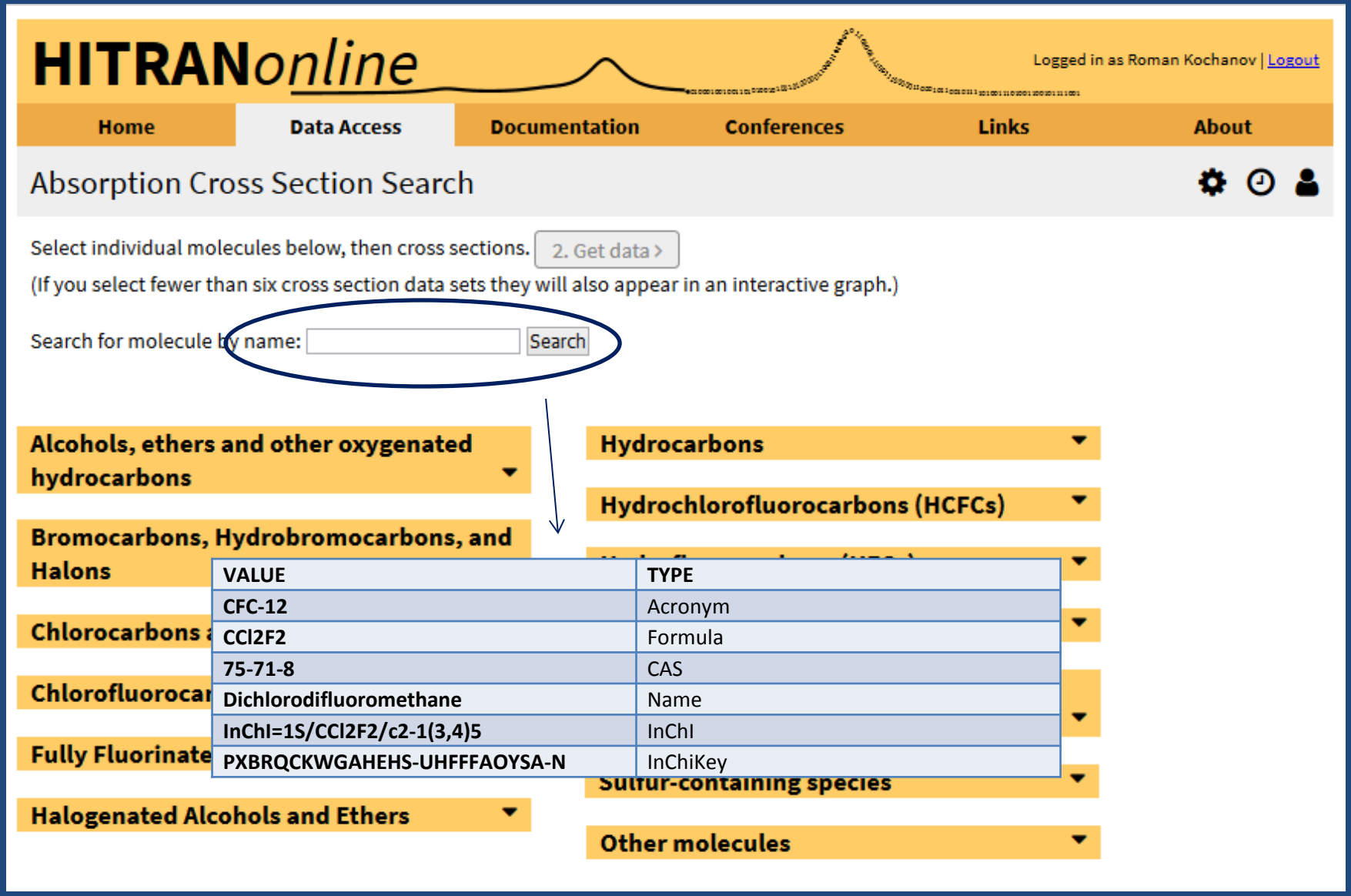


HITRAN2016 IR cross-sections

- **HITRAN2016 update features:**
- **275 new molecules (=>325 in total)**
- **2780 cross-section (T,p)-sets in total**
- **Contains categorized compounds for remote sensing, environment monitoring, climate applications, industrial pollution tracking, instrument calibration…**
- **Atmospherically relevant temperature and pressure range**
- **(temperature 180-362K, pressure up to 760Torr)**
- **Update contains spectra with features in near, middle and far infrared.**
- **Measurements:**
  - CRDS (Ethane, 200 kHz resolution, Reed & Hodges. JQSRT 2015)
  - FTS (0.005-2 cm-1 resolution)
  - Spectra broadened by air, N2, He, and pure

HITRAN*online* absorption cross-section search

http://hitran.org



HITRAN*online* absorption cross-section search

http://hitran.org

Search for molecule by name: Search

PXBRQCKWGAHEHS-UHFFFAOYSA-N found as CFC-12

Alcohols, ethers and other oxygenated hydrocarbons

Bromocarbons, Hydrobromocarbons, and Halons

Chlorocarbons and Hydrochlorocarbons

Chlorofluorocarbons (CFCs)

IR	UV/Vis	Common Name	Formula
⊘	○	CFC-113a	$C_2Cl_3F_3$
⊘	○	CFC-114a	$C_2Cl_2F_4$
⊘	○	CFC-112a	
⊘	○	CFC-112	
⊘	○	CFC-11	
⊘	○	CFC-12	CCl_2F_2
⊘	○	CFC-113	$C_2Cl_3F_3$
⊘	○	CFC-114	$C_2Cl_2F_4$
⊘	○	CFC-115	C_2ClF_5
⊘	○	CFC-13	$CClF_3$
⊘	○	Hexachlorocyclopentadiene	C_5Cl_6

CFC-12: CCl_2F_2

IR cross sections

	ν range /cm^{-1}	*T*/K	*p*/Torr	Resolution	npts	Broadener
☐	500.0 - 1499.9	296.0	700.0	0.5 cm-1	8297	air
☐	600.0 - 6500.0	298.15	760.0	0.112 cm-1	97903	N2
☐	600.0 - 6500.0	323.15	760.0	0.112 cm-1	97903	N2
☐	600.0 - 6500.0	278.15	760.0	0.112 cm-1	97903	N2
☐	799.8 - 1300.3	293.0	750.0	0.5 cm-1	1039	N2
☐	800.0 - 1270.0	216.2	129.4	0.02 cm-1	187181	air
☐	800.0 - 1270.0	189.5	170.4	0.03 cm-1	187181	air
☐	800.0 - 1270.0	216.2	379.5	0.03 cm-1	187181	air
☐	800.0 - 1270.0	233.1	197.2	0.03 cm-1	187181	air
☐	800.0 - 1270.0	233.2	380.8	0.03 cm-1	187181	air
☐	800.0 - 1270.0	244.8	171.0	0.03 cm-1	187180	air
☐	800.0 - 1270.0	244.8	444.6	0.03 cm-1	187180	air
☐	800.0 - 1270.0	244.8	550.0	0.03 cm-1	187180	air
☐	800.0 - 1270.0	269.0	169.8	0.03 cm-1	187180	air

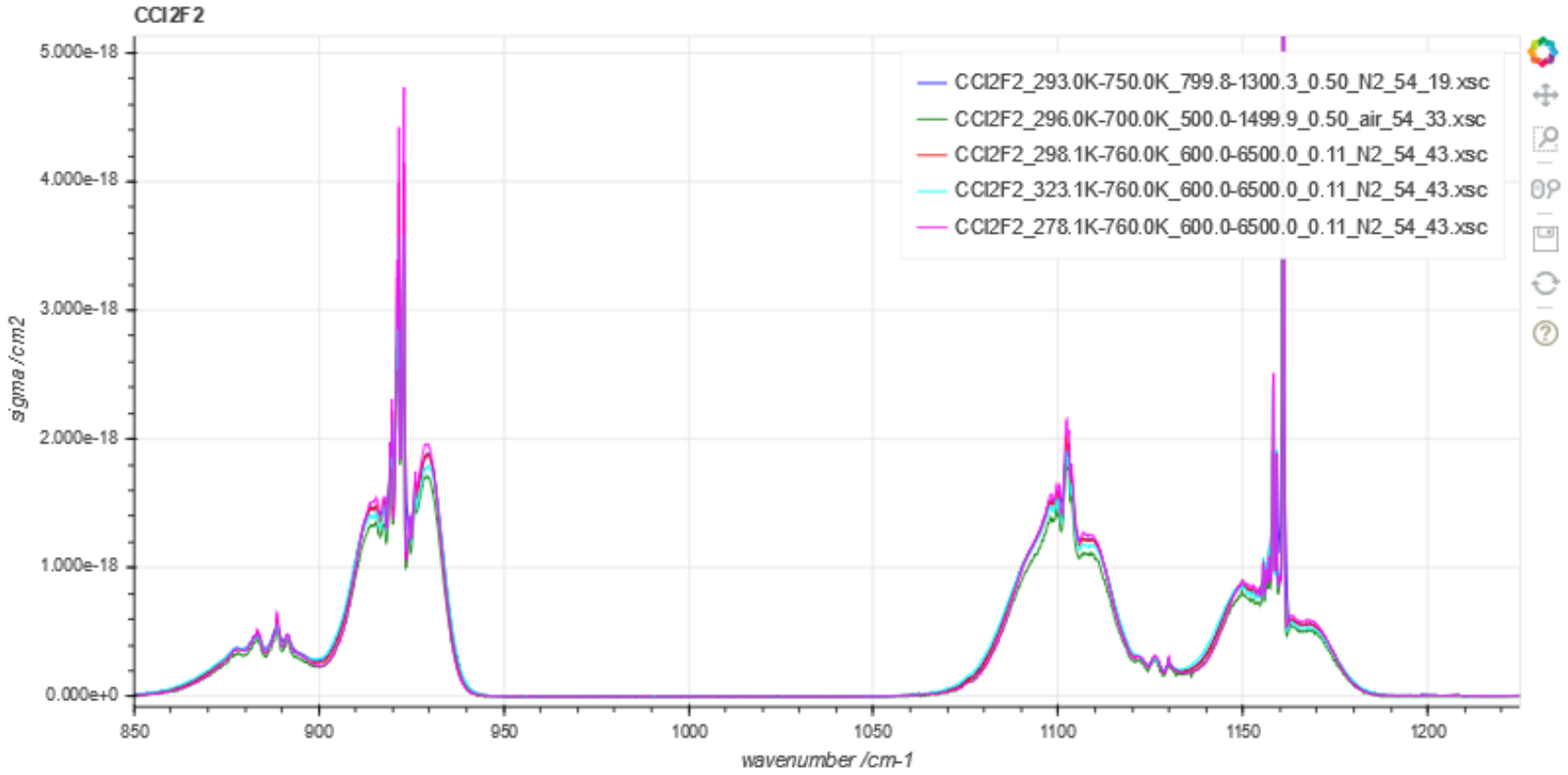
576. J.J. Harrison, "New and improved infrared absorption cross sections for dichlorodifluoromethane (CFC-12)", *Atmospheric Measurement Techniques* **8**, 3197-3207 (2015). [ADS]

CCl_2F_2

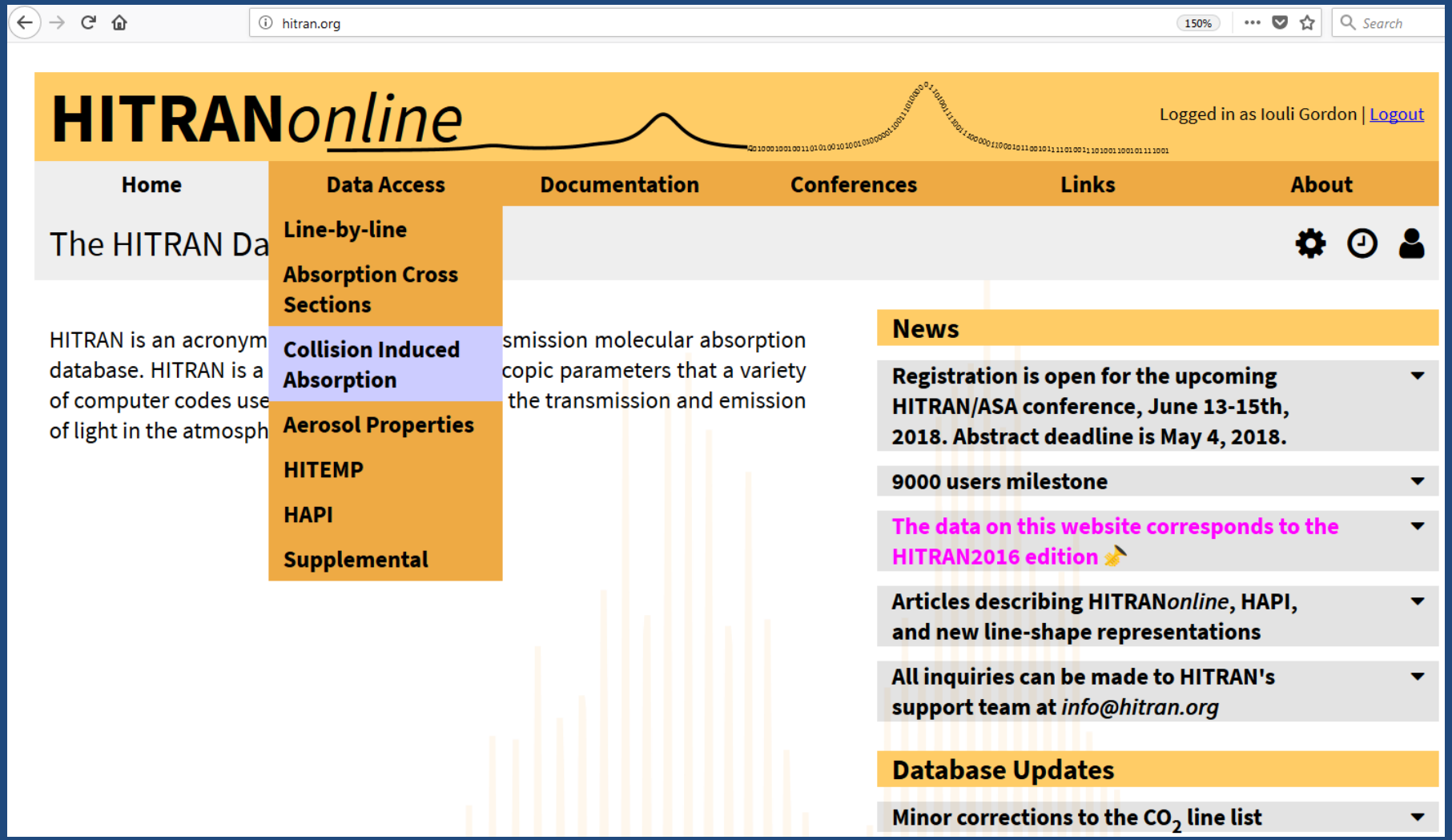
5 cross sections were found.

CCl2F2_293.0K-750.0K_799.8-1300.3_0.50_N2_54_19.xsc	[10.5 KB]	Cross section file (HITRAN .xsc format)
CCl2F2_296.0K-700.0K_500.0-1499.9_0.50_air_54_33.xsc	[82.8 KB]	Cross section file (HITRAN .xsc format)
CCl2F2_298.1K-760.0K_600.0-6500.0_0.11_N2_54_43.xsc	[975.4 KB]	Cross section file (HITRAN .xsc format)
CCl2F2_323.1K-760.0K_600.0-6500.0_0.11_N2_54_43.xsc	[975.4 KB]	Cross section file (HITRAN .xsc format)
CCl2F2_278.1K-760.0K_600.0-6500.0_0.11_N2_54_43.xsc	[975.4 KB]	Cross section file (HITRAN .xsc format)
test.bib.html	[2.5 KB]	List of sources (HTML format)
test.bib	[2.1 KB]	List of sources (BibTeX format)

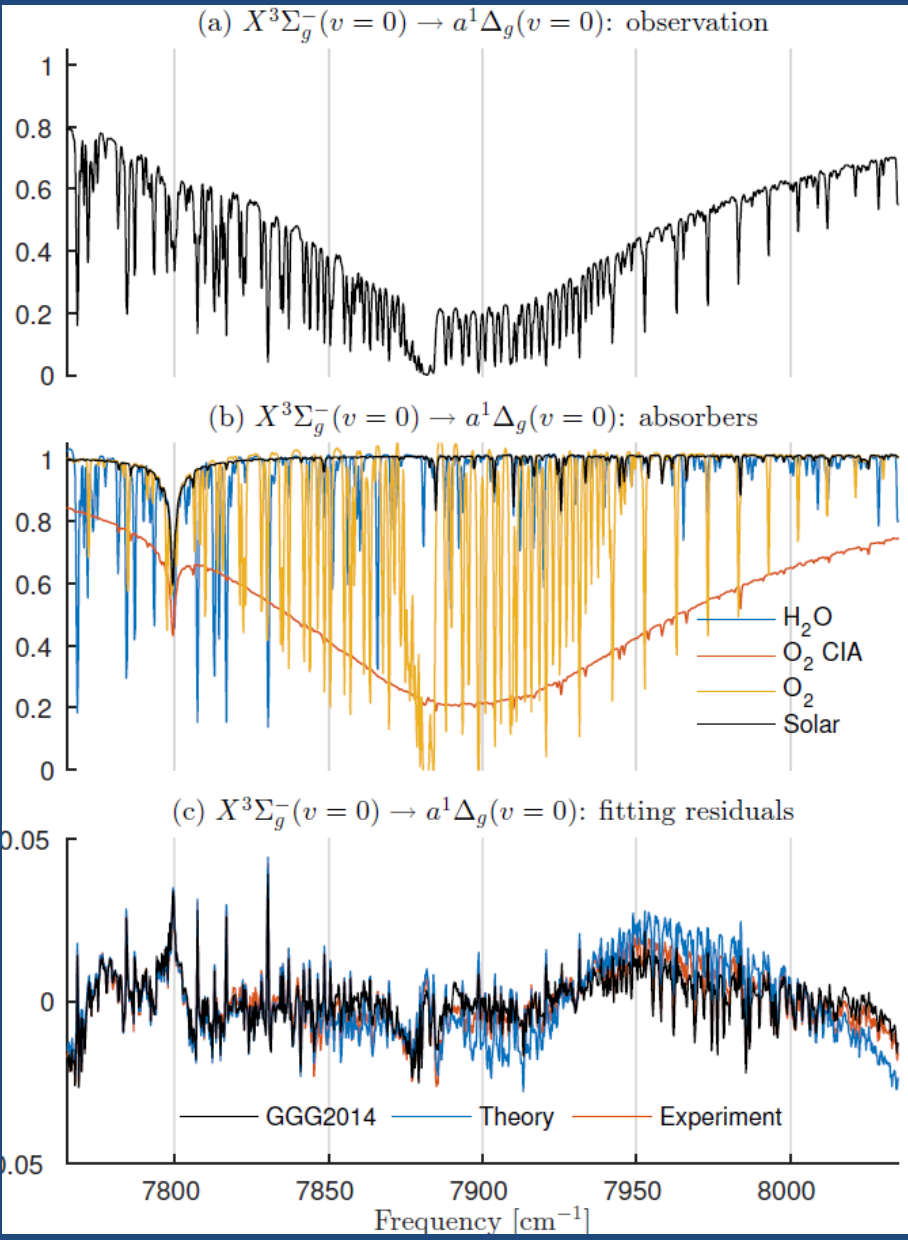
ZIP archive: test.zip

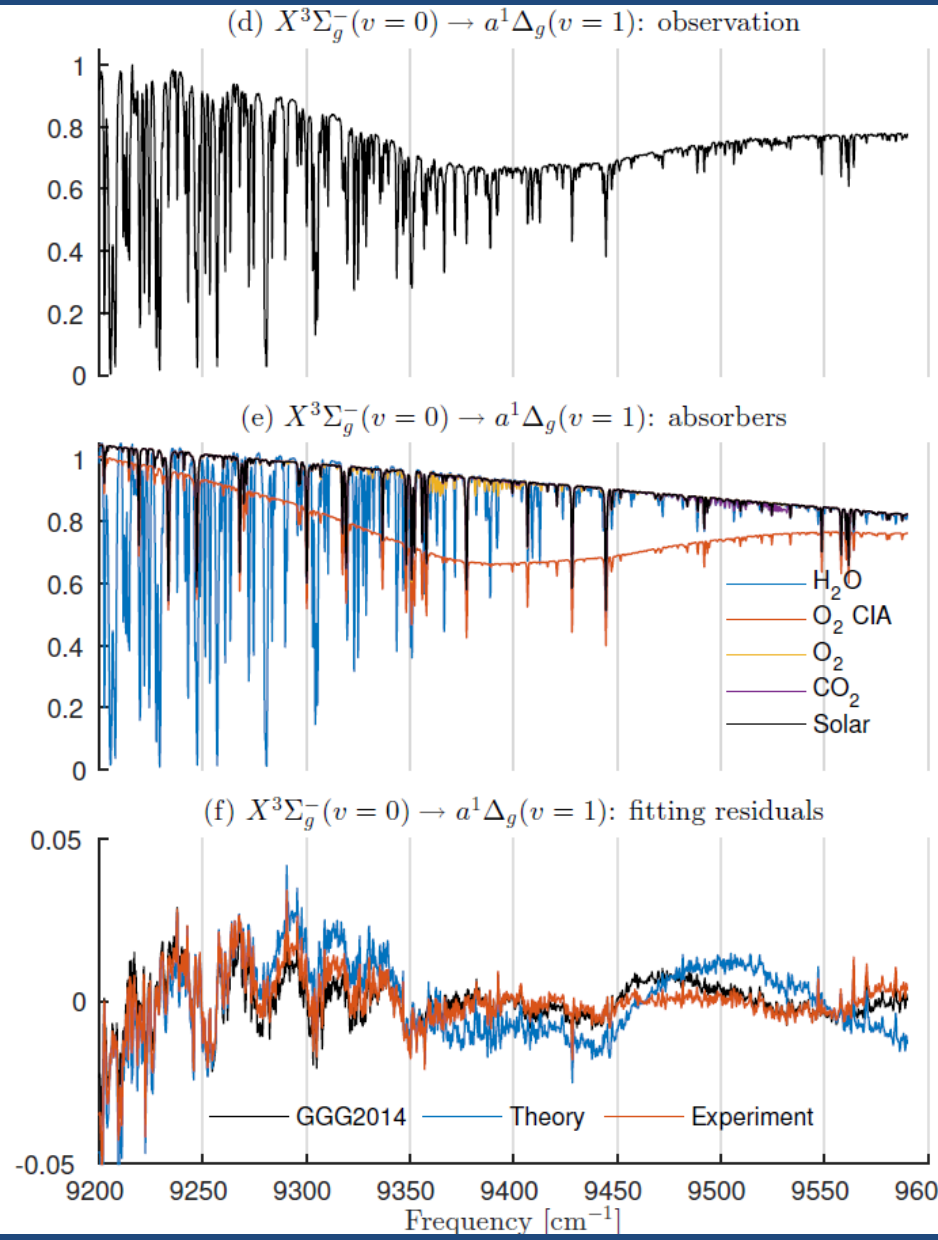


Collision Induced Absorption (CIA)



Example of importance of CIA in atmospheric spectra





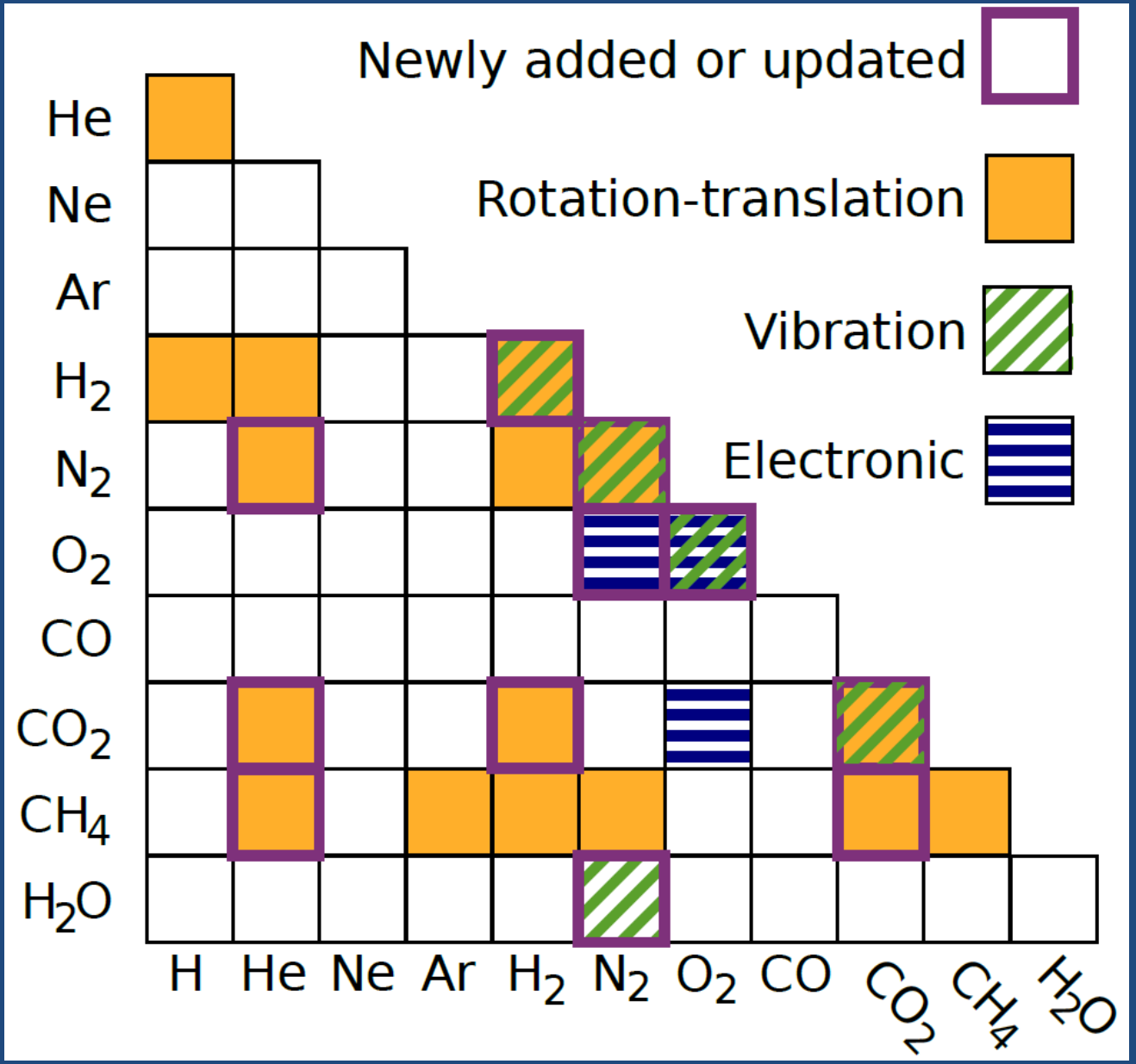
Collision Induced Absorption (CIA)

CIA system	Spectral range (cm^{-1})	Temperature range (K)	Number of sets	Band(s)
N_2–N_2	0.02 – 554	40 – 400	10	Roto-translational
	2000 – 2698	228 – 272	5	Fundamental
	1850 – 3000	300 – 362	5	Fundamental
N_2–H_2	0.02 – 1886	40 – 400	10	Roto-translational
N_2–CH_4	0.02 – 1379	40 – 400	10	Roto-translational
H_2–H_2	0.02 – 2400[a]/2400[b]	40 – 400	10	Roto-translational
	20 – 10000	200 – 3000	113	Roto-translational, Fundamental, 1st overtone
H_2–He	0.02 – 2400[a]/2400[b]	40 – 400	10	Roto-translational
	20 – 20000	200 – 9900	334	Roto-translational, Fundamental, 1st to 4th overtone
H_2–CH_4	0.02 – 1946[a]/1946[b]	40 – 400	10	Roto-translational
H_2–H	100 – 10000	1000 – 2500	4	Roto-translational, Fundamental, 1st overtone
He–H	50 – 11000	1500 – 10000	10	Roto-translational
O_2–O_2	1150 – 1950	193 – 353	15	Fundamental
	7450 – 8487	253 – 296	3	$a^1\Delta_g \leftarrow X^3\Sigma_g^-$ (0–0)
	9001 – 9997	296	1	$a^1\Delta_g \leftarrow X^3\Sigma_g^-$ (1–0)
	12600 – 13839	200 – 300[c]	1	A Band
	14996 – 29790	294	1	$a^1\Delta_g$+$a^1\Delta_g$, $b^1\Sigma_g^-$+$a^1\Delta_g$, and $b^1\Sigma_g^-$+ $b^1\Sigma_g^-$
O_2–N_2	7500 – 8600	200 – 295	7	$a^1\Delta_g \leftarrow X^3\Sigma_g^-$ (0–0)
	9000 – 10000	200 – 295	5	$a^1\Delta_g \leftarrow X^3\Sigma_g^-$ (1–0)
	12600 – 13839	200 – 300[c]	1	A Band
O_2–CO_2	12600 – 13839	200 – 300[c]	1	A Band
CO_2–CO_2	1 – 250	200 – 800	7	Roto-translational
CH_4–CH_4	0.02 – 990	40 – 400	10	Roto-translational
CH_4–Ar	1 – 697	70 – 296	5	Roto-translational

Systems highlighted in orange are provided in the main folder, while systems highlighted in green are provided in the alternate folder.
[a] refers to the "equilibrium" data
[b] refers to the "normal" data
[c] in this specific case, data between 200 and 300 K are the same and the temperature chosen for HITRAN is 296 K (room-temperature)

C. Richard, I.E. Gordon, L.S. Rothman, M. Abel, L. Frommhold, M. Gustafsson, J.-M. Hartmann, C. Hermans, W.J. Lafferty, G. Orton, K.M. Smith, H. Tran "New section of the HITRAN database: Collision-induced absorption (CIA)," *JQSRT* **113**, 1276-1285 (2012).

Upcoming update of the CIA section



HITRAN Application Programming Interface (HAPI)

Home | Data Access | Documentation | Conferences | Links | About

- Line-by-line
- Absorption Cross Sections
- Collision Induced Absorption
- Aerosol Properties
- HITEMP
- HAPI
- Supplemental

HAPI: The HITR Programming Interface

.1.1.0.7

al.pdf documentation

Int

The *ogramming Interface* (HAPI)[1] is a set of routines in Python which aims to pro unctionality and data given by the HITRAN*online*. At the present time, the API d process line-by-line transition data.

The API is to extend the functionality of the main site, in particular, in the calculation of spectra using several types of line shape, including the flexible HT (Hartmann-Tran) profile[2] and optionally accounting for instrumental functions. Each feature of the API is represented by a Python function taking a set of arguments which describe the parameters defining the task.

The current version is in the beta stage. All comments and suggestions are welcome: please email rkochanov@cfa.harvard.edu.

Features

Some of the prominent current features of HAPI are:

1. Downloading line-by-line data from the HITRAN*online* site to a local machine;
2. Filtering and processing the data in SQL-like fashion;
3. Conventional Python structures (lists, tuples, and dictionaries) for representing spectroscopic data;

HITRAN Application Programming interface (HAPI) examples

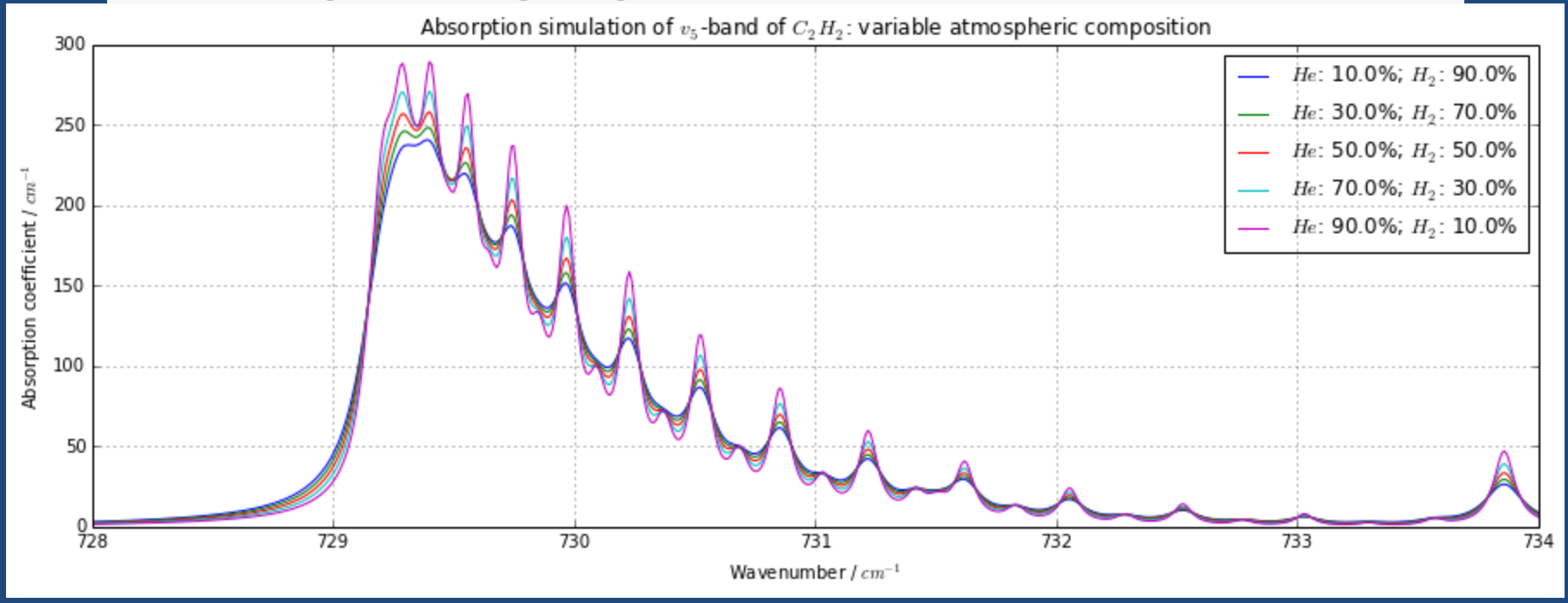
```
01. # Import functions for data download (fetch),
02. #  filtering (select) and processing (abscoef)
03. from hapi import fetch,select,abscoef
04.
05. # Download the data for H2O molecule
06. #  in 2100,2100 wavenumber range.
07. # The molecule is given in the HITRAN
08. #  nomenclature (N_mol,N_isot)
09. fetch('h2o',1,1,2000,2100)
10.
11. # Select all lines with intensity
12. #  greater than 1e-26 cm-1/(molecule.cm-2)
13. select('h2o',DestinationTableName='h2o_cut',
14.        Conditions=('>','sw',1e-25))
15.
16. # Calculate absorption coefficient
17. nu,coef = abscoef('h2o_cut')
```

```
fetch_by_ids('O2',[36,37,38],12000,14000,ParameterGroups=['160-char','Galatry'])
```

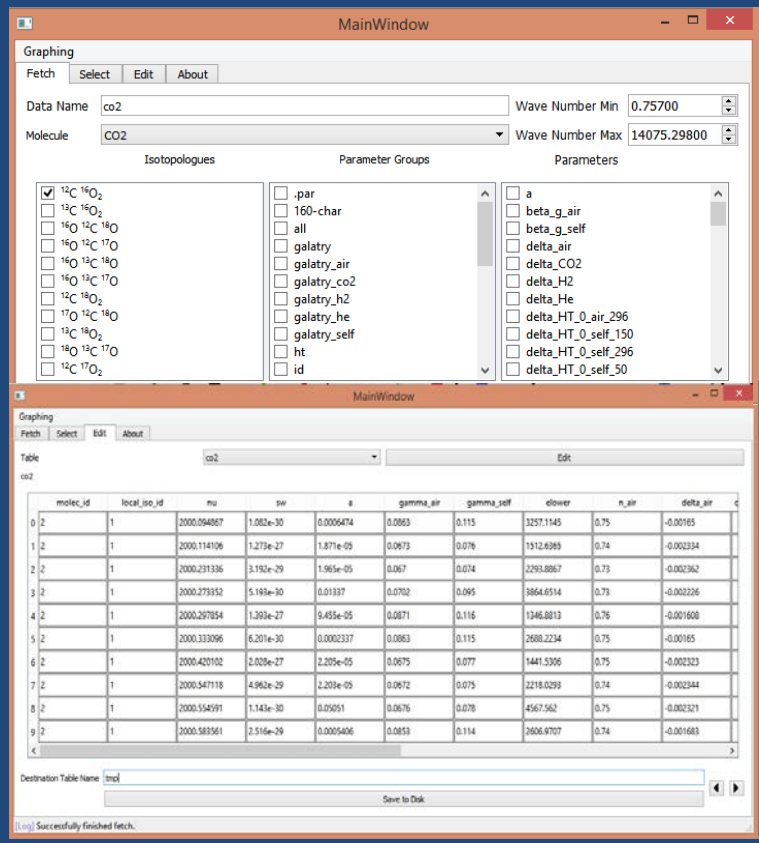
```
fetch_by_ids('H2',[103],2500,3500,ParameterGroups=['160-char'],
             Parameters=['gamma_HT_0_self_296', 'n_HT_self_296',
                         'gamma_HT_2_self_296', 'delta_HT_0_self_296',
                         'deltap_HT_0_self_296','delta_HT_2_self_296',
                         'nu_HT_self','kappa_HT_self','eta_HT_self'])
```

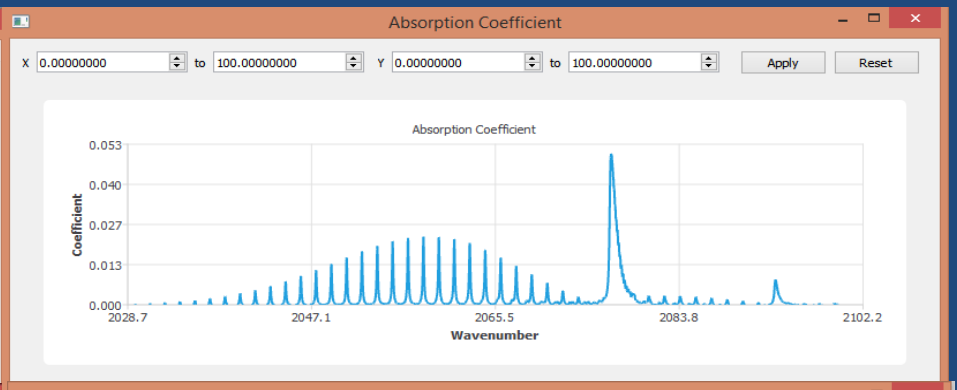
HAPI code example: modeling of C_2H_2 ν_5-band absorption in a He+H_2 atmosphere

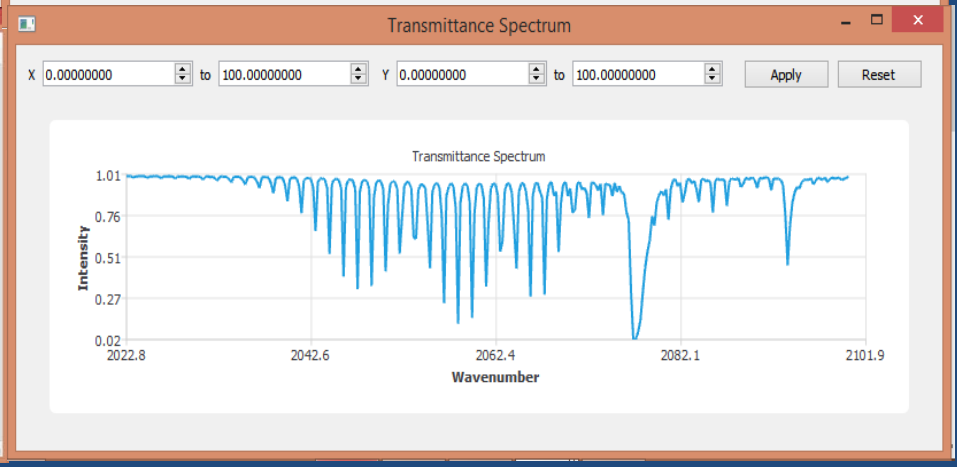
```
alphas = [0.1, 0.3, 0.5, 0.7, 0.9]
leg = []
for alpha in alphas:
    He_frac = alpha; H2_frac = 1-alpha
    nu,coef = absorptionCoefficient_Voigt(SourceTables='c2h2_v5',WavenumberRange=[727.,735.],
                                          Diluent={'He':He_frac,'H2':H2_frac},HITRAN_units=False)
    plot(nu,coef)
    #leg.append('%.1f'%alpha)
    leg.append('$He$: %.1f%%; $H_2$: %.1f%%'%(He_frac*100,H2_frac*100))
title('Absorption simulation of $v_5$-band of $C_2H_2$: variable atmospheric composition')
xlabel('Wavenumber / $cm^{-1}$'); ylabel('Absorption coefficient / $cm^{-1}$')
xlim(728,734); grid(True); legend(leg)
```



HITRAN Application Programming Interface and Efficient Spectroscopic Tools (HAPIEST)

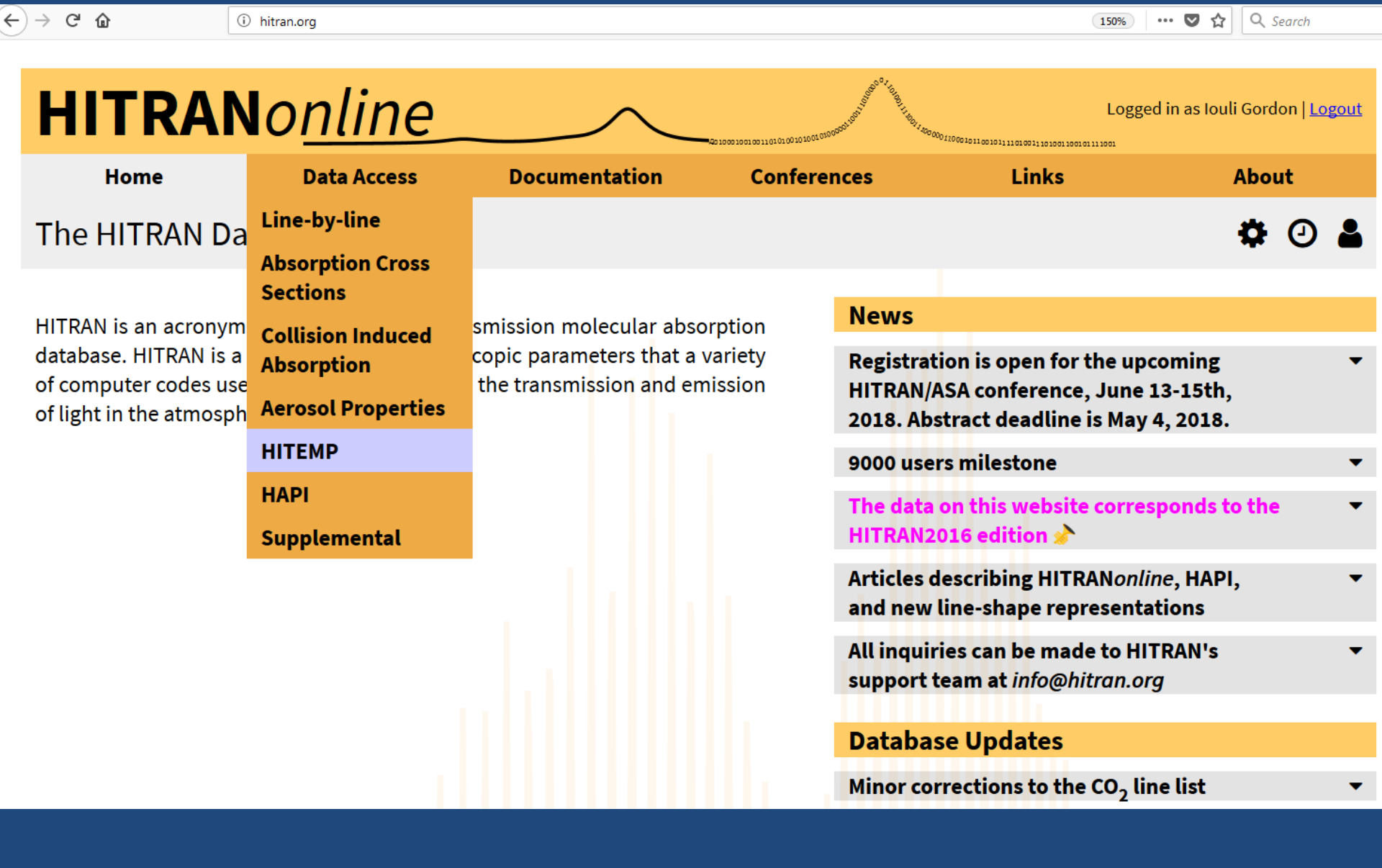






https://github.com/hitranonline/hapiest

HITEMP database



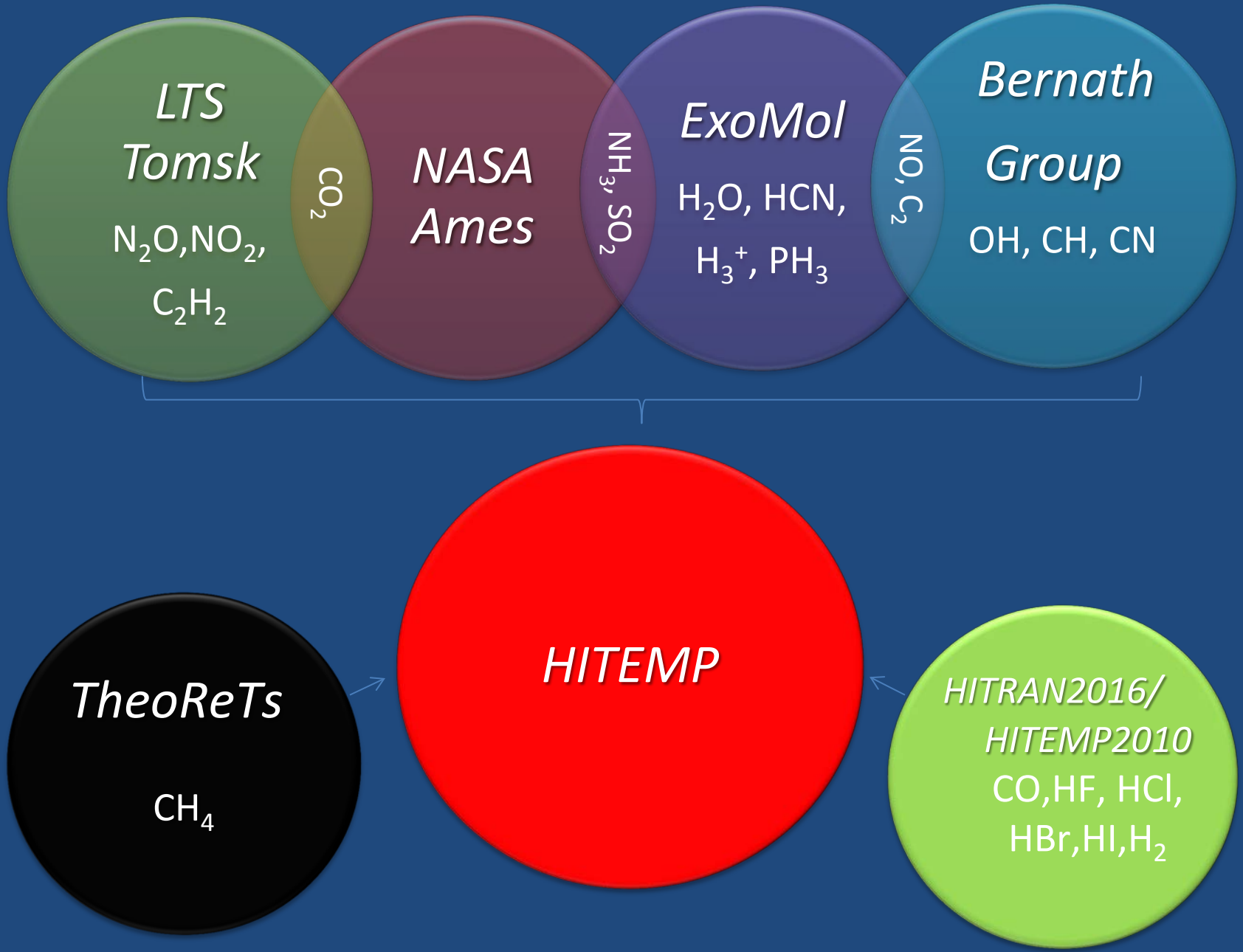
HITEMP 2010 database

Molecule	Spectral coverage (cm^{-1})	Number of isotopologues[a] (HITEMP2010)	Number of transitions (HITEMP2010)	Number of transitions[b] (HITRAN)
H_2O	0–30,000	6	111,377,777	69,201
CO_2	258–9648	7	11,167,618	312,479
CO	0–8465	6	115,218	4,477
NO	0–9274	3	105 633	105,079
OH	0–19,268	3	40,055	31,976

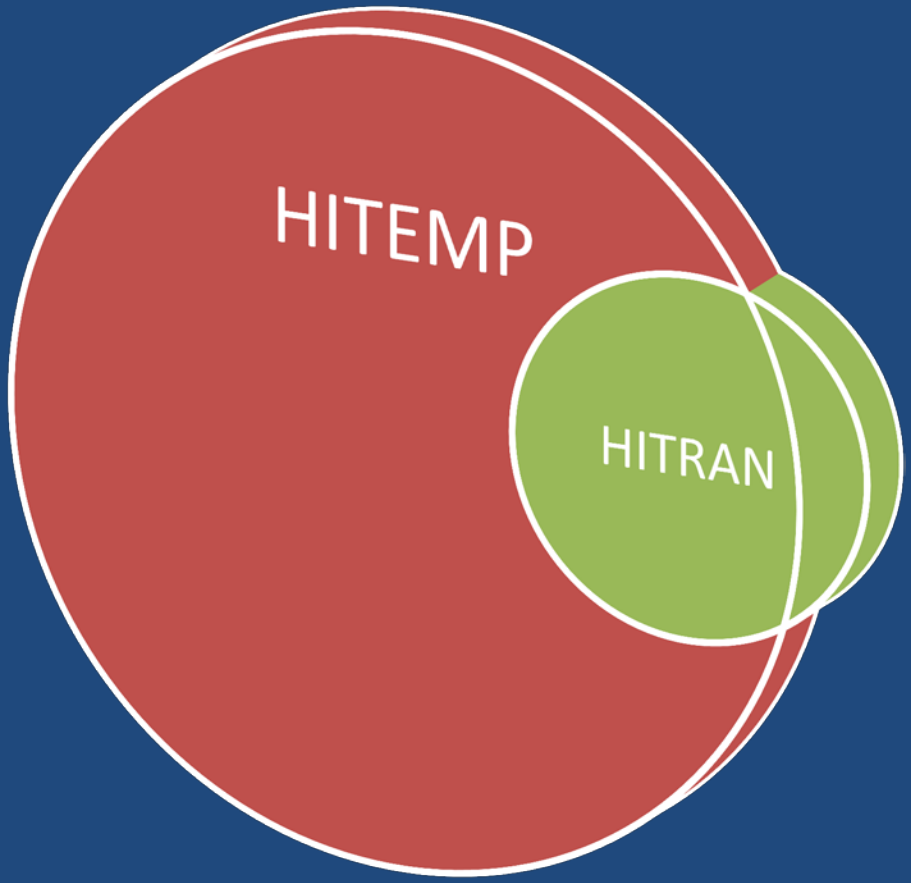
L.S. Rothman, I.E. Gordon, R.J. Barber, H. Dothe, R.R. Gamache, A. Goldman, V. Perevalov, S.A. Tashkun, and J. Tennyson, *J. Quant. Spectrosc. and Rad. Transfer* **111,** 2139-2150 (2010)

HITRAN 2012 data for HF, HCl, HBr, HI and H_2 are suitable for use at thousands of Kelvin!

Data for new HITEMP



Line parameters in HITEMP will be common with HITRAN wherever possible



Direct fit approach

- Calculate expectation values using empirical potential of Coxon and Hajigeorgiou *J. Chem. Phys.* **121,** 2992 (2004)
- Employ Le Roy's LEVEL program.
- Do a least squares fit to obtain M_i coefficients. Every measurement is included with appropriate weight

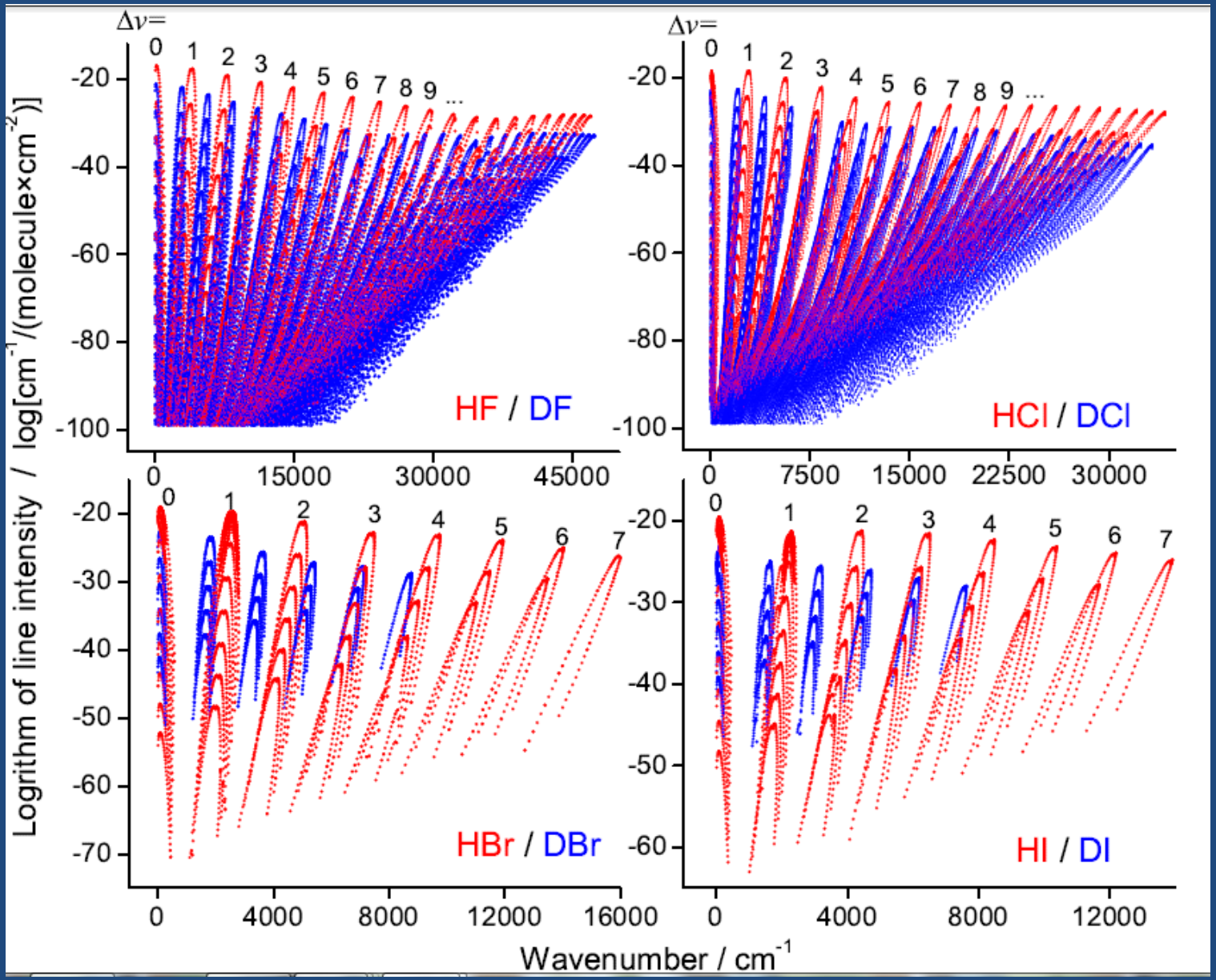
$$\langle vJ' | M(x) | 0J'' \rangle = \sum_{i=1}^{n} M_i \langle vJ' | x^i | 0J'' \rangle$$

- Include long-range ab initio data and create a piecewise dipole moment function

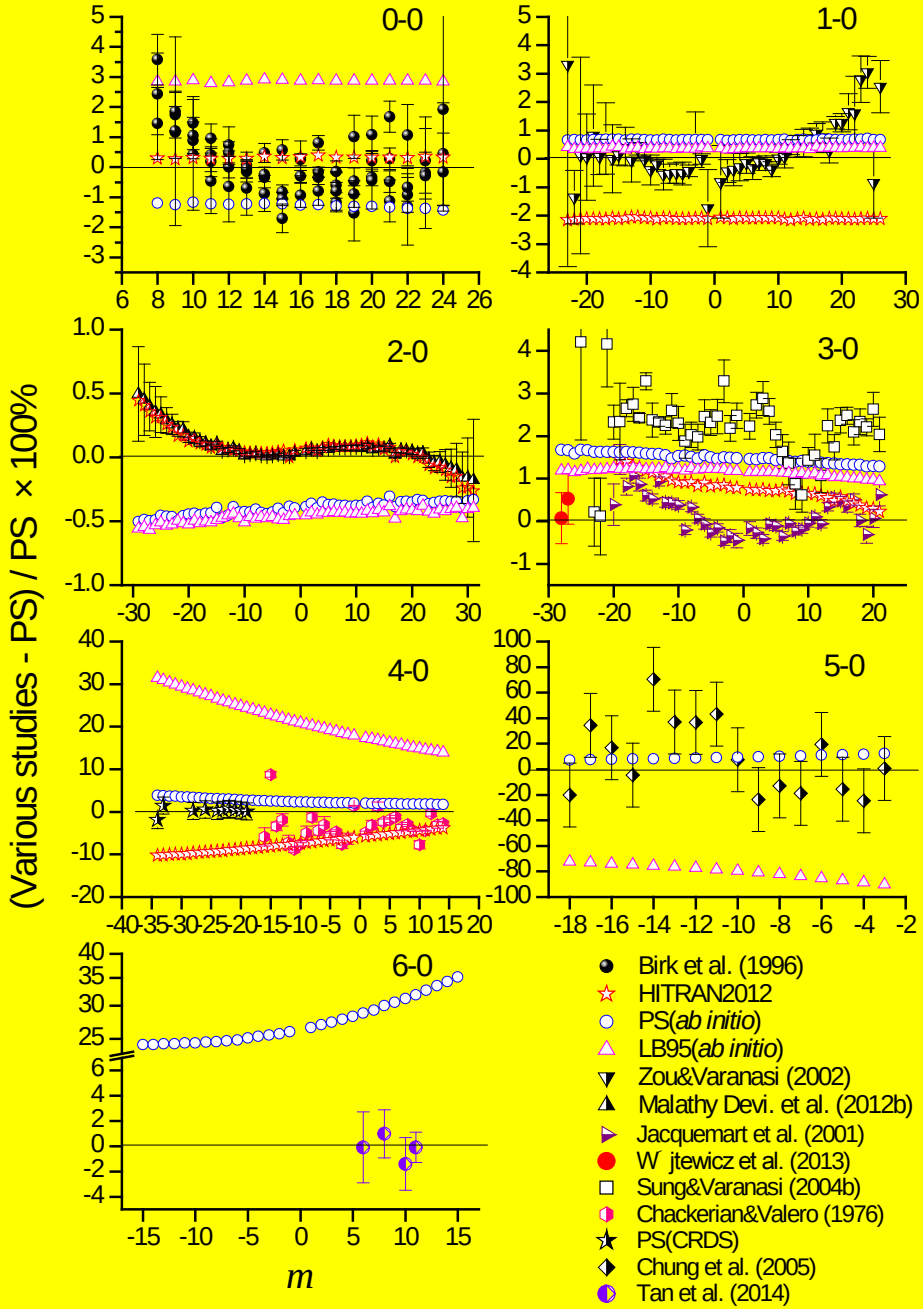
G. Li, I.E. Gordon, P.F. Bernath, and L.S. Rothman, "Direct fit of experimental ro-vibrational intensities to the dipole moment function: Application to HCl," *JQSRT* 112, 1543-1550 (2011).

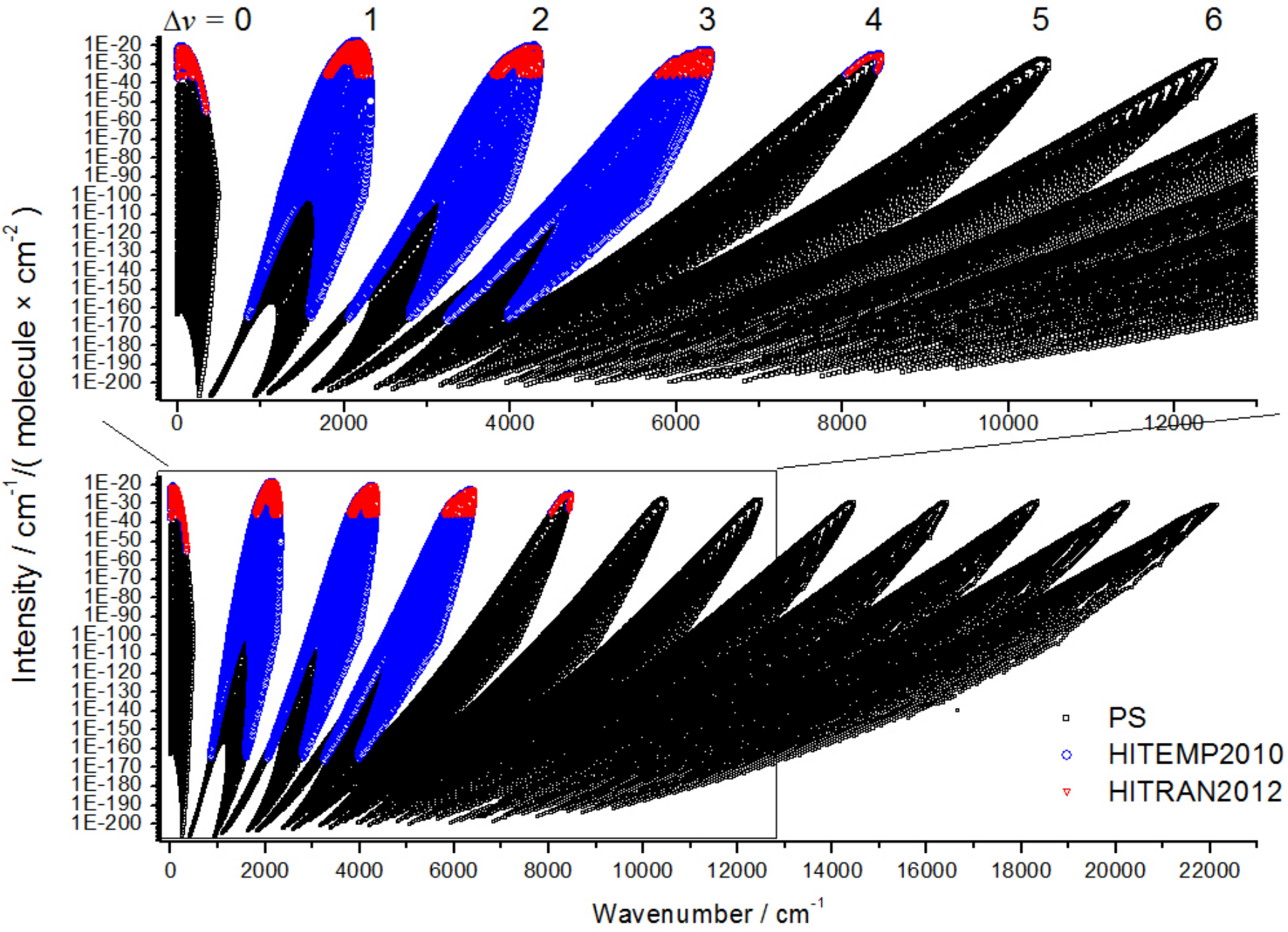
G. Li, I. E. Gordon, R.J. Le Roy, P.G. Hajigeorgiou, J.A. Coxon, P.F. Bernath, and L.S. Rothman, "Reference spectroscopic data for hydrogen halides. Part I: Construction and validation of the ro-vibrational dipole moment functions," *JQSRT* ***121, 78-90 (2013)***

Overview of new line lists



Comparison of CO intensities from different sources





Li et al APJS (2015)

Summary comparison of CO rotation-vibration line lists

	This work	HITEMP 2010	HITRAN 2012	Goorvitch (1994)
Stable isotopologues	6	6	6	6
Maximum v''	41	20	4	20
Maximum J''	150	149	94	149
Maximum Δv	11	4	4	3
Temperature range (K)	1-9000	70-3000	70-3000	500-10000
Spectral range (cm^{-1})	2 - 22149	3 - 8464	3 - 8464	849 - 6417
Number of lines	752,976	113,631	4,606	113,022
Radioactive isotopologues	3	None	None	None
Maximum v''	41			
Maximum J''	150			
Maximum Δv	11			
Temperature range (K)	1-9000			
Spectral range (cm^{-1})	2 - 21293			
Number of lines	376,488			

Example of validation of line-lists for inclusion into HITEMP

Journal of Quantitative Spectroscopy & Radiative Transfer 177 (2016) 43–48

Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: www.elsevier.com/locate/jqsrt

NOSD-1000, the high-temperature nitrous oxide spectroscopic databank

S.A. Tashkun [a,*], V.I. Perevalov [a], N.N. Lavrentieva [b]

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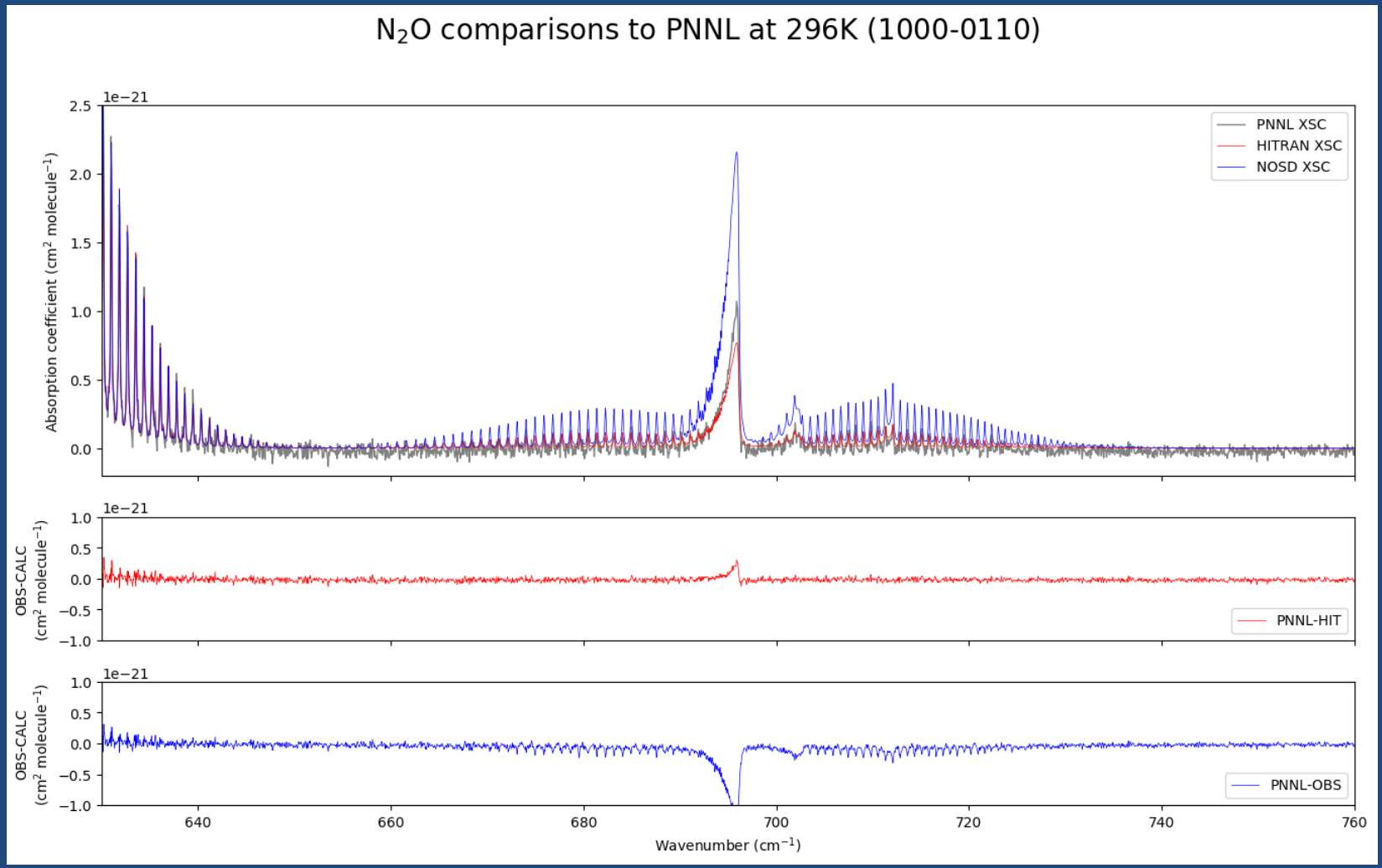
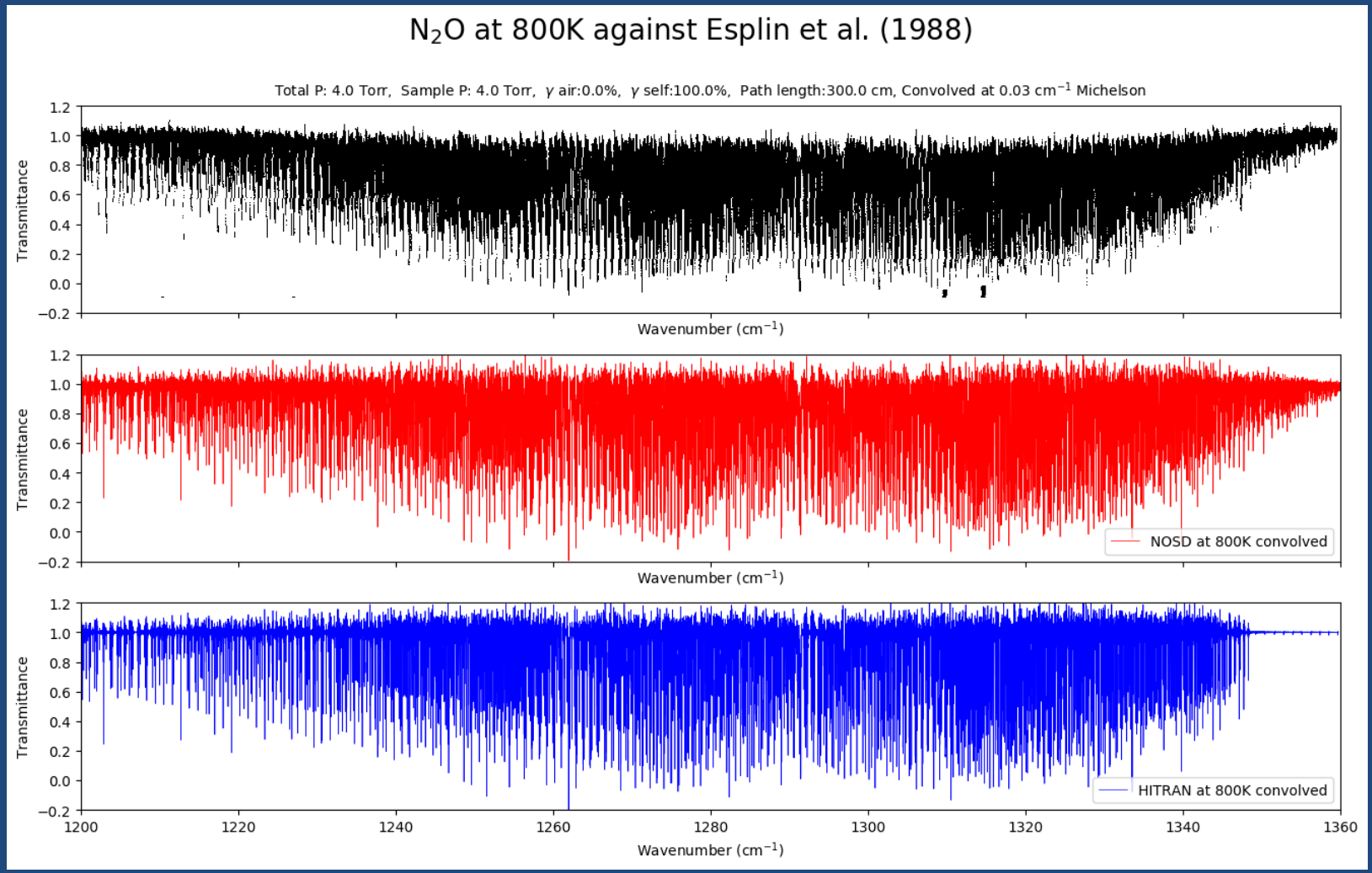
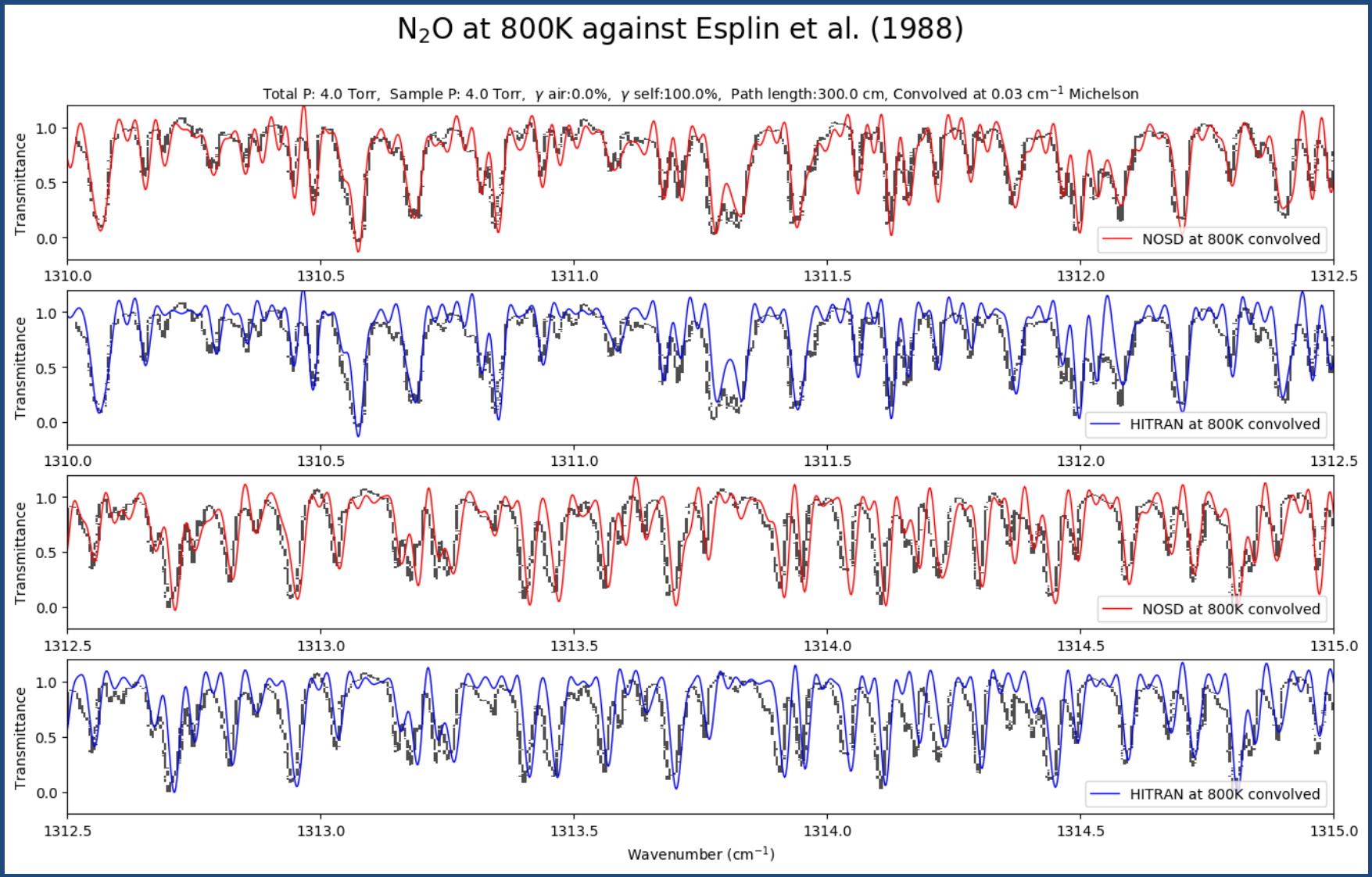
Comparison with PNNL cross-sections



Comparison with Esplin et al (1998) high temperature measurements



Comparison with Esplin et al (1998) high temperature measurements



Improvements and enhancements to the compilation being considered

- More bands and isotopologues for line-by-line; Improved accuracy
- Continue Refining line-shape parameters
- Additional line-mixing algorithms
- Additional Temperature-pressure sets of cross-sections (now with more UV)
- Additional high-temperature parameters (for HITEMP)
- Molecules for astrophysics applications
- More Collision-Induced Absorption bands as they become available

Next HITRAN/ASA Meeting

June 13-15, 2018

Harvard-Smithsonian Center for Astrophysics

Cambridge, MA

http://hitran.org/conferences/hitran-15-2018/

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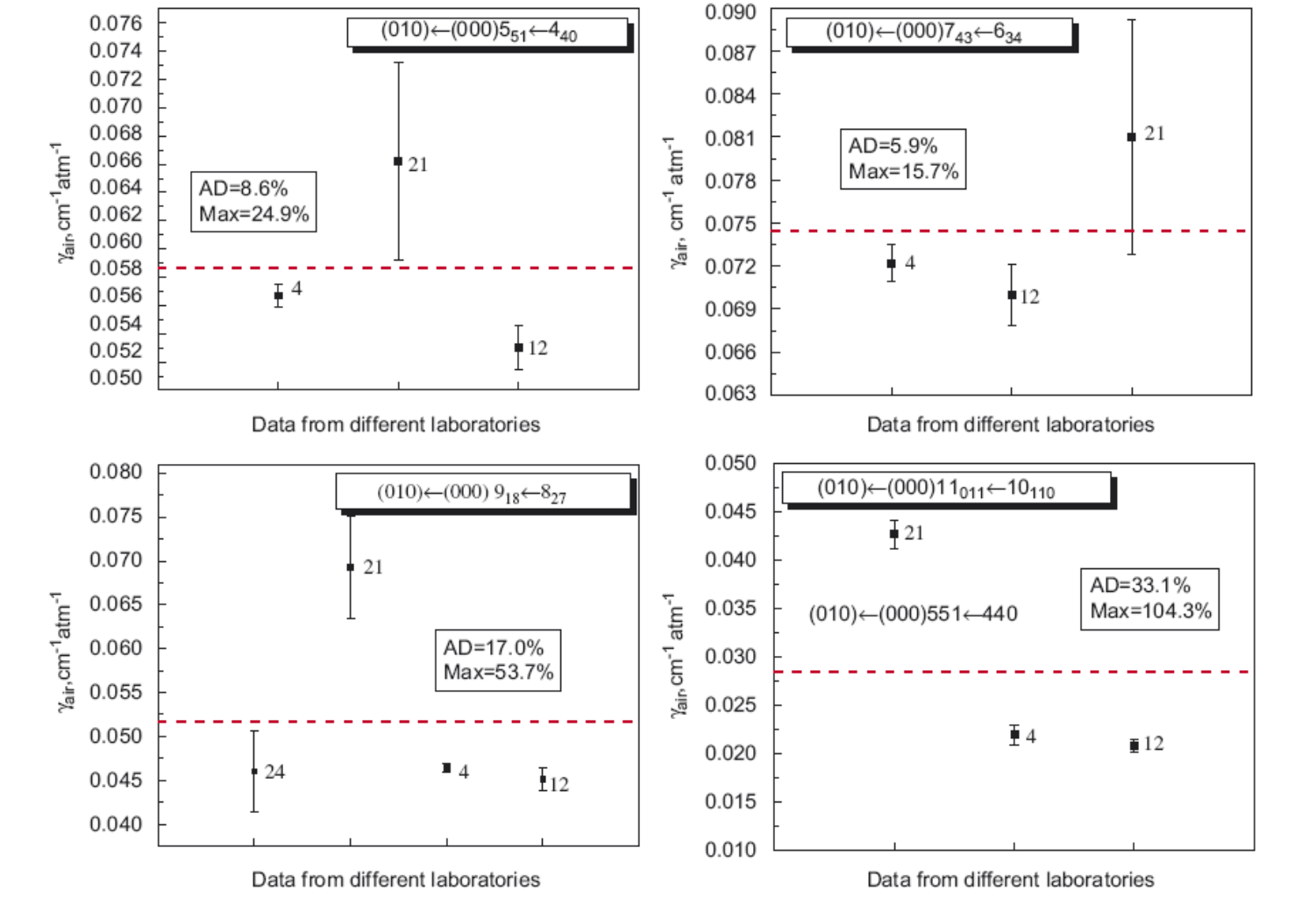
Funding Support

NASA Earth Observing System
NASA Planetary Atmospheres Program
NASA Planetary Data Archiving and Restoration Tools

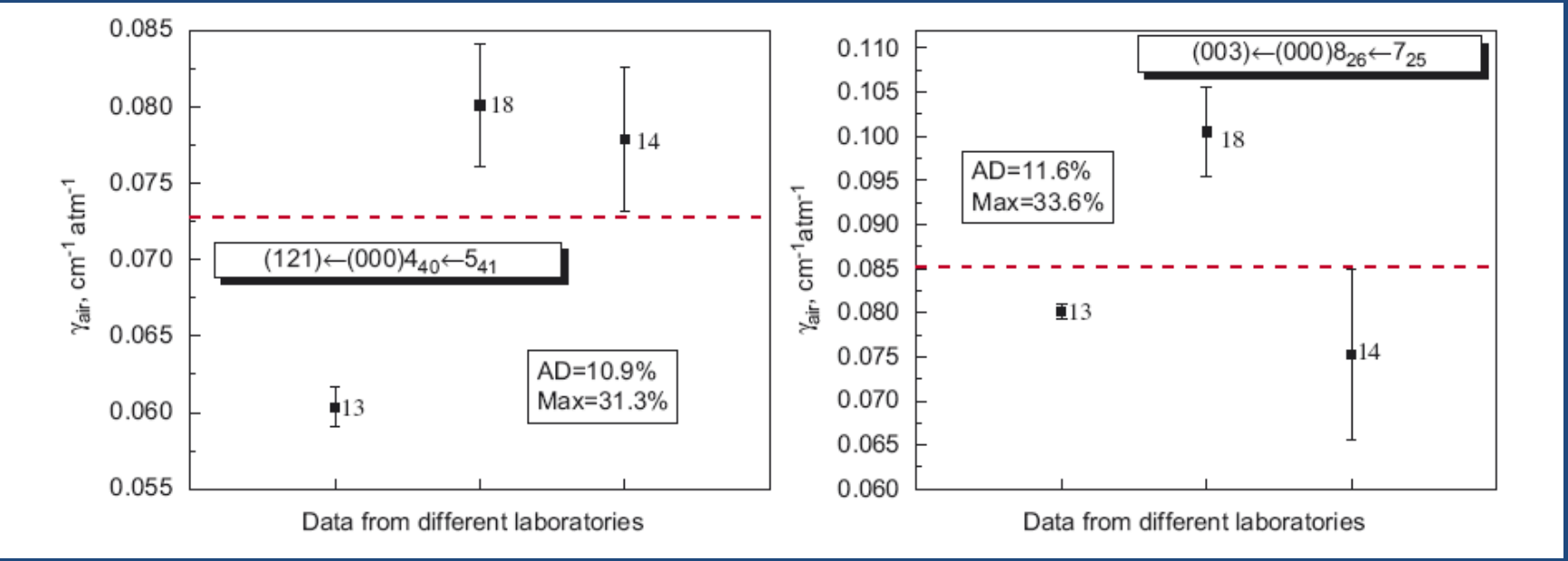
Pros and Cons of Experimental Data

- Advantages
  - Low uncertainty in determining parameters of relatively strong unblended lines
  - Direct observation of perturbations which often hard to account for with theoretical methods
- Disadvantages
  - Large uncertainty in determining parameters of weak or saturated lines
  - Sensitivity to impurities and congested spectra
  - Difficulties in controlling the conditions
  - Difficulties in covering large spectral and dynamic ranges simultaneously

Intercomparison of experimental measurements of water lines air-broadening in different laboratories



Intercomparison of experimental data



Gordon *et al*, *JQSRT* **108** (2007) 389–402

Pros and Cons of Theoretical and Semi-Empirical Data

- Advantages
  - Completeness, i.e. prediction of parameters that could not be measured by experiment
  - Can be easily adjusted to match high quality experiments
- Disadvantages
  - Rarely can compete with experimental uncertainty
  - Sometimes the model is oversimplified
  - Semi-empirical methods often lead to large errors when used for extrapolating the data