

Extensions to the HITRAN broadening parameters & Future Plans for HITEMP

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HARVARD-SMITHSONIAN
CENTER FOR ASTROPHYSICS

**ExoMol Conference:
Spectroscopy of Exoplanets**

Cumberland Lodge, Windsor, UK

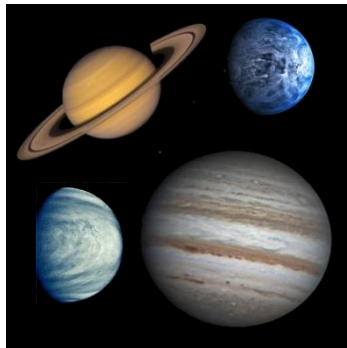
Monday 9th July, 2018

Overview



Brief introduction to the HITRAN2016 database

- Downloading data
- HAPI
- Additional parameters



Outline of latest additions for foreign broadening parameters

- Of relevance to planetary/exoplanetary atmospheres
- H_2 , He, CO_2 , H_2O broadening



The future of HITEMP

- Of relevance to exoplanet observations
- Proposed summary for data to be collected
- Example for N_2O

Current HITRAN Database

Journal of Quantitative Spectroscopy & Radiative Transfer 203 (2017) 3–69



Contents lists available at [ScienceDirect](#)

Journal of Quantitative Spectroscopy & Radiative Transfer

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



Credit: Y. Tan

The HITRAN2016 molecular spectroscopic database



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54 authors from **30** laboratories worldwide

67 pages, almost **650** references

The HITRAN community is **much larger** than the author list!

Brief overview of HITRAN

Credit: Y. Tan

- **Line-by-line (high precision)** : HITRAN2016 molecules (49 molecules)

Species (isotopologues) in line-by-line portion of HITRAN

H₂O (6)	NO (3)	HCl (4)	N ₂ (2)	COF ₂ (2)	NO ⁺ (1)	C ₄ H ₂ (1)
CO ₂ (10)	SO ₂ (2)	HBr (4)	HCN (3)	SF ₆ (1)	HOBr (2)	HC ₃ N (1)
O ₃ (5)	NO ₂ (1)	HI (2)	CH ₃ Cl (2)	H ₂ S (3)	C ₂ H ₄ (2)	H₂ (2)
N₂O (5)	NH ₃ (2)	ClO (2)	H ₂ O ₂ (1)	HCOOH (1)	CH ₃ OH (1)	CS (4)
CO (6)	HNO ₃ (2)	OCS (5)	C ₂ H ₂ (3)	HO ₂ (1)	CH ₃ Br (2)	SO ₃ (1)
CH ₄ (4)	OH (3)	H ₂ CO (3)	C ₂ H ₆ (2)	O (1)	CH ₃ CN (1)	C₂N₂ (1)
O₂ (3)	HF (2)	HOCl (2)	PH ₃ (1)	ClONO ₂ (2)	CF ₄ (1)	COCl₂(2)

- **Absorption cross sections** : (~320 molecules, with ~2000 experimental cross sections!)
 - Primarily from the PNNL database [1] and the Hodnebrog review [2].
- **HAPI (the HITRAN Application Programming Interface) [3]**
 - A free open source Python module (library) for working with HITRAN data.
- **Aerosol Properties**
- **Collision-Induced Absorption (CIA)**

[1] S. Sharpe, et al., (2004), *App. Spectrosc.* 58, 1452.
[2] Ø. Hodnebrog, et al. (2013), *Rev. Geophys.* 51, 300.
[3] R. V. Kochanov, et al. (2016), *JQSRT* 177, 15.

Brief overview of HITRAN

Credit: Y. Tashkun

○ Line-by-line (high resolution)

Species	
H ₂ O (6)	NO (3)
CO ₂ (10)	SO ₂ (2)
O ₃ (5)	NO ₂ (1)
N ₂ O (5)	NH ₃ (2)
CO (6)	CH ₄ (4)
CH ₄ (4)	OH (3)
O ₂ (3)	HF (2)

○ Absorption cross sections

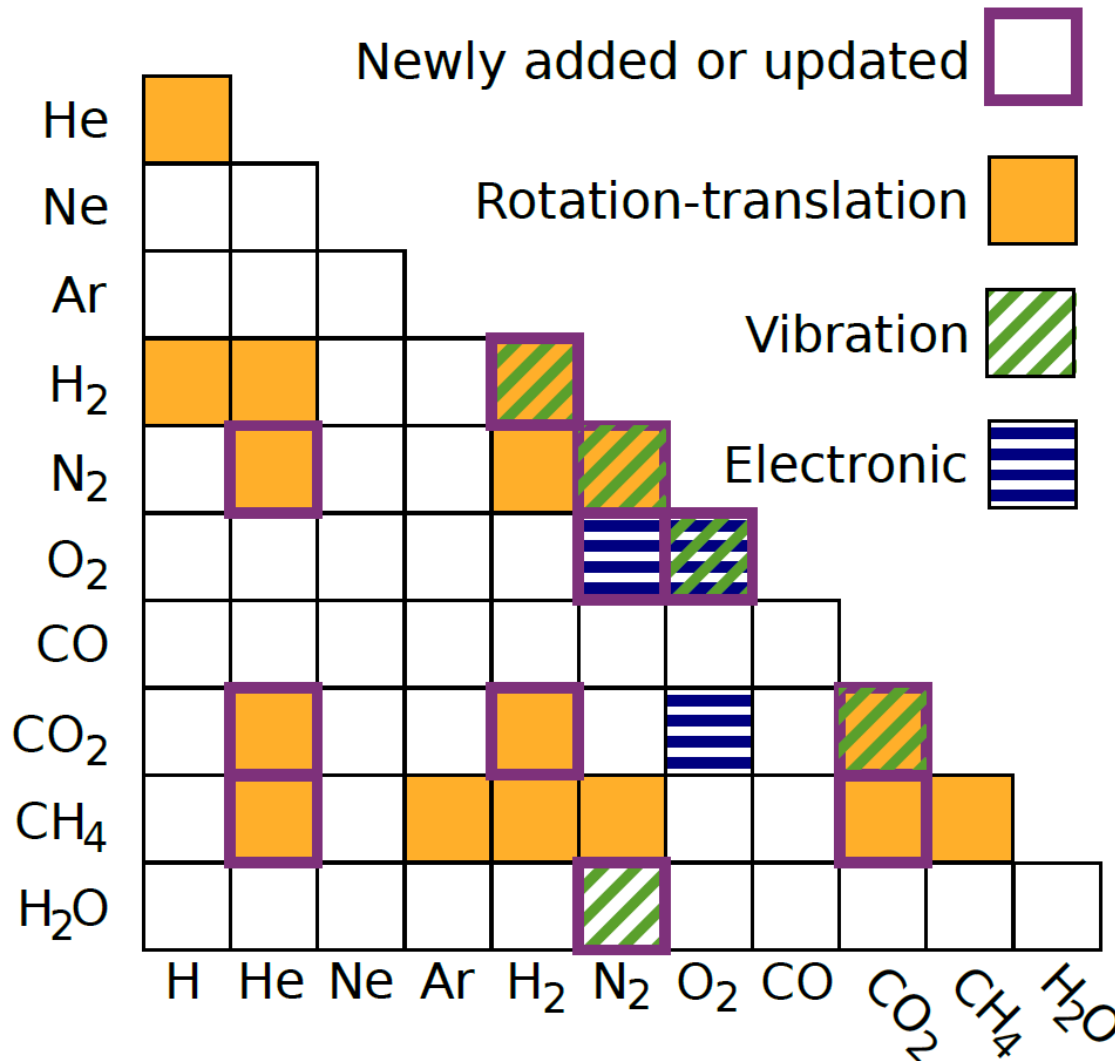
○ Continuum (primarily from

○ HITRAN (the HITRAN

○ Continuum free open

○ Aerosol Properties

○ Collision-Induced Absorption (CIA)



Species	
C ₄ H ₂ (1)	
HC ₃ N (1)	
H ₂ (2)	
CS (4)	
SO ₃ (1)	
C ₂ N ₂ (1)	
COCl ₂ (2)	

cross sections!)

[1] S. Sharpe, et al., (2004), *App. Spectrosc.* 58, 1452.
 [2] Ø. Hodnebrog, et al. (2013), *Rev. Geophys.* 51, 300.
 [3] R. V. Kochanov, et al. (2016), *JQSRT* 177, 15.

Accessing HITRANonline

Credit: Y. Tan

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The HITRAN Database

HITRAN is an acronym for the HITRAN database. HITRAN is a collection of computer codes used to calculate the transmission and emission of light in the atmosphere.

Data Access

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

News

- Registration is open for the upcoming HITRAN/ASA conference, June 13-15th, 2018. Abstract deadline is May 4, 2018.
- 9000 users milestone
- The data on this website corresponds to the HITRAN2016 edition
- Articles describing HITRANonline, HAPI, and new line-shape representations
- All inquiries can be made to HITRAN's support team at info@hitran.org

Database Updates

- Minor corrections to the CO₂ line list

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Line-by-Line Search

1. Select Molecules

Select individual molecules below or [Select all](#) [Select first 7](#) then: [2. Select Isotopologues >](#)

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		304225	8.400×10^{-5}	25710.825	1.055×10^{-39}	2.662×10^{-18}	
<input type="checkbox"/> 2	CO ₂	Carbon Dioxide		559874	0.757	14075.298	5.937×10^{-36}	3.542×10^{-18}	
<input type="checkbox"/> 3	O ₃	Ozone		449570	0.026	6996.681	1.498×10^{-31}	4.059×10^{-20}	
<input type="checkbox"/> 4	N ₂ O	Nitrous Oxide		160287	0.791	10363.675	1.000×10^{-29}	1.004×10^{-18}	
<input type="checkbox"/> 5	CO	Carbon Monoxide		5381	3.402	14477.377	1.013×10^{-45}	4.556×10^{-19}	
<input checked="" type="checkbox"/> 6	CH ₄	Methane		450332	0.001	11501.872	1.052×10^{-37}	2.114×10^{-19}	
<input type="checkbox"/> 7	O ₂	Molecular Oxygen		14085	6.440×10^{-7}	17272.060	1.960×10^{-54}	8.797×10^{-24}	
<input type="checkbox"/> 8	NO	Nitric Oxide		105079	1.000×10^{-6}	9273.214	1.451×10^{-95}	2.322×10^{-20}	
<input checked="" 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"/> 11	NH ₃	Ammonia		67148	0.058	10348.719	2.115×10^{-39}	5.493×10^{-19}	
<input type="checkbox"/> 12	HNO ₃	Nitric Acid		1008972	0.007	1769.982	3.246×10^{-29}	3.198×10^{-20}	
<input type="checkbox"/> 13	OH	Hydroxyl Radical		33058	0.003	35874.955	8.504×10^{-84}	6.449×10^{-17}	
<input checked="" type="checkbox"/> 14	HF	Hydrogen Fluoride		20010	13.620	32351.592	1.009×10^{-99}	1.460×10^{-17}	
<input type="checkbox"/> 15	HCl	Hydrogen Chloride		53252	5.342	20231.245	1.003×10^{-99}	5.038×10^{-19}	
<input type="checkbox"/> 16	HBr	Hydrogen Bromide		8980	7.656	16033.492	3.148×10^{-71}	1.214×10^{-19}	
<input type="checkbox"/> 17	HI	Hydrogen Iodide		4751	5.888	13907.689	9.342×10^{-64}	3.420×10^{-20}	
<input type="checkbox"/> 18	ClO	Chlorine Monoxide		11501	0.015	1207.639	5.944×10^{-30}	3.196×10^{-21}	
<input type="checkbox"/> 19	OCS	Carbonyl Sulfide		33030	0.396	7821.109	3.000×10^{-28}	1.248×10^{-18}	
<input type="checkbox"/> 20	H ₂ CO	Formaldehyde		44601	1.000×10^{-6}	3099.958	4.441×10^{-39}	7.436×10^{-20}	
<input type="checkbox"/> 21	HOCl	Hypochlorous Acid		16276	1.081	3799.682	1.720×10^{-24}	3.360×10^{-20}	

C. Hill, et al., *JQSRT* 177, 4 (2016).

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Line-by-Line Search

1. Select Molecules

Select individual molecules by:

ID	Formula	Name
<input type="checkbox"/> 1	H ₂ O	Water
<input type="checkbox"/> 2	CO ₂	Carbon Dioxide
<input type="checkbox"/> 3	O ₃	Ozone
<input type="checkbox"/> 4	N ₂ O	Nitrous Oxide
<input type="checkbox"/> 5	CO	Carbon Monoxide
<input checked="" type="checkbox"/> 6	CH ₄	Methane
<input type="checkbox"/> 7	O ₂	Molecular Oxygen
<input type="checkbox"/> 8	NO	Nitric Oxide
<input checked="" type="checkbox"/> 9	SO ₂	Sulfur Dioxide
<input type="checkbox"/> 10	NO ₂	Nitrogen Dioxide
<input type="checkbox"/> 11	NH ₃	Ammonia
<input type="checkbox"/> 12	HNO ₃	Nitric Acid
<input type="checkbox"/> 13	OH	Hydroxyl Radical
<input checked="" type="checkbox"/> 14	HF	Hydrogen Fluoride
<input type="checkbox"/> 15	HCl	Hydrogen Chloride
<input type="checkbox"/> 16	HBr	Hydrogen Bromide
<input type="checkbox"/> 17	HI	Hydrogen Iodide
<input type="checkbox"/> 18	ClO	Chlorine Monoxide
<input type="checkbox"/> 19	OCS	Carbonyl Sulfide
<input type="checkbox"/> 20	H ₂ CO	Formaldehyde
<input type="checkbox"/> 21	HOCl	Hypochlorous Acid

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Line-by-Line Search

2. Select Isotopologues

Select isotopologues for the following molecules then [3. Select wavenumber / wavelength range >](#)

Select one isotopologue only to search by vibrational band.

CH₄ [Select all](#)

ID	Formula	AFGL Code	Abundance	Line count	$\nu_{\min} / \text{cm}^{-1}$	$\nu_{\max} / \text{cm}^{-1}$	$S_{\min} / \text{cm}^{-1} / (\text{molec} \cdot \text{cm}^{-2})$	$S_{\max} / \text{cm}^{-1} / (\text{molec} \cdot \text{cm}^{-2})$
<input checked="" type="checkbox"/> 1	¹² CH ₄	211	0.988274	313943	0.001	11501.872	1.052×10^{-37}	2.114×10^{-19}
<input checked="" type="checkbox"/> 2	¹³ CH ₄	311	0.011103	77626	0.032	11318.537	4.100×10^{-34}	2.363×10^{-21}
<input type="checkbox"/> 3	¹² CH ₃ D	212	6.157510×10^{-4}	54550	7.760	6510.324	3.528×10^{-30}	5.714×10^{-23}
<input type="checkbox"/> 4	¹³ CH ₃ D	312	6.917850×10^{-6}	4213	959.394	1694.123	2.768×10^{-29}	1.398×10^{-25}

SO₂ [Select all](#)

ID	Formula	AFGL Code	Abundance	Line count	$\nu_{\min} / \text{cm}^{-1}$	$\nu_{\max} / \text{cm}^{-1}$	$S_{\min} / \text{cm}^{-1} / (\text{molec} \cdot \text{cm}^{-2})$	$S_{\max} / \text{cm}^{-1} / (\text{molec} \cdot \text{cm}^{-2})$
<input checked="" type="checkbox"/> 1	³² S ¹⁶ O ₂	626	0.945678	72460	0.017	4092.948	3.101×10^{-30}	4.851×10^{-20}
<input type="checkbox"/> 2	³⁴ S ¹⁶ O ₂	646	0.041950	22661	0.103	2500.400	4.191×10^{-30}	2.100×10^{-21}

HF [Select all](#)

ID	Formula	AFGL Code	Abundance	Line count	$\nu_{\min} / \text{cm}^{-1}$	$\nu_{\max} / \text{cm}^{-1}$	$S_{\min} / \text{cm}^{-1} / (\text{molec} \cdot \text{cm}^{-2})$	$S_{\max} / \text{cm}^{-1} / (\text{molec} \cdot \text{cm}^{-2})$
<input checked="" type="checkbox"/> 1	H ¹⁹ F	19	0.999844	8090	24.129	32351.592	1.009×10^{-99}	1.460×10^{-17}
<input type="checkbox"/> 2	D ¹⁹ F	29	1.557410×10^{-4}	11920	13.620	20829.169	1.018×10^{-99}	8.601×10^{-22}

C. Hill, et al., *JQSRT* 177, 4 (2016).

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Credit: I. Gordon

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Line-by-Line Search

1. Select Molecules

Select individual molecules for the following search:

ID	Formula	Name
<input type="checkbox"/> 1	H ₂ O	Water
<input type="checkbox"/> 2	CO ₂	Carbon Dioxide
<input type="checkbox"/> 3	O ₃	Ozone
<input type="checkbox"/> 4	N ₂ O	Nitrous Oxide
<input type="checkbox"/> 5	CO	Carbon Monoxide
<input checked="" type="checkbox"/> 6	CH ₄	Methane
<input type="checkbox"/> 7	O ₂	Molecular Oxygen
<input type="checkbox"/> 8	NO	Nitric Oxide
<input checked="" type="checkbox"/> 9	SO ₂	Sulfur Dioxide
<input type="checkbox"/> 10	NO ₂	Nitrogen Dioxide
<input type="checkbox"/> 11	NH ₃	Ammonia
<input type="checkbox"/> 12	HNO ₃	Nitric Acid
<input type="checkbox"/> 13	OH	Hydroxyl Radical
<input checked="" type="checkbox"/> 14	HF	Hydrogen Fluoride
<input type="checkbox"/> 15	HCl	Hydrogen Chloride
<input type="checkbox"/> 16	HBr	Hydrogen Bromide
<input type="checkbox"/> 17	HI	Hydrogen Iodide
<input type="checkbox"/> 18	ClO	Chlorine Monoxide
<input type="checkbox"/> 19	OCS	Carbonyl Sulfide
<input type="checkbox"/> 20	H ₂ CO	Formaldehyde
<input type="checkbox"/> 21	HOCl	Hypochlorous Acid

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Line-by-Line Search

2. Select Isotopologues

Select isotopologues for the following search:

Select one isotopologue only

CH₄ [Select all](#)

ID	Formula	AFGL Code	Abundance
<input checked="" type="checkbox"/> 1	¹² CH ₄	211	0.9883
<input checked="" type="checkbox"/> 2	¹³ CH ₄	311	0.0111
<input type="checkbox"/> 3	¹² CH ₃ D	212	6.11e-05
<input type="checkbox"/> 4	¹³ CH ₃ D	312	6.91e-05

SO₂ [Select all](#)

ID	Formula	AFGL Code	Abundance
<input checked="" type="checkbox"/> 1	³² S ¹⁶ O ₂	626	0.9457
<input type="checkbox"/> 2	³⁴ S ¹⁶ O ₂	646	0.0043




HF [Select all](#)

ID	Formula	AFGL Code	Abundance
<input checked="" type="checkbox"/> 1	H ¹⁹ F	19	0.9998
<input type="checkbox"/> 2	D ¹⁹ F	29	1.56e-05

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Line-by-Line Search   

3. Select Wavenumber / Wavelength Range

Select wavenumber range below (leave blank to select all lines for the selected isotopologues) then:

4. Select output options >

v_{min}: cm⁻¹
v_{max}: cm⁻¹ (leave blank for no upper limit)

Selected isotopologues are:

CH₄

ID	Formula	AFGL Code	Abundance	v _{min} /cm ⁻¹	v _{max} /cm ⁻¹
1	¹² CH ₄	211	0.9883	0.001	11501.872
2	¹³ CH ₄	311	0.0111	0.032	11318.537

SO₂

ID	Formula	AFGL Code	Abundance	v _{min} /cm ⁻¹	v _{max} /cm ⁻¹
1	³² S ¹⁶ O ₂	626	0.9457	0.017	4092.948

HF

ID	Formula	AFGL Code	Abundance	v _{min} /cm ⁻¹	v _{max} /cm ⁻¹
1	H ¹⁹ F	19	0.9998	24.129	32351.592

C. Hill, et al., *JQSRT* 177, 4 (2016).

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Line-by-Line Search

1. Select Molecules

Select individual molecules to search:

ID	Formula	Name
<input type="checkbox"/> 1	H ₂ O	Water
<input type="checkbox"/> 2	CO ₂	Carbon Dioxide
<input type="checkbox"/> 3	O ₃	Ozone
<input type="checkbox"/> 4	N ₂ O	Nitrous Oxide
<input type="checkbox"/> 5	CO	Carbon Monoxide
<input checked="" type="checkbox"/> 6	CH ₄	Methane
<input type="checkbox"/> 7	O ₂	Molecular Oxygen
<input type="checkbox"/> 8	NO	Nitric Oxide
<input checked="" type="checkbox"/> 9	SO ₂	Sulfur Dioxide
<input type="checkbox"/> 10	NO ₂	Nitrogen Dioxide
<input type="checkbox"/> 11	NH ₃	Ammonia
<input type="checkbox"/> 12	HNO ₃	Nitric Acid
<input type="checkbox"/> 13	OH	Hydroxyl Radical
<input checked="" type="checkbox"/> 14	HF	Hydrogen Fluoride
<input type="checkbox"/> 15	HCl	Hydrogen Chloride
<input type="checkbox"/> 16	HBr	Hydrogen Bromide
<input type="checkbox"/> 17	HI	Hydrogen Iodide
<input type="checkbox"/> 18	ClO	Chlorine Monoxide
<input type="checkbox"/> 19	OCS	Carbonyl Sulfide
<input type="checkbox"/> 20	H ₂ CO	Formaldehyde
<input type="checkbox"/> 21	HOCl	Hypochlorous Acid

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Line-by-Line Search

2. Select Isotopologues

Select isotopologues for the molecule:

Select one isotopologue only

CH₄ Select all

ID	Formula	AFGL Code	Abundance
<input checked="" type="checkbox"/> 1	¹² CH ₄	211	0.9998
<input checked="" type="checkbox"/> 2	¹³ CH ₄	311	0.0001
<input type="checkbox"/> 3	¹² CH ₃ D	212	6.11e-05
<input type="checkbox"/> 4	¹³ CH ₃ D	312	6.91e-06

SO₂ Select all

ID	Formula	AFGL Code	Abundance
<input checked="" type="checkbox"/> 1	³² S ¹⁶ O ₂	626	0.994
<input type="checkbox"/> 2	³⁴ S ¹⁶ O ₂	646	0.004

HF Select all

ID	Formula	AFGL Code	Abundance
<input checked="" type="checkbox"/> 1	H ¹⁹ F	19	0.9998
<input type="checkbox"/> 2	D ¹⁹ F	29	1.56e-05

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Line-by-Line Search

3. Select Wavenumber

Select wavenumber range below:

V_{min}: 2500 cm⁻¹
V_{max}: 2600 cm⁻¹

4. Select output options

Selected isotopologues are:

CH₄

ID	Formula	AFGL
1	¹² CH ₄	211
2	¹³ CH ₄	311

SO₂

ID	Formula	AFGL
1	³² S ¹⁶ O ₂	626

HF

ID	Formula	AFGL
1	H ¹⁹ F	19

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Line-by-Line Search

4. Select or Create Output Format

Select an output format or create a new one, then [5. Start Data Search >](#)

Available Output Formats

.par (160 chars)

Planetary_Extras

[Create New Output Format](#)

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	Fortran Format	Err	Ref
1 Molecule ID		I2		
1 Isotopologue ID		I1		
1 ν	cm ⁻¹	F12.6	✓	✓
1 S	cm ⁻¹ /(molec·cm ⁻²)	E10.3	✓	✓
1 A	s ⁻¹	E10.3		
1 ν _{air}	cm ⁻¹ ·atm ⁻¹	F5.4	✓	✓
1 ν _{self}	cm ⁻¹ ·atm ⁻¹	F5.3	✓	✓
1 E''	cm ⁻¹	F10.4		
1 n _{air}		F4.2	✓	✓
1 δ _{air}	cm ⁻¹ ·atm ⁻¹	F8.6	✓	✓
1 Global upper quanta		A15		
1 Global lower quanta		A15		
1 Local upper quanta		A15		
1 Local lower quanta		A15		
1 Error indices		6I1		
1 References		6I2		
1 Line mixing flag		A1		
1 g'		F7.1		
1 g''		F7.1		

C. Hill, et al., JQSRT
177, 4 (2016).

Accessing HITRANonline

Credit: I. Gordon

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Line-by-Line Search

New Output Format

Edit this output format by clicking on the + and x icons (or double-clicking the parameter rows). Reorder them by dragging rows within the selected parameters table.

Save and Return to Data Search Cancel

Output Format Name:

Description:

Example for a selection of additional parameters of relevance to planetary atmospheres. This example includes H2, He and CO2 broadening (and shifts), as well as alternative lineshape parameters for Hartmann-Tran profiles.

Field separator: ☒ Fixed width format **i**

Line endings: ☐ Output header line

☐ HDF5 output

New Output Format

Parameter	Units	Fortran Format	Err	Ref
x i Molecule ID		I2		
x i Isotopologue ID		I1		
x i ν	cm ⁻¹	F12.6	O	O
x i S	cm ⁻¹ /(molec·cm ⁻²)	E10.3	O	O
x i γ_{H2}	cm ⁻¹ ·atm ⁻¹	F6.4	O	O
x i η_{H2}		F7.4	O	O
x i δ_{H2}	cm ⁻¹ ·atm ⁻¹	F9.6	O	O
x i γ_{He}	cm ⁻¹ ·atm ⁻¹	F6.4	O	O
x i δ_{He}	cm ⁻¹ ·atm ⁻¹	F9.6	O	O
x i γ_{CO2}	cm ⁻¹ ·atm ⁻¹	F6.4	O	O
x i η_{CO2}		F7.4	O	O
x i $\delta_{HT_0_self}(296)$	cm ⁻¹ ·atm ⁻¹	F9.6	O	O
x i $\delta'_{HT_0_self}(296)$	cm ⁻¹ ·atm ⁻¹ ·K ⁻¹	F9.6	O	O
x i $\gamma_{HT_0_self}(296)$	cm ⁻¹ ·atm ⁻¹	F6.4	O	O
x i $\eta_{HT_0_self}(296)$		F7.4	O	O
x i $\delta_{HT_2_self}(296)$	cm ⁻¹ ·atm ⁻¹	F9.6	O	O
x i $\gamma_{HT_2_self}(296)$	cm ⁻¹ ·atm ⁻¹	F6.4	O	O
x i η_{HT_self}		F7.4	O	O
x i γ_{HT_self}	cm ⁻¹ ·atm ⁻¹	F7.4	O	O
x i η_{HT_self}		F7.4	O	O

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Line-by-Line Search

1. Select Molecules

Select individual molecules to be included in the search

ID	Formula	Name
<input type="checkbox"/> 1	H ₂ O	Water
<input type="checkbox"/> 2	CO ₂	Carbon Dioxide
<input type="checkbox"/> 3	O ₃	Ozone
<input type="checkbox"/> 4	N ₂ O	Nitrous Oxide
<input type="checkbox"/> 5	CO	Carbon Monoxide
<input checked="" type="checkbox"/> 6	CH ₄	Methane
<input type="checkbox"/> 7	O ₂	Molecular Oxygen
<input type="checkbox"/> 8	NO	Nitric Oxide
<input checked="" type="checkbox"/> 9	SO ₂	Sulfur Dioxide
<input type="checkbox"/> 10	NO ₂	Nitrogen Dioxide
<input type="checkbox"/> 11	NH ₃	Ammonia
<input type="checkbox"/> 12	HNO ₃	Nitric Acid
<input type="checkbox"/> 13	OH	Hydroxyl Radical
<input checked="" type="checkbox"/> 14	HF	Hydrogen Fluoride
<input type="checkbox"/> 15	HCl	Hydrogen Chloride
<input type="checkbox"/> 16	HBr	Hydrogen Bromide
<input type="checkbox"/> 17	HI	Hydrogen Iodide
<input type="checkbox"/> 18	ClO	Chlorine Monoxide
<input type="checkbox"/> 19	OCS	Carbonyl Sulfide
<input type="checkbox"/> 20	H ₂ CO	Formaldehyde
<input type="checkbox"/> 21	HOCl	Hypochlorous Acid

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Line-by-Line Search

2. Select Isotopologues

Select isotopologues for the following molecule

Select one isotopologue only

CH₄ Select all

ID	Formula	AFGL Code	Abundance
<input checked="" type="checkbox"/> 1	¹² CH ₄	211	0.99985
<input checked="" type="checkbox"/> 2	¹³ CH ₄	311	0.00015
<input type="checkbox"/> 3	¹² CH ₃ D	212	6.11e-05
<input type="checkbox"/> 4	¹³ CH ₃ D	312	6.91e-06

SO₂ Select all

ID	Formula	AFGL Code	Abundance
<input checked="" type="checkbox"/> 1	³² S ¹⁶ O ₂	626	0.995
<input type="checkbox"/> 2	³⁴ S ¹⁶ O ₂	646	0.004

HF Select all

ID	Formula	AFGL Code	Abundance
<input checked="" type="checkbox"/> 1	H ¹⁹ F	19	0.99985
<input type="checkbox"/> 2	D ¹⁹ F	29	1.51e-05

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Line-by-Line Search

3. Select Wavenumber Range

Select wavenumber range below

4. Select output options

Select an output format or create a new one

Available Output Formats

.par (160 chars)

Planetary_Extras

Create New Output Format

V_{min}: 2500 cm⁻¹

V_{max}: 2600 cm⁻¹

Selected isotopologues are:

CH₄

ID	Formula	AFGL
1	¹² CH ₄	211
2	¹³ CH ₄	311

SO₂

ID	Formula	AFGL
1	³² S ¹⁶ O ₂	626

HF

ID	Formula	AFGL
1	H ¹⁹ F	19

HITRANonline

Home Data Access Documentation Conferences Links About

Line-by-Line Search

4. Select or Create Output Format

Select an output format or create a new one

Available Output Formats

.par (160 chars)

Planetary_Extras

Create New Output Format

V_{min}: 2500 cm⁻¹

V_{max}: 2600 cm⁻¹

Selected isotopologues are:

CH₄

ID	Formula	AFGL
1	¹² CH ₄	211
2	¹³ CH ₄	311

SO₂

ID	Formula	AFGL
1	³² S ¹⁶ O ₂	626

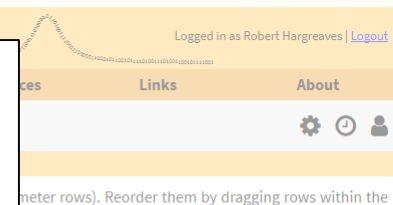
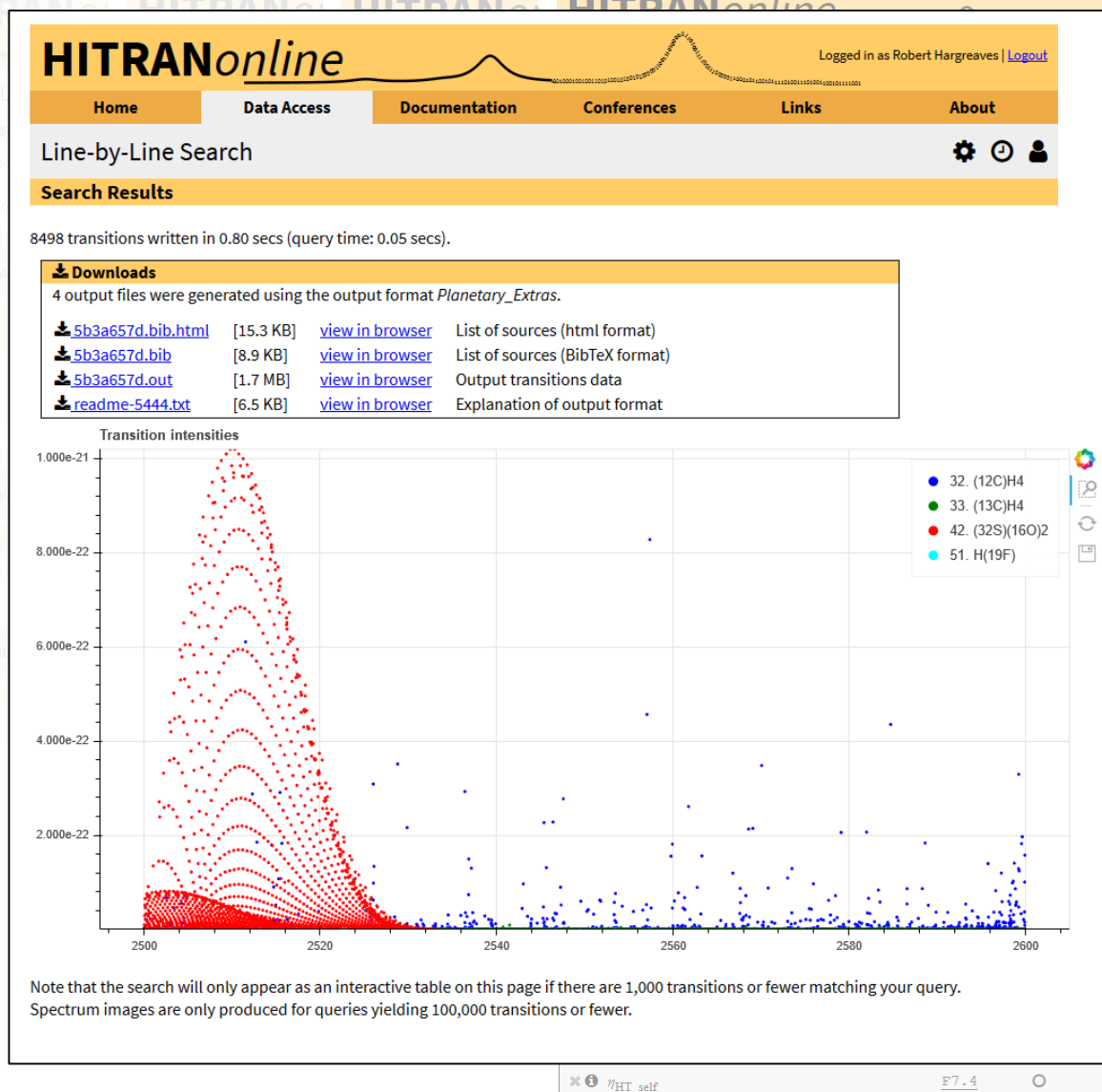
HF

ID	Formula	AFGL
1	H ¹⁹ F	19

C. Hill, et al., JQSRT
177, 4 (2016).

Accessing HITRANonline

Credit: I. Gordon



Available Parameters

Parameter
Global isotopologue ID
A
γ_{air}
γ_{self}
η_{air}
ϕ_{air}
E''
g'
g''
ϕ'_{air}

Grouped Parameters

Parameter Group
HT Profile Parameters

C. Hill, et al., *JQSRT*
177, 4 (2016).

Accessing HITRAN with HAPI

○ HAPI (the HITRAN Application Programming Interface) [1]

- A free open source Python module (library) which provides a set of tools for working with structured spectroscopic data from different sources.

```
# Import HAPI functions for downloading the data:
from hapi import *

# Fetch the CH4 data for the main isotopologue, in the 2500-2600 wavenumber range:
fetch('ch4', 6, 1, 2500, 2600)

# Select the lines with and intensity greater than 1.0x10e-21 cm/molecule:
select('ch4', DestinationTableName='ch4_strong', Conditions=('>', 'sw', 1e-21))

# Calculate absorption coefficient:
nu_coeff= abscoef('ch4_strong')

# Repeat the fetching for other molecules and isotopologues in previous example:
fetch('ch4', 6, 2, 2500, 2600)
fetch('so2', 9, 1, 2500, 2600)
fetch('hf', 14, 2, 2500, 2600)

# Print a list of unique IDs:
getHelp(ISO_ID)

# Fetch the CH4 data for the two strongest isotopologues, in the 2500-2600
# wavenumber range, including the additional broadening parameters:
fetch_by_ids('ch4', [32, 33], 2500, 2600, ParameterGroups=['160-char'], Parameters[
    'gamma_H2', 'delta_H2', 'gamma_He', 'delta_H2', 'gamma_CO2', 'delta_CO2', ... ])
```

Import HAPI library

Easy command to
download data

Tools for working with the
data

Embedded help
(and tutorials)

Many more options to
include additional
parameters, filtering etc.

Broadening, temperature dependence & pressure shifts in planetary atmospheres

Credit: I. Gordon

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 , SiH_4 , 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, ...

HITRAN contains **self-** and **air-** broadening parameters for all line-by-line molecules

Foreign broadening gas

Gas being broadened



Broadening, temperature dependence & pressure shifts in planetary atmospheres

- A consequence of dominant gases in planetary atmospheres
- **PART 1:** This work has recently expanded for H₂, He and CO₂

Molecule	Parameter	Perturbed by H ₂	Perturbed by He	Perturbed by CO ₂
SO ₂	γ	2	2	1
	n	1	1	0
	δ	0	0	0
NH ₃	γ	3	3	2-3
	n	2-3	1	0
	δ	2-3	2-3	2
HF	γ	1	1	1-2
	n	0	1	0
	δ	0	1	1
HCl	γ	1	1-2	1-2
	n	1	0	0
	δ	1	1-2	1-2
OCS	γ	1	1	1-2
	n	0	0	0
	δ	0	0	0
C ₂ H ₂	γ	3	3	1
	n	1	1	0
	δ	1	1-2	0-1

γ = Broadening coefficient (Lorentz)

n = Temperature dependence:

$$\gamma(T) = \gamma(T_{ref}) \cdot \left(\frac{T_{ref}}{T} \right)^n$$

δ = Pressure shifts

0 = No data available

1 = Few data available

2 = Some measurements available
allowing semi-empirical extrapolations

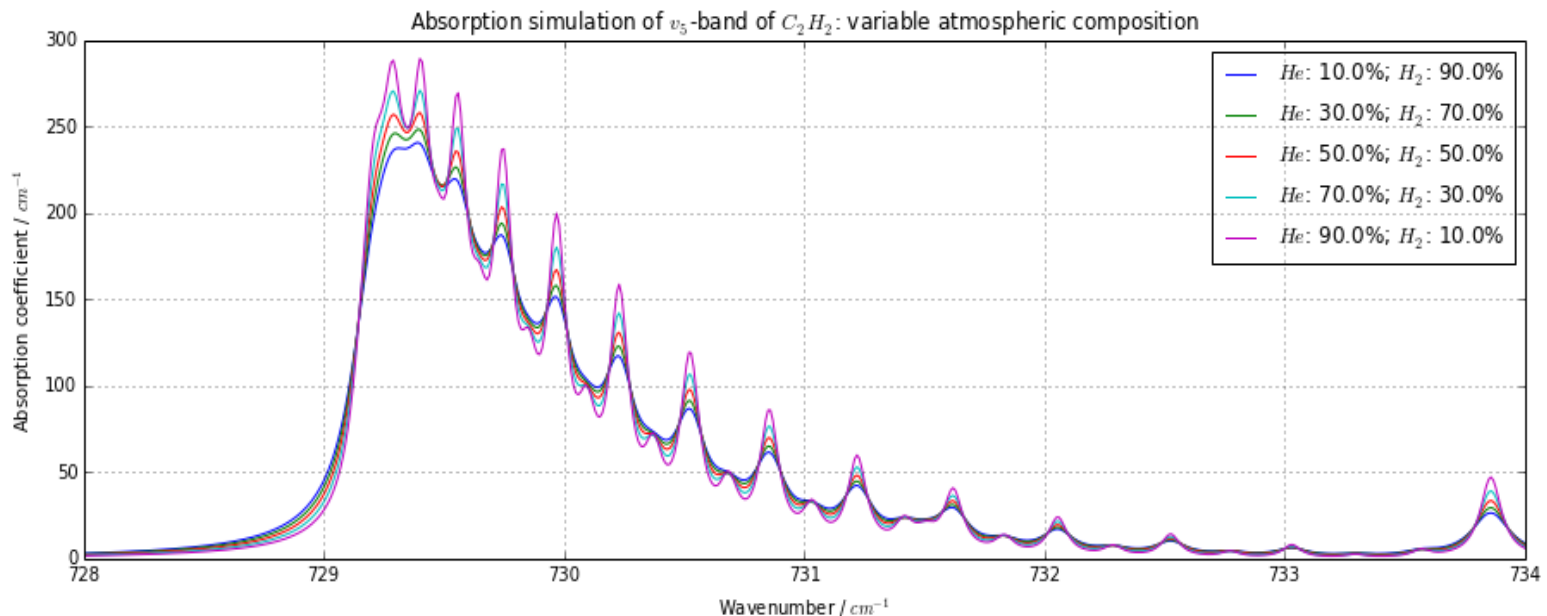
3 = Relatively complete set of
measurements and/or calculations
available at least at room temperature

Broadening calculations with HAPI

- Example of modelling the 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('$He$: %.1f%%; $H_2$: %.1f%%'%(He_frac*100,H2_frac*100))
title('Absorption simulation of  $\nu_5$  band of  $C_2H_2$ : variable atmospheric composition')
xlabel('Wavenumber /  $cm^{-1}$ '); ylabel('Absorption coefficient /  $cm^{-1}$ ')
xlim(728,734); grid(True); legend(leg)
```



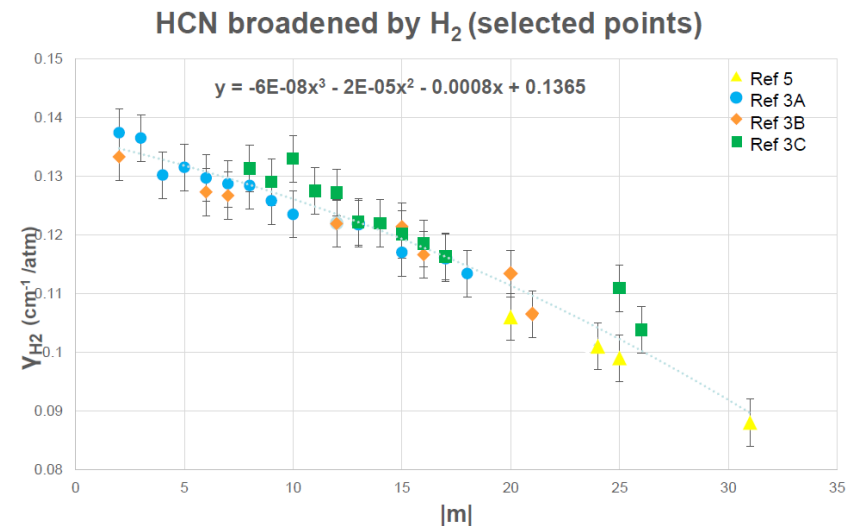
See: "H₂, He, and CO₂ line-broadening coefficients, pressure shifts and temperature-dependence exponents for the HITRAN database. Part 1: SO₂, NH₃, HF, HCl, OCS and C₂H₂"
J. S. Wilzewski, et al. (2016), *JQSRT* 168, 193.

Broadening, temperature dependence & pressure shifts in planetary atmospheres

Credit: S. Samuels

- PART 2:** This work has recently expanded for H₂, He and CO₂
 - Includes line broadening coefficients (γ), temperature dependence exponents (n) and pressure shifts (δ)
 - CO₂, N₂O, OH, H₂CO, HCN, H₂S

Molecule	Parameter	Perturbed by H ₂	Perturbed by He	Perturbed by CO ₂
HCN	γ	3	2	0
	n	1	1	0
	δ	1	1	0
CO ₂	γ	1	1	3
	n	1	1	3
	δ	0	1	3
N ₂ O	γ	0	1 or 2	1 or 2
	n	0	1	1
	δ	0	1 or 2	0
H ₂ CO	γ	2	2	0
	n	0	0	0
	δ	1	0	0
H ₂ S	γ	1	2	2
	n	0	0	0
	δ	0	0	0



0 = no data available
 1 = few data available
 2 = some measurements available allowing semi-empirical extrapolations
 3 = relatively complete set of measurements and/or calculations available at least at room temperature

- “H₂, He and CO₂ Line-Broadening Coefficients for Molecules in the HITRAN Database. Part II: CO₂, N₂O, H₂CO, HCN, H₂S, OH”

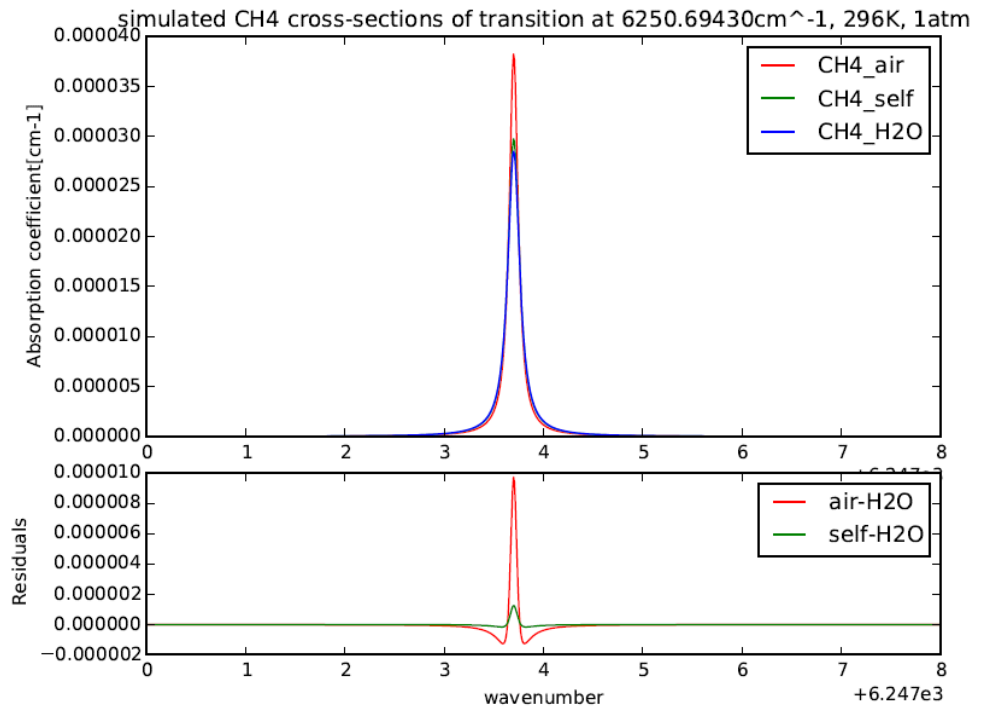
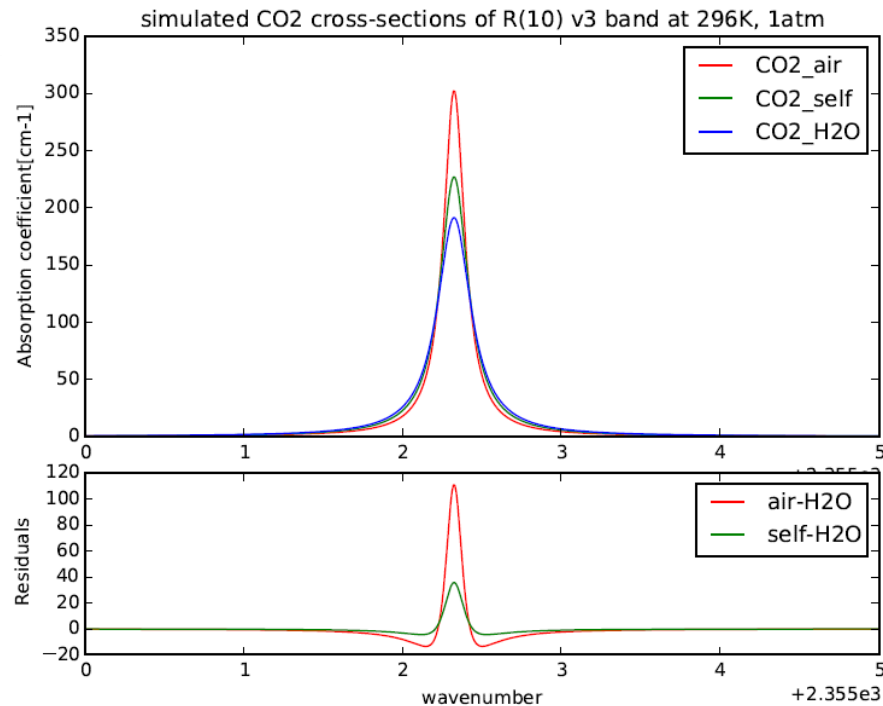
S. Samuels, Y. Tan, R. V. Kochanov, L. S. Rothman, I. E., Gordon, *in preparation*

What about water?

Credit: Y. Tan

- Water vapor is a very **efficient** broadening gas
 - Compared to N_2 and O_2
- For the Earth's lower atmosphere water vapor is **highly variable**
- Some rocky exoplanets have been predicted to have “**steamy**” atmospheres

Simulated effect of water broadening of CO_2 and CH_4



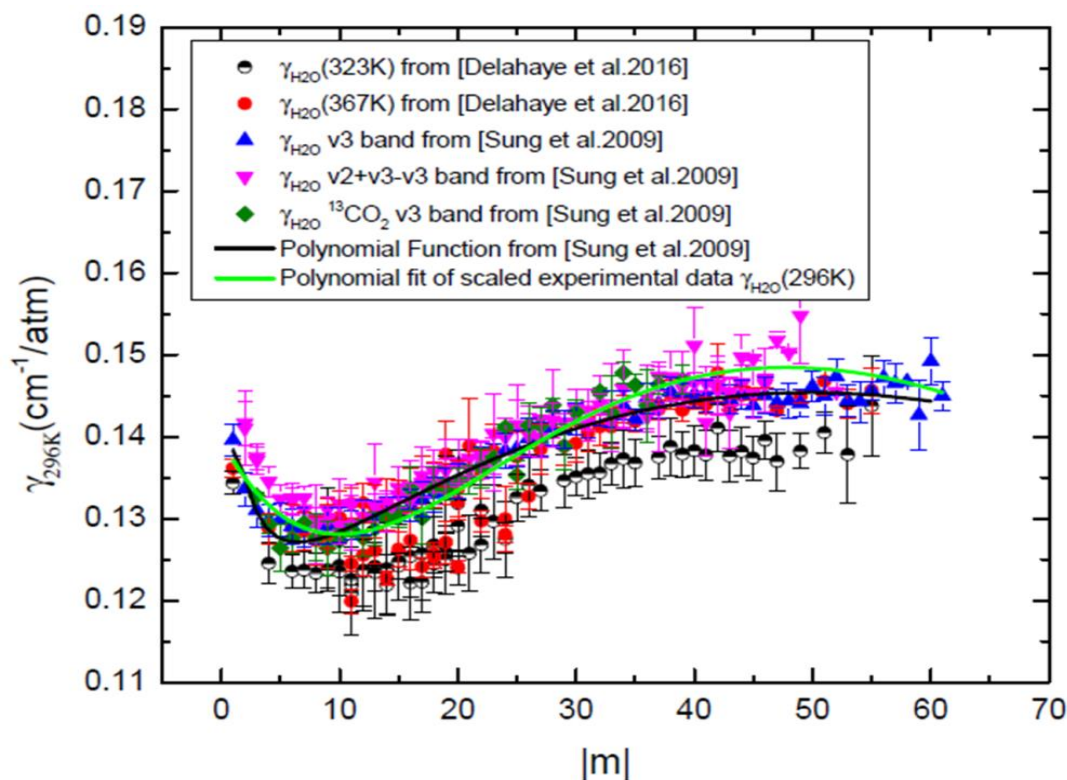
What about water?

Credit: Y. Tan

- H₂O broadening coefficients of CO₂, O₂, CH₄, CO, NH₃, N₂O and H₂S
- Example for CO₂:

Polynomial function in the quantum index m :

$$\gamma(m) = c_0 + c_1 \cdot m + c_2 \cdot m^2 + c_3 \cdot m^3 + c_4 \cdot m^4 + c_5 \cdot m^5$$



Molecule \ Parameter	γ	n
CO ₂	3	3
O ₂	3	2
CH ₄	1	0
CO	2	2
NH ₃	1	0
N ₂ O	1	0
H ₂ S	1	0

Data Availability in **Table**:

- **0** = No data available;
- **1** = Few data available, new HITRAN file contains mostly averages;
- **2** = Some measurements available, allowing semi-classical extrapolations;
- **3** = Relatively complete set of measurements or calculations available - at least for room temperature.

Current HITEMP

○ High-Temperature Molecular Spectroscopic Database

- 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. Rad. Transf.* **111**, 2139-2150 (2010)

HITRANonline

Home	Data Access	Documentation	Conferences	Links				
HITEMP	<ul style="list-style-type: none">Line-by-lineAbsorption Cross SectionsCollision Induced AbsorptionAerosol PropertiesHITEMPHAPISupplemental	<p>The HITEMP database is described in the article "HITEMP, the high-temperature molecular spectroscopic database" (2010)[1]. This replaces the earlier edition [2], "HITRAN, HAWKS and HITEMP High Temperature Molecular Spectroscopic Database" (1995).</p> <p>This database has been placed on the FTP server.</p> <p>Log in with anonymous and your email address as the password.</p> <p>To access the database directly by from the command line:</p> <pre>ftp user = anonymous password = e-mail address cd /pub/HITEMP-2010</pre> <p>In the directory /pub/HITEMP-2010 you will find five folders:</p> <table border="1"><thead><tr><th>Folder</th><th>Number of isotopologues</th><th>Total number of transitions</th><th>Spectral Coverage (cm⁻¹)</th></tr></thead></table>			Folder	Number of isotopologues	Total number of transitions	Spectral Coverage (cm ⁻¹)
Folder	Number of isotopologues	Total number of transitions	Spectral Coverage (cm ⁻¹)					

Current HITEMP

- Line-by-line data is at 296 K like HITRAN
- Currently only five molecules:

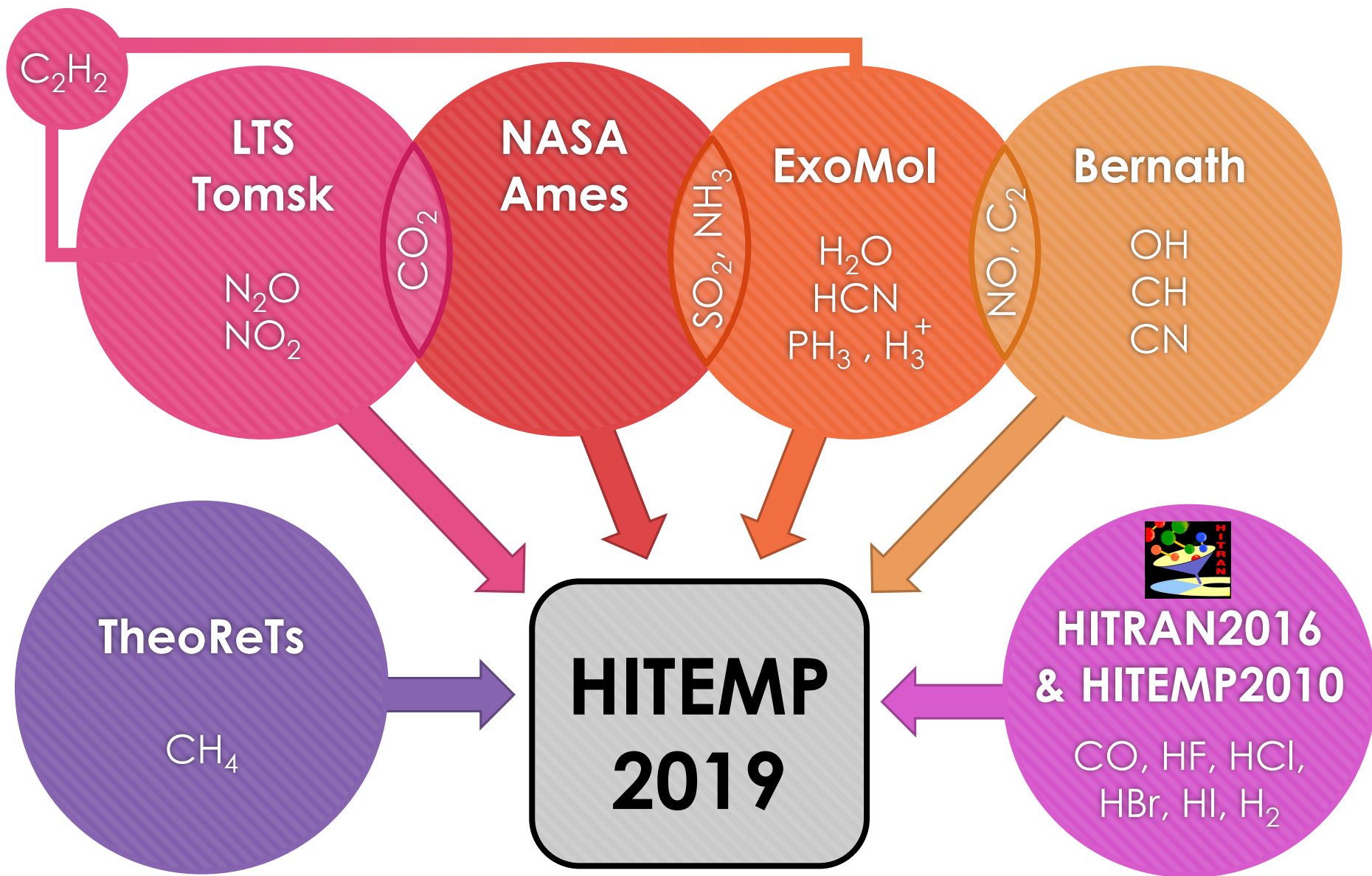
Molecule	Spectral Coverage (cm ⁻¹)	Number of Isotopologues	Number of Transitions
H ₂ O	0 – 30,000	6*	111,241,164
CO ₂	5 – 12,785	7	11,193,608
NO	0 – 9,274	3*	115,610
CO	0 – 8,465	6	113,631
OH	0 – 19,268	3*	41,557

*only principal isotopologue

- **HITRAN2016** data for HF, HCl, HBr, HI and H₂
 - Also suitable for 1000's of Kelvin
 - **TIPS** up to 9000 K for some molecules
- Line parameters in HITEMP will be consistent with HITRAN
 - Where possible



Proposed data for HITEMP

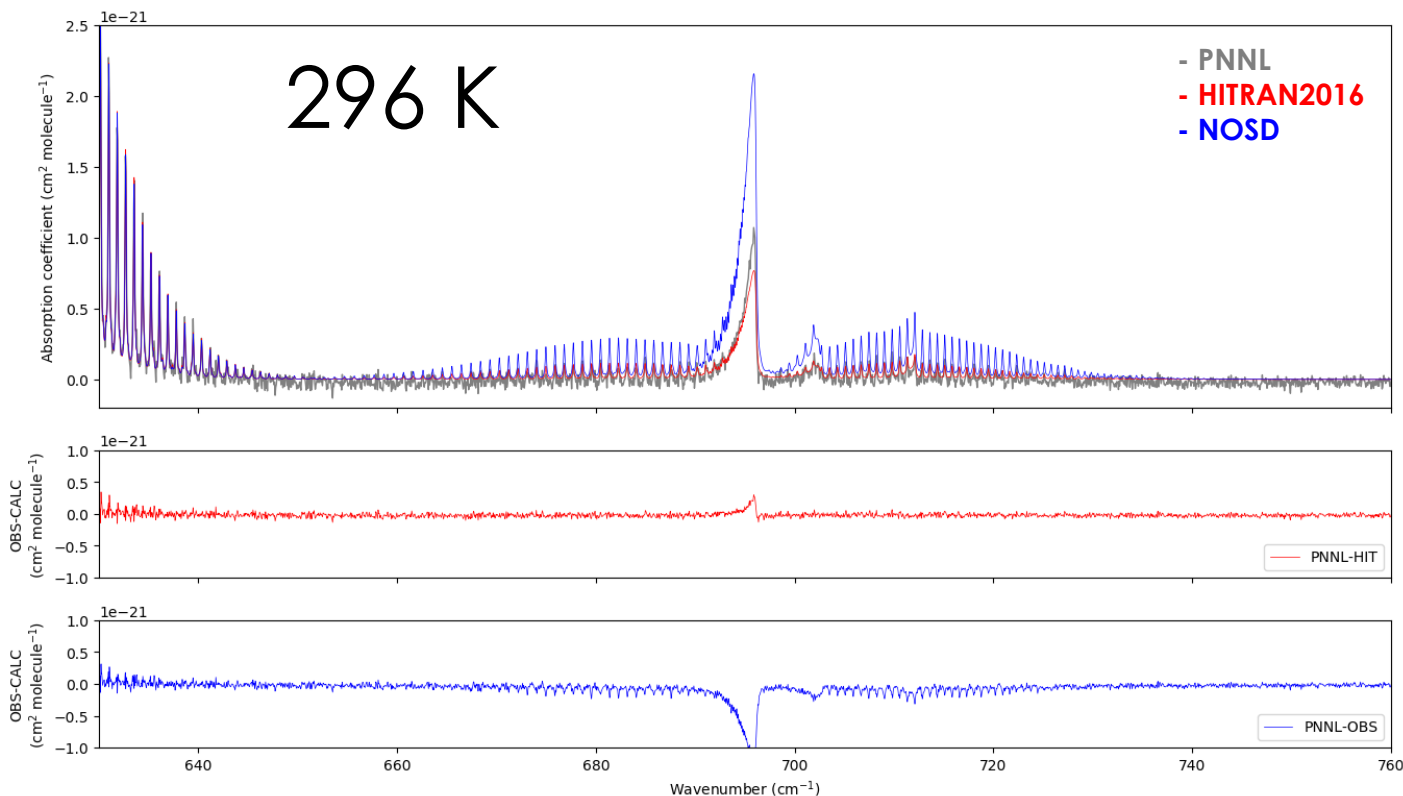


N₂O for HITEMP

- Available **NOSD-1000** from LTS Tomsk group:



N₂O comparisons to PNNL at 296K (1000-0110)



- Noticeable differences
 - PNNL
 - HITRAN2016
- Band intensity was corrected

N₂O for HITEMP

- Recalculated by S. A. Tashkun

- @ 296 K

- @ 500 K

- @ 1000 K

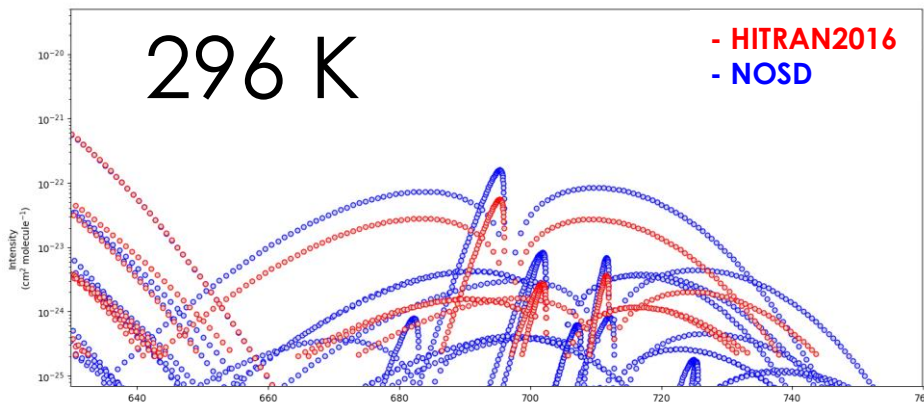
- Updated line list for HITEMP

- $>1.0 \times 10^{-26}$ cm molecule⁻¹

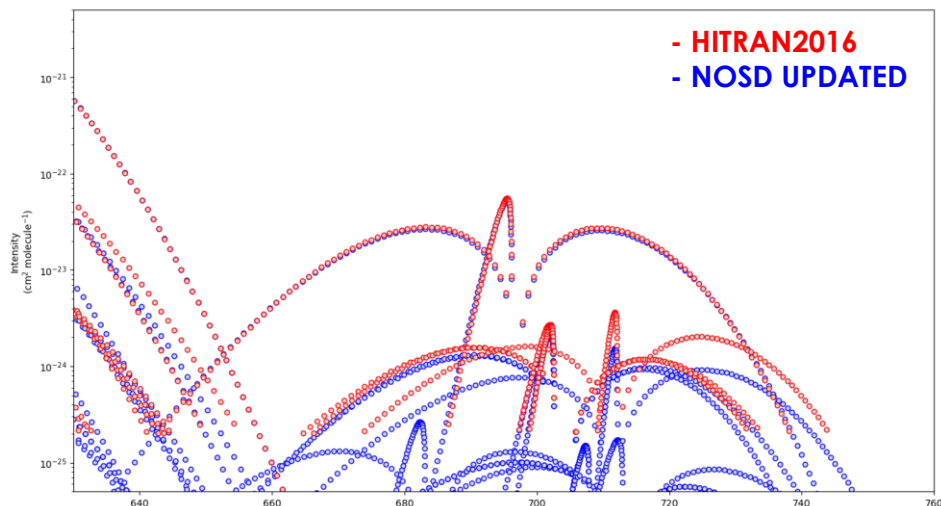
- At all temperatures

- HITRAN replacements

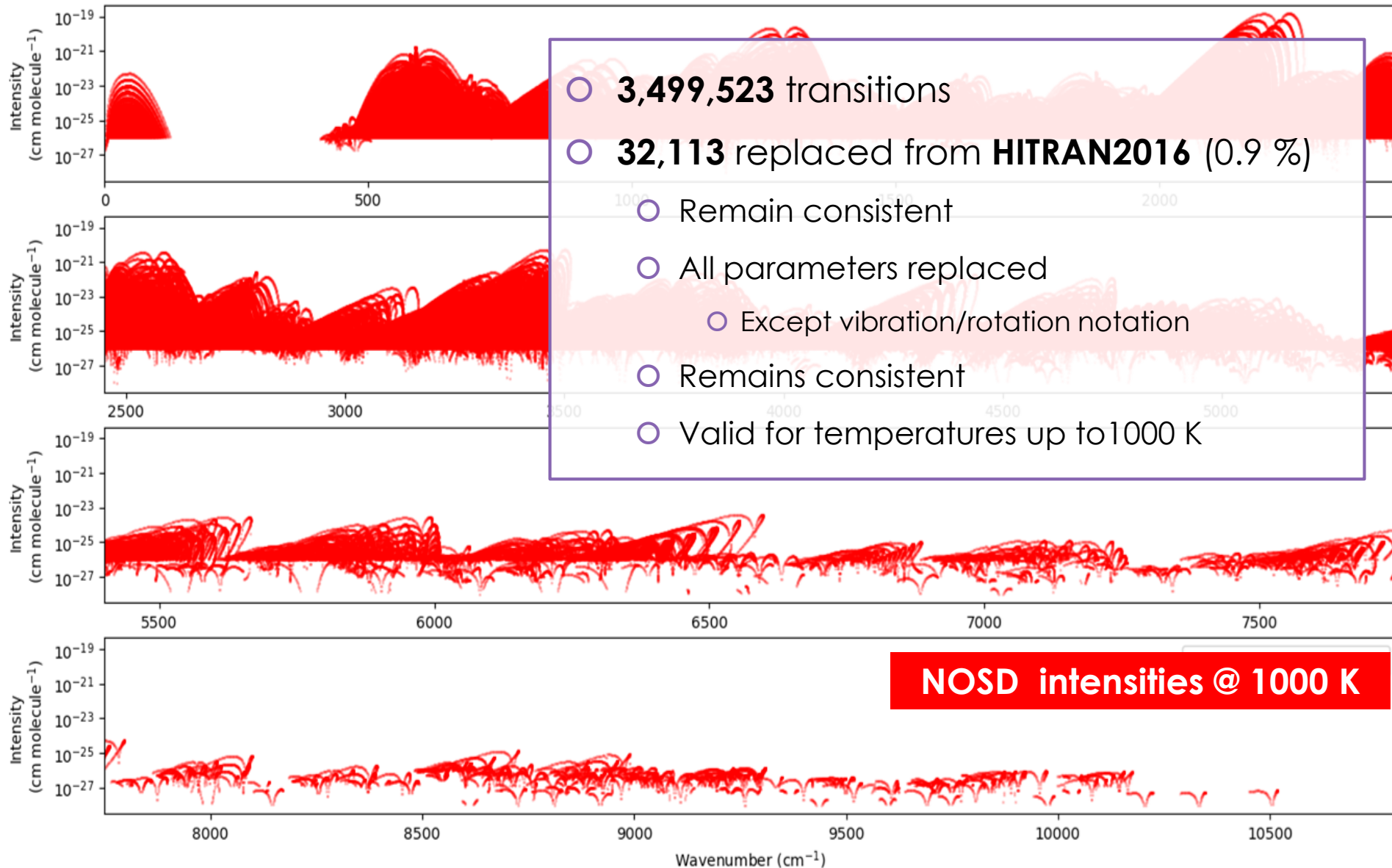
N₂O at 296K (1000-0110)



N₂O at 1000K (1000-0110)

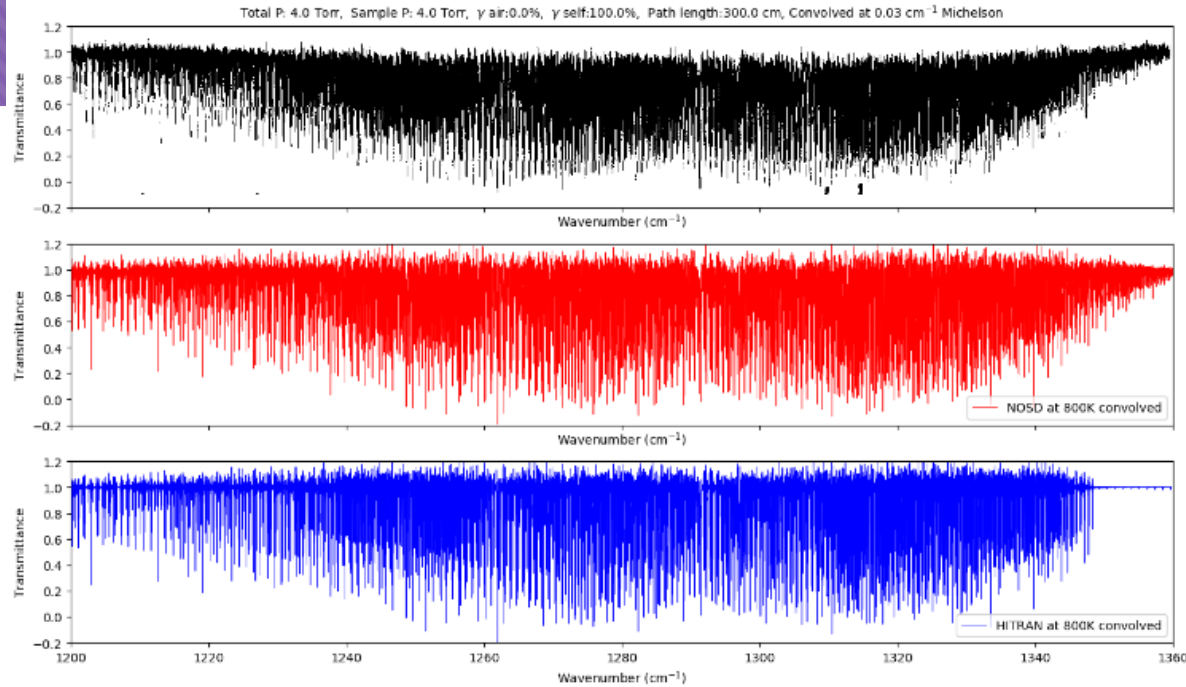


N₂O overview for HITEMP



800 K

N₂O at 800K against Esplin et al. (1988)

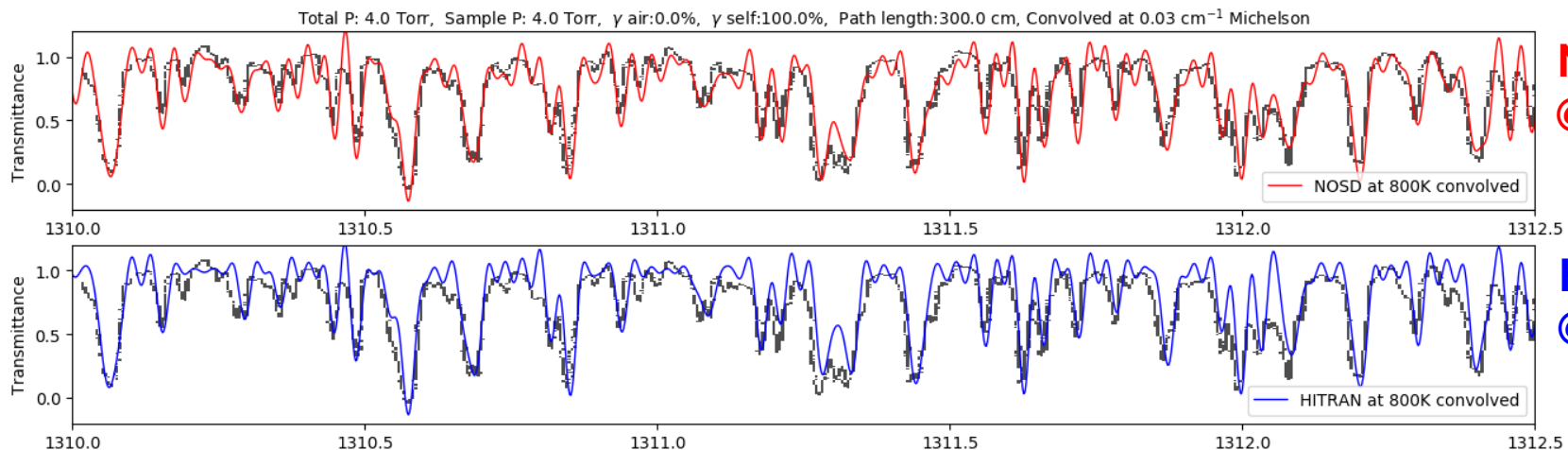


- High temperature comparison

- M. P. Esplin et al. *Mikrochim. Acta* 2, 403 (1988)

- Calculated using HAPI tools

- R. V. Kochanov et al. *JQSRT* 177, 15 (2016)



**NOSD
@ 800 K**

**HITRAN
@ 800 K**

Summary

○ HITRAN freely available online

- Line-by-line data and cross sections available (among other information)
- HAPI Python libraries to download
 - Easy to work with HITRAN data
- Broadening, temperature dependence and shifts parameters are being updated for **foreign broadeners relevant to planets/exoplanets**
 - Numerous molecules

○ Work towards the next HITEMP update **underway!**

- Expected... 2019
 - Some molecules easier to validate than others
- More high temperature measurements needed for validation
- Data will be relevant for hot exoplanets
- Further molecules will be added in secondary update



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Dr Yan Tan [Email](#)
Postdoctoral Fellow



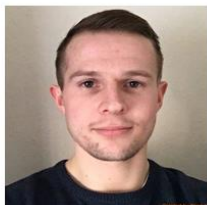
Shanelle Samuels
[Email](#)
Intern from U Mass Lowell



Dr Christian Hill [Email](#) | [www](#)
Visiting Scientist



Dr Geoffrey C. Toon
[Email](#)
Visiting Scientist



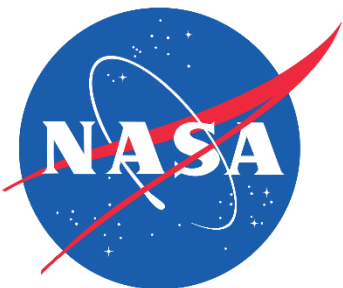
Eamon Conway [Email](#)
Predoctoral fellow

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