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HITRAN2020: Practicality, Accuracy, Completeness, Traceability (PACT)

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Roman Kochanov, Yan Tan, Christian Hill

and

HITRAN contributors and validators world wide

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The HITRAN Da

HITRAN is an acronym database. HITRAN is a of computer codes use of light in the atmosph



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mission molecular absorption copic parameters that a variety the transmission and emission



News

Sep 2022 | **25000 users milestone**

Oct 2021 | **The data on this website corresponds to the HITRAN2020 edition**

Apr 2021 | **History of HITRAN by Dr. Laurence S. Rothman**

Apr 2020 | **HITEMP now includes methane**

Jul 2015 | **All inquiries can be made to HITRAN's support team at info@hitran.org**

Database Updates

Aug 2022 | **Updated broadening parameters for CO₂ and H₂**

May 2022 | **H₂O line list update above 4340 cm⁻¹**

Nov 2021 | **Lines of ¹⁶O₃ in 850-980 cm⁻¹ region restored**

New quadrennial edition

Journal of Quantitative Spectroscopy & Radiative Transfer 277 (2022) 107949



Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

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



- Article describing the HITRAN2020 edition is in Open Access in JQSRT

The HITRAN2020 molecular spectroscopic database

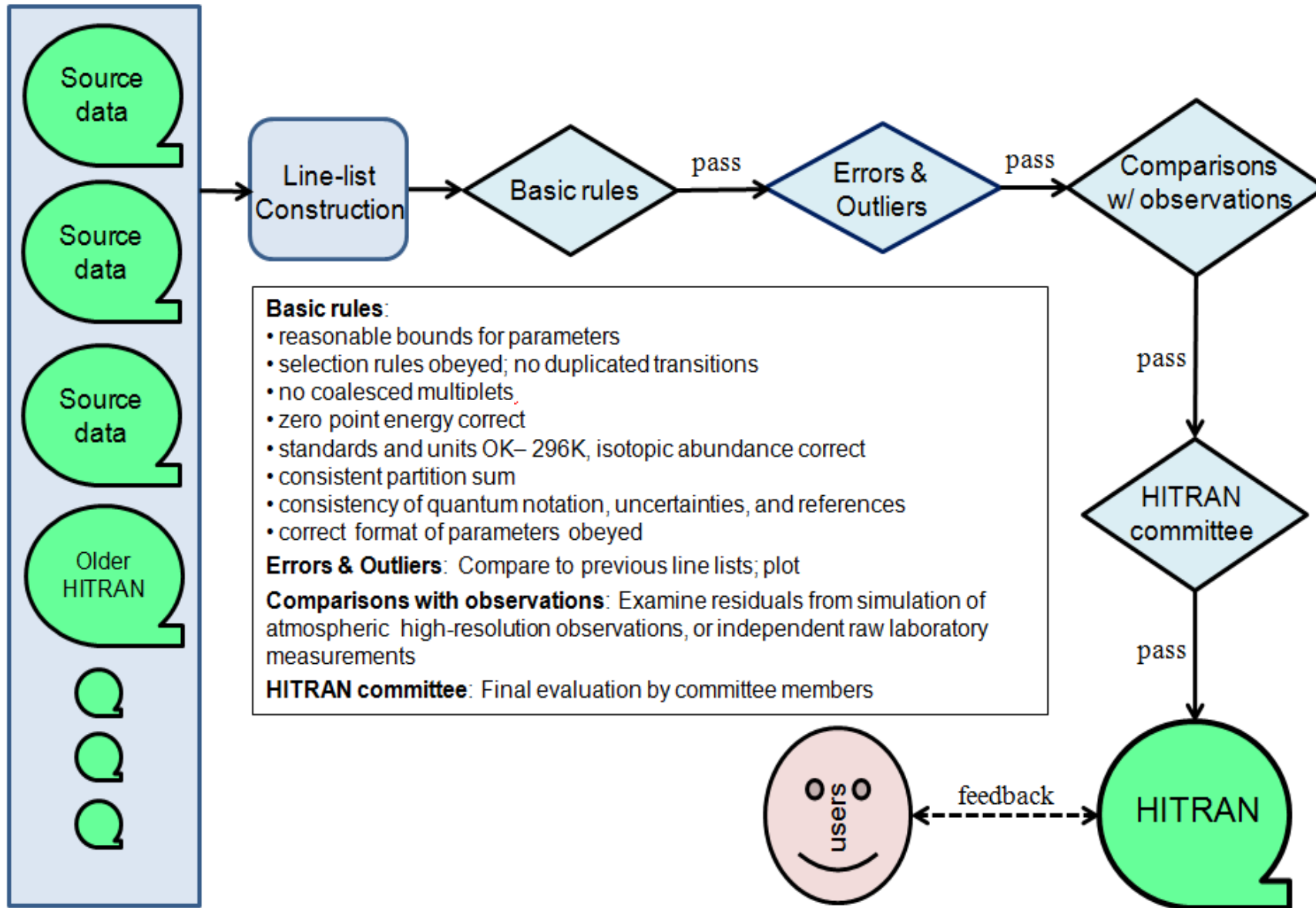
I.E. Gordon^{a,*}, L.S. Rothman^a, R.J. Hargreaves^a, R. Hashemi^a, E.V. Karlovets^a, F.M. Skinner^a, E.K. Conway^a, C. Hill^b, R.V. Kochanov^{a,c,d}, Y. Tan^{a,e}, P. Wcisło^f, A.A. Finenko^{a,g}, K. Nelson^a, P.F. Bernath^h, M. Birkⁱ, V. Boudon^j, A. Campargue^k, K.V. Chance^a, A. Coustenis^l, B.J. Drouin^m, J.-M. Flaud^s, R.R. Gamache^o, J.T. Hodges^p, D. Jacquemart^q, E.J. Mlawer^r, A.V. Nikitin^c, V.I. Perevalov^c, M. Rotger^t, J. Tennyson^u, G.C. Toon^m, H. Tran^l, V.G. Tyuterev^{t,d,c}, E.M. Adkins^p, A. Bakerⁿ, A. Barbe^t, E. Canè^w, A.G. Császár^{y,z}, A. Dudaryonok^c, O. Egorov^c, A.J. Fleisher^p, H. Fleurbaey^k, A. Foltynowicz^A, T. Furtenbacher^y, J.J. Harrison^{B,C,D}, J.-M. Hartmann^v, V.-M. Horneman^E, X. Huang^F, T. Karman^a, J. Karns^{a,W,X}, S. Kassi^k, I. Kleiner^M, V. Kofman^R, F. Kwabia-Tchana^M, N.N. Lavrentieva^c, T.J. Lee^G, D.A. Long^p, A.A. Lukashetskaya^c, O.M. Lyulin^c, V.Yu. Makhnev^N, W. Matt^{a,X}, S.T. Massie^H, M. Melosso^x, S.N. Mikhailenko^c, D. Mondelain^k, H.S.P. Müller^l, O.V. Naumenko^c, A. Perrin^L, O.L. Polyansky^{u,N}, E. Raddaoui^q, P.L. Raston^{J,K}, Z.D. Reed^p, M. Rey^t, C. Richard^j, R. Tóbiás^y, I. Sadiek^{A,O}, D.W. Schwenke^G, E. Starikova^c, K. Sung^m, F. Tamassia^w, S.A. Tashkun^c, J. Vander Auwera^p, I.A. Vasilenko^c, A.A. Viggasin^Q, G.L. Villanueva^R, B. Vispoel^{T,S,o}, G. Wagnerⁱ, A. Yachmenev^{U,V}, S.N. Yurchenko^u



Summary:

- 88 authors
- 82 pages
- 909 references

Scheme for Construction



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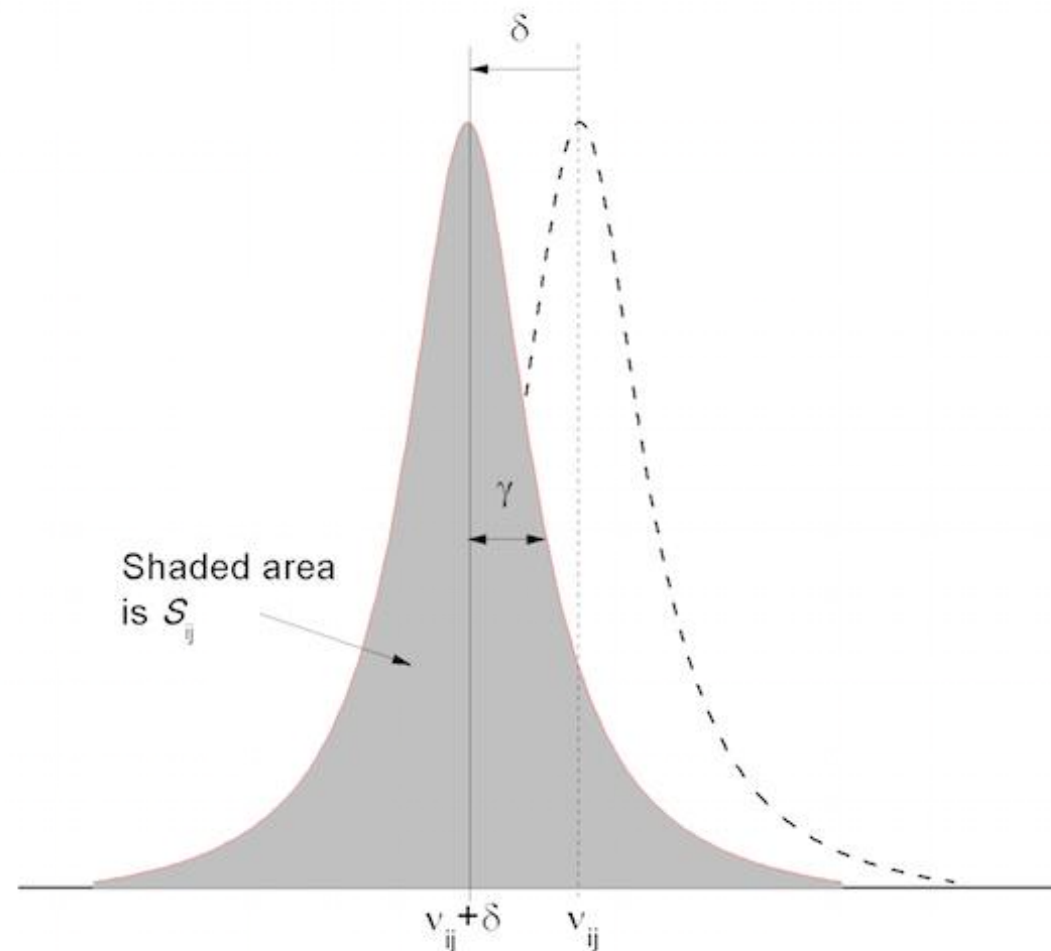
HITRAN is an acronym database. HITRAN is a of computer codes use of light in the atmosph



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Tutorials



HITRAN2020 line-by-line section (55 molecules)

Molecules (isotopologues) in the line-by-line portion of HITRAN

H₂O (7)	SO₂ (4)	HI (2)	H ₂ O ₂ (1)	HO ₂ (1)	CH ₃ CN (1)	COCl ₂ (2)
CO₂ (12)	NO₂ (2)	ClO (2)	C₂H₂ (3)	O (1)	CF ₄ (1)	SO (3)
O₃ (5)	NH₃ (2)	OCS (6)	C₂H₆ (3)	ClONO ₂ (2)	C ₄ H ₂ (1)	CH₃F (1)
N₂O (5)	HNO ₃ (2)	H₂CO (3)	PH₃ (1)	NO ⁺ (1)	HC₃N (1)	GeH₄ (4)
CO (6+3) 	OH (3)	HOCl (2)	COF ₂ (2)	HOBr (2)	H₂ (2)	CS₂ (4)
CH₄ (4)	HF (2)	N ₂ (2)	SF₆ (1)	C ₂ H ₄ (2)	CS (4)	CH₃I (1)
O₂ (3)	HCl (4)	HCN (3)	H₂S (3)	CH ₃ OH (1)	SO ₃ (1)	NF₃ (1)
NO (3)	HBr (4)	CH ₃ Cl (2)	HCOOH (1)	CH ₃ Br (2)	C ₂ N ₂ (1)	

Molecules for which the line lists were updated/extended with respect to HITRAN2016 are in bold
 New molecules or increased amount of isotopologues for existing molecules are highlighted in red;

Updates in the line by line section

- Improved quality of the existing parameters

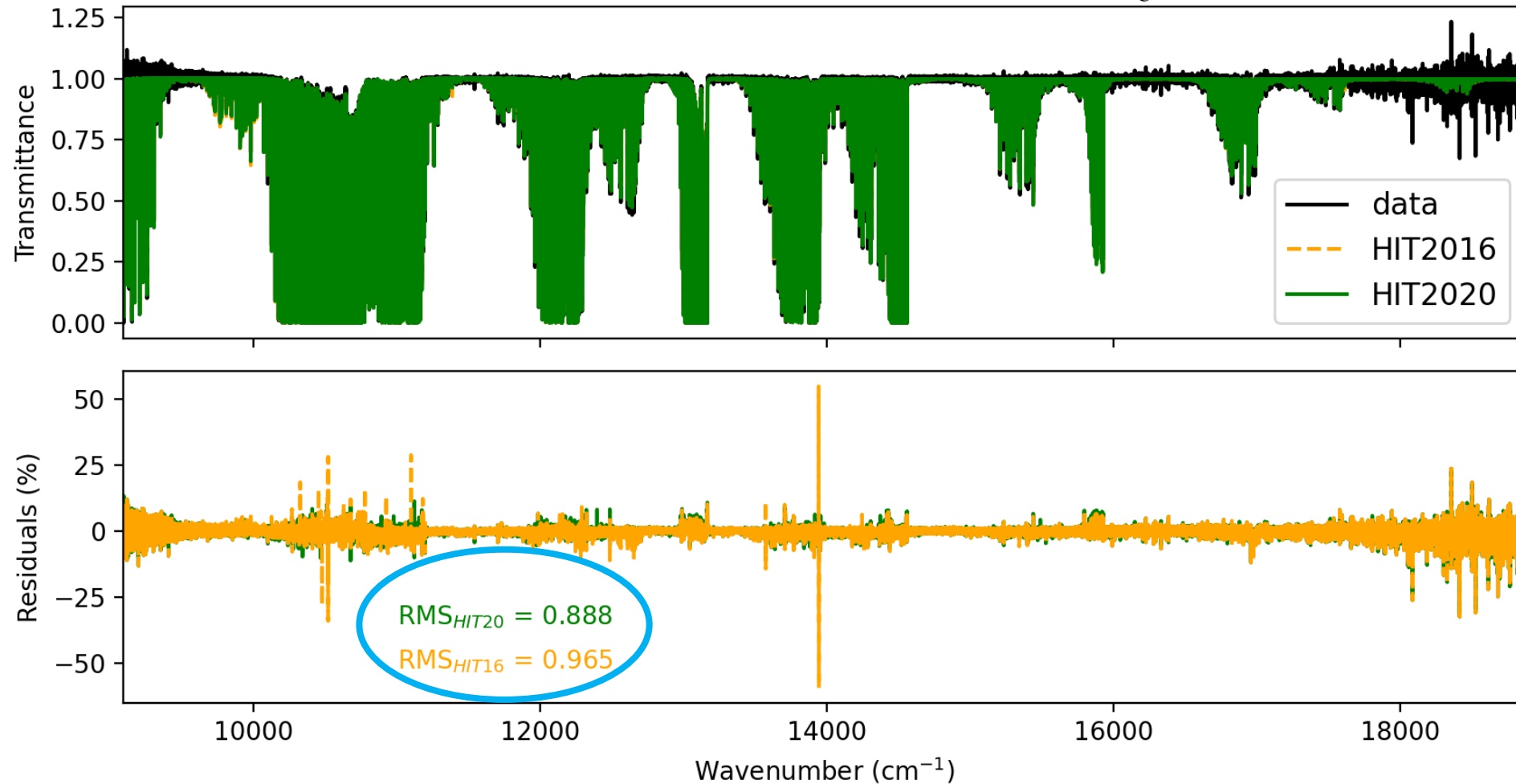
For many molecules in the database, but some are particularly important for the spectroscopy of the atmosphere.

- Many added bands for most species in the database
- Partition sums are (re)calculated for all species (Gamache et al. JQSRT 271 (2021) 107713)
- Line shapes:
 - VP updated form many molecules
 - SDV parameterization (incl. CO₂, CO, N₂O)
 - Additional broadening by various perturbers (incl. H₂O)

Validations of H₂O in HITRAN2020

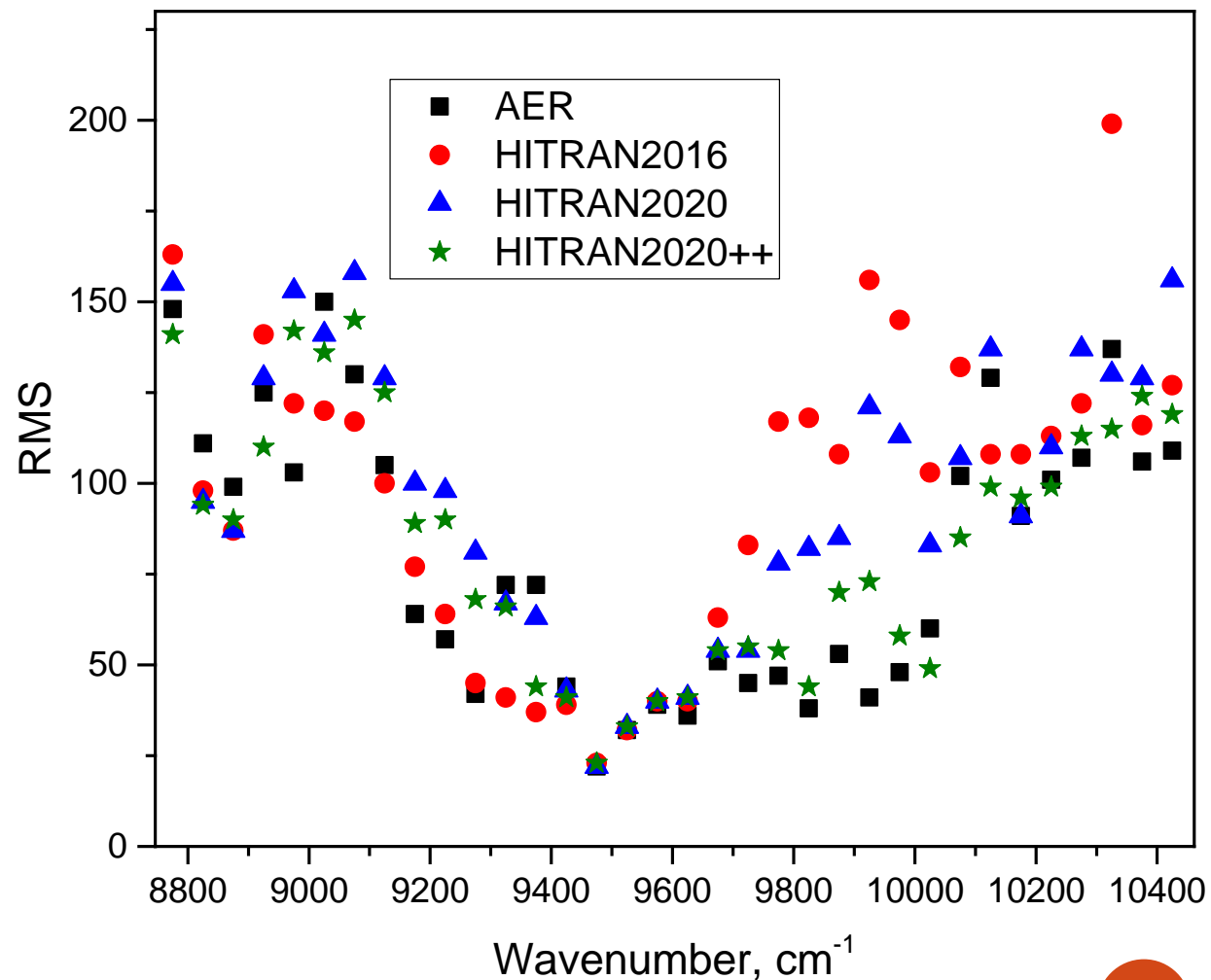
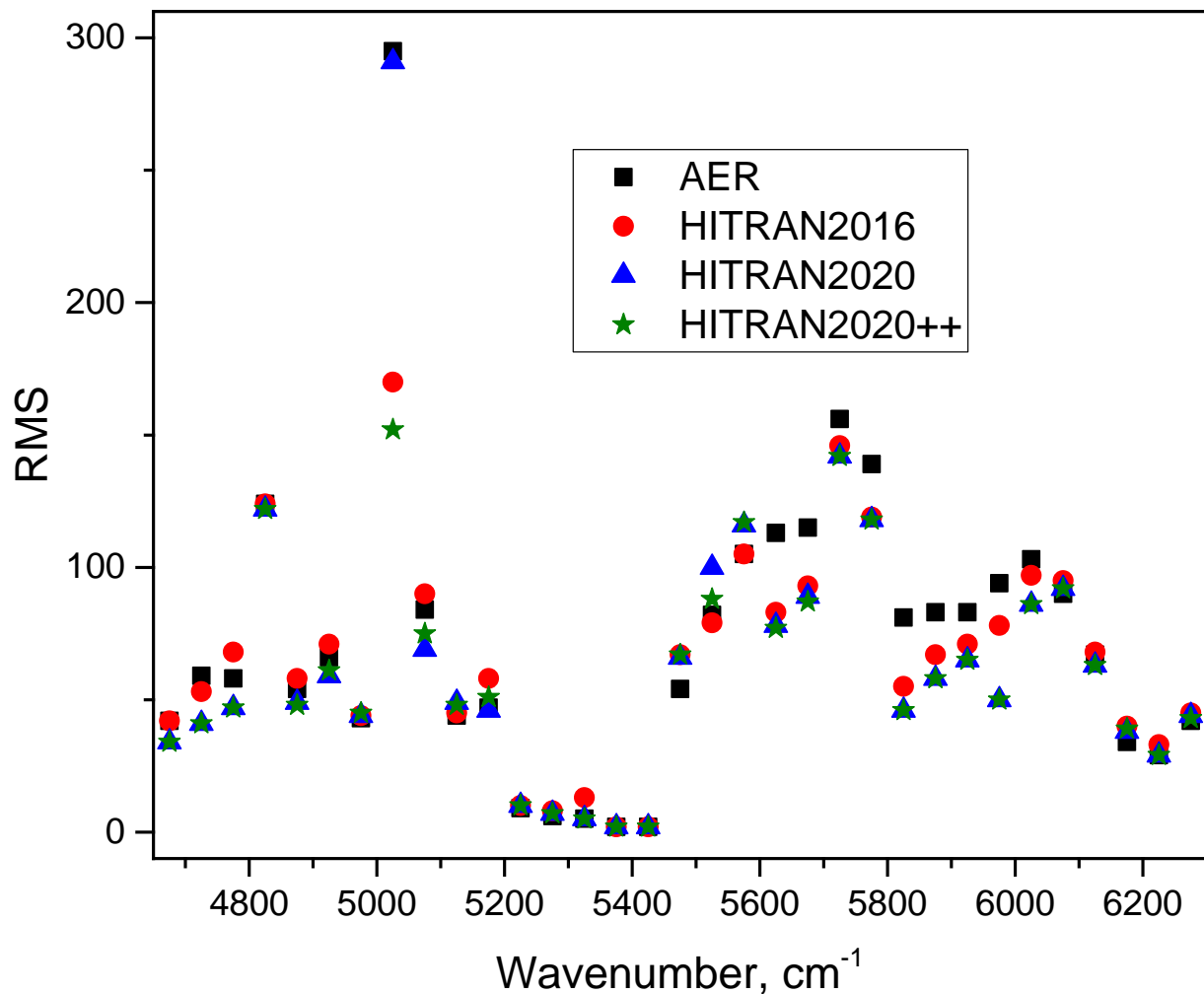
HITRAN2020 and HITRAN2016 compared at modelling the atmospheric transmittance. Compared to high-resolution solar spectrum Baker et al. ApJ 2020

Figure credit: A. Baker (Caltech)



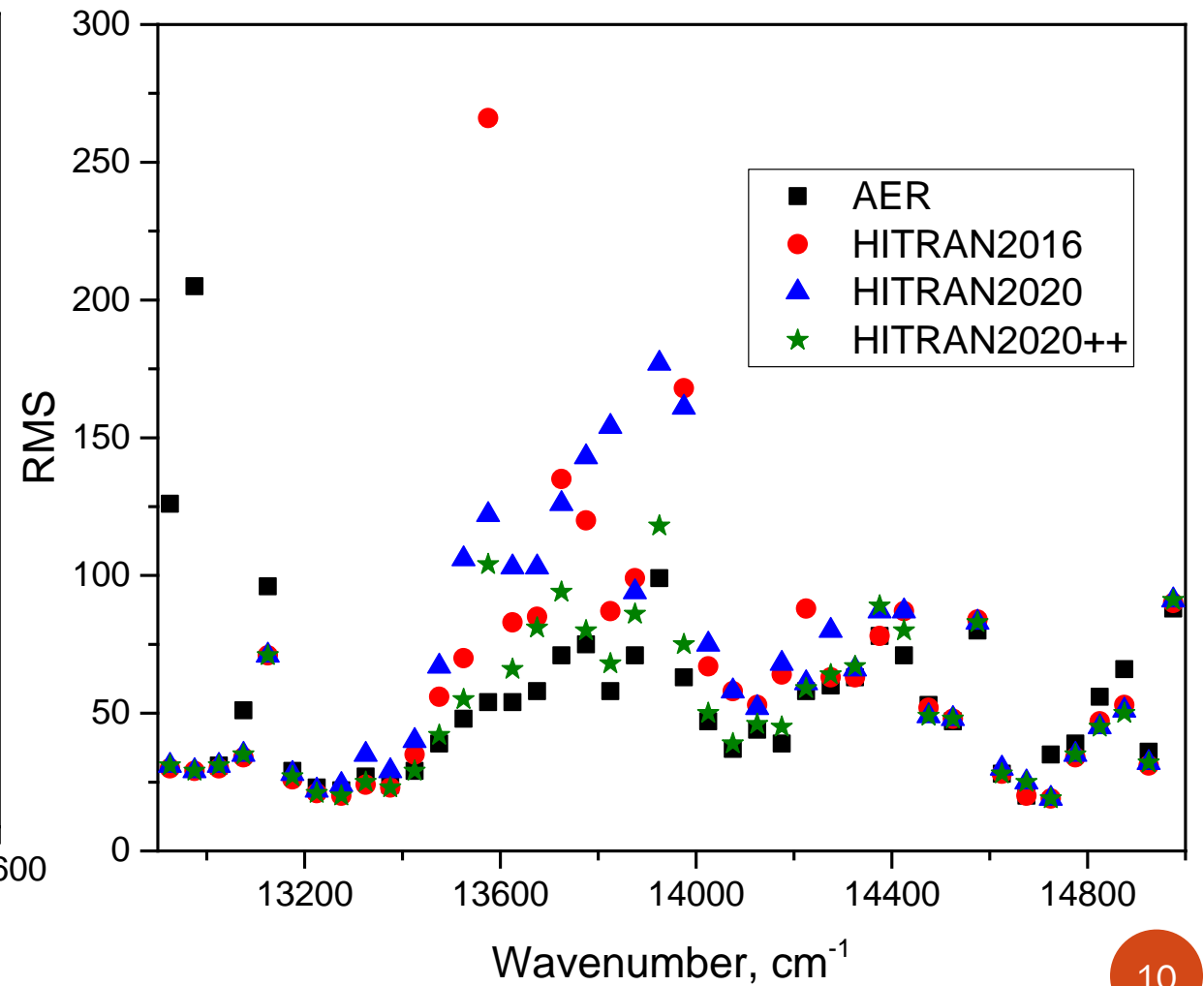
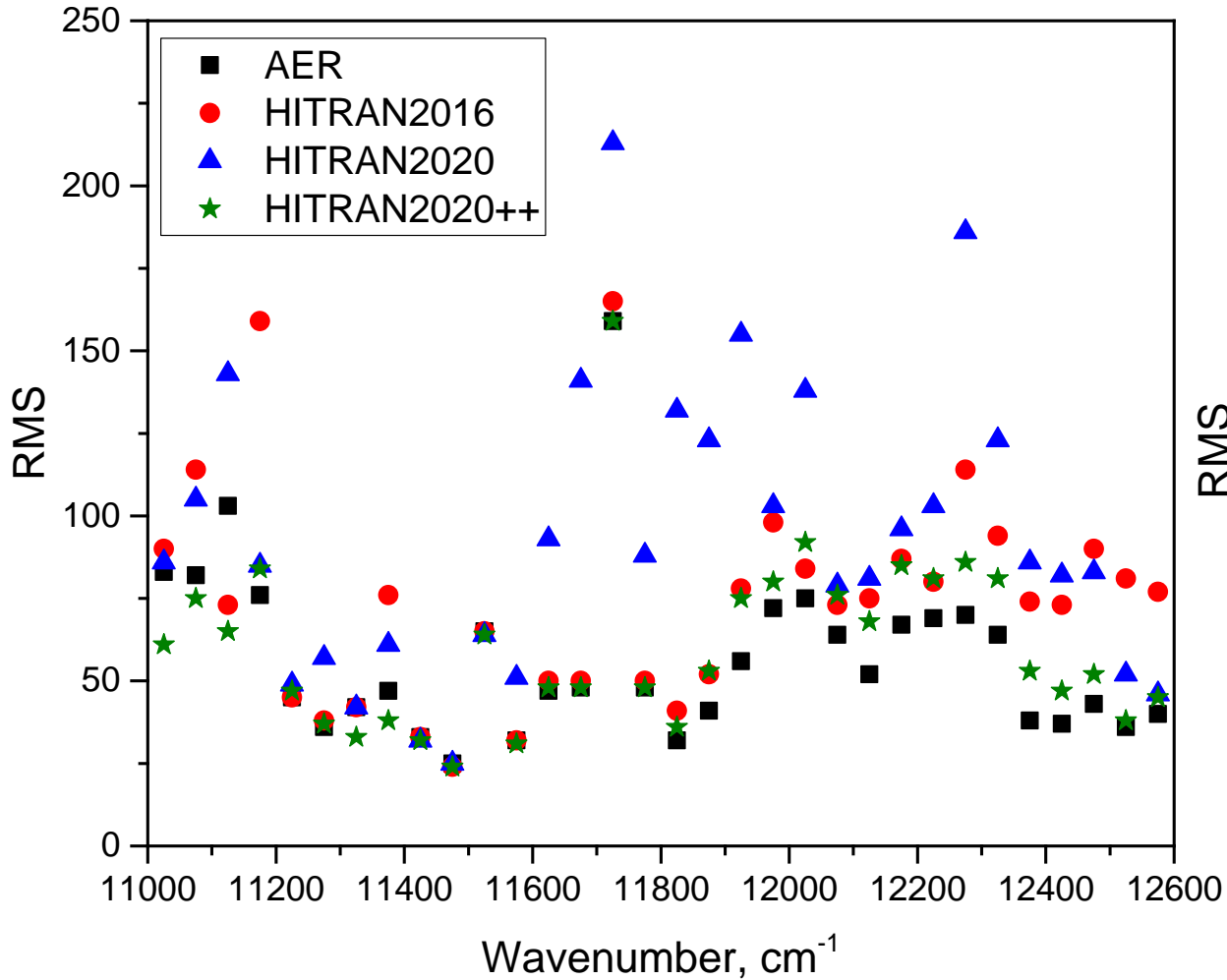
Further Validations of H₂O in HITRAN2020 Using TCCON

△ Eli Mlawer and Mike Iacono (AER)




Major culprit: broadening and shifts

Further Validations of H₂O in HITRAN2020 Using TCCON



Example: ozone improvements

- Major overhaul of the O₃ line list and cross-sections from MW to UV.

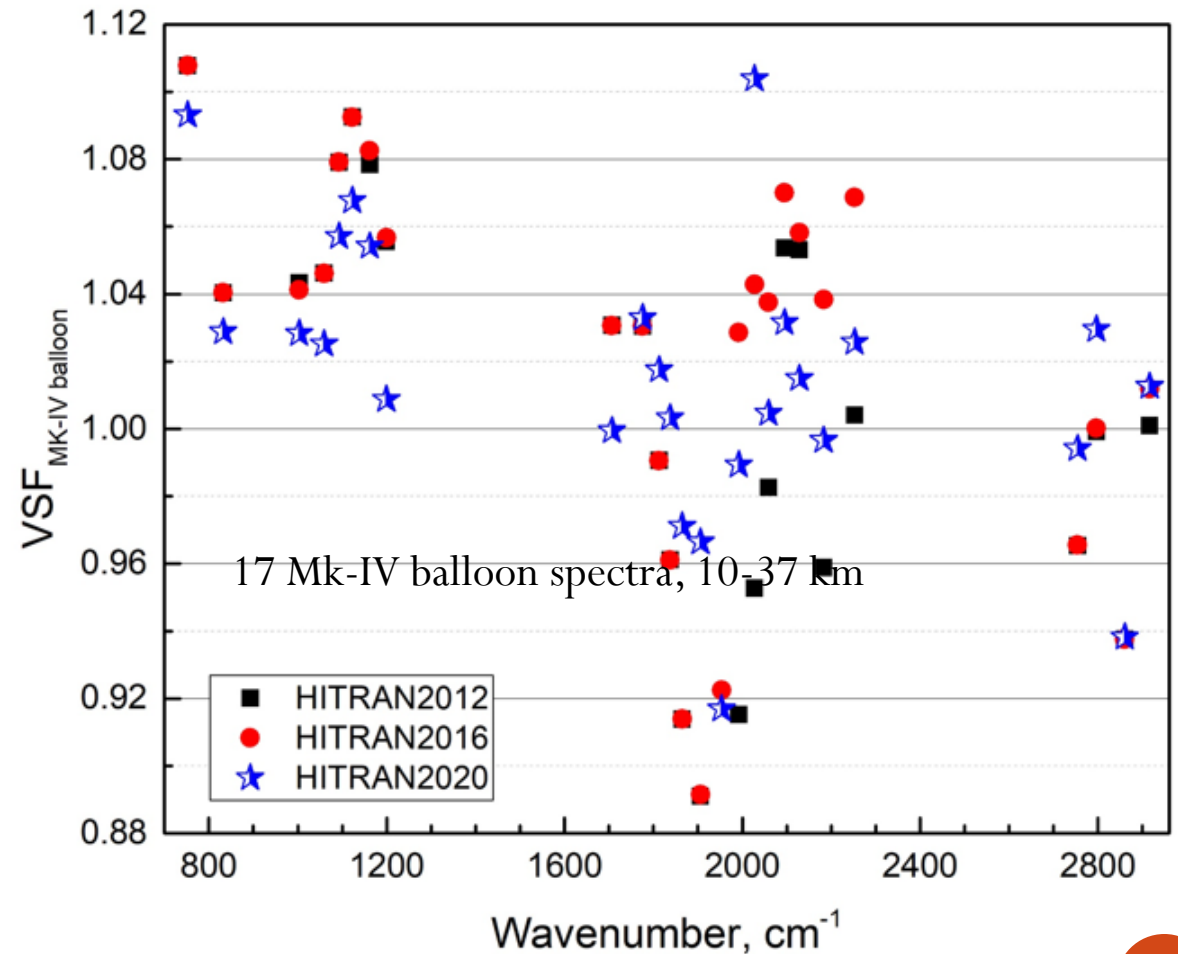
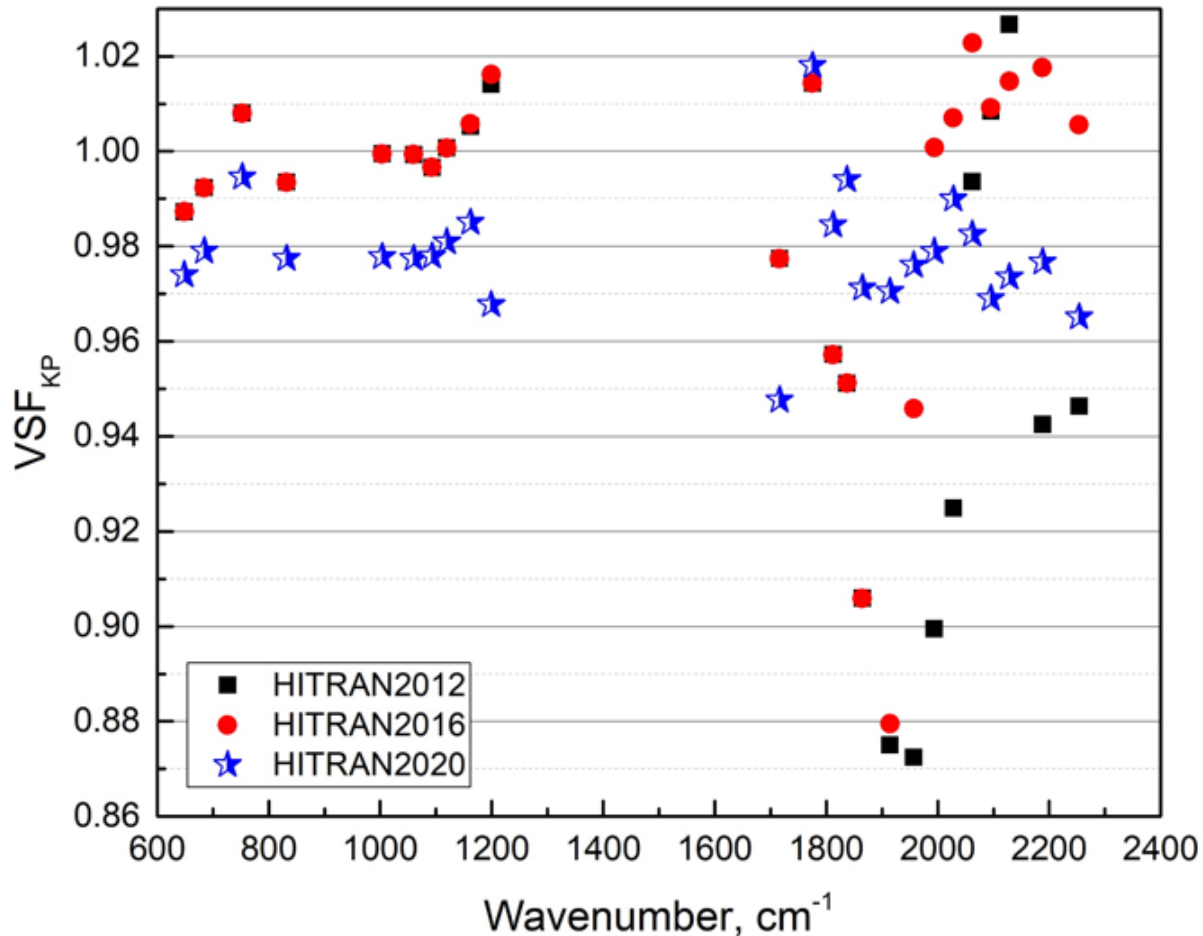
- 
- MW** ❖ In the region of pure rotational transitions, the values from the JPL catalogue were chosen
 - FIR** ❖ Below 1180 cm⁻¹ the DLR line list (which includes new broadening).
<https://dx.doi.org/10.5281/zenodo.4428825>
 - MIR** ❖ Above 1180 cm⁻¹ and up to 5791 cm⁻¹ new S&MPO line list partially described in Tyuterev et al., (2021) JQSRT, 272, 107801 is used except for the 2975-3205 cm⁻¹ region, where UCL/Paris line list is used (Jacquemart et al., (2021) JQSRT 269, 107651)
 - NIR** ❖ Above 5791 cm⁻¹ HITRAN2016 line list is retained for HITRAN2020
 - UV** ❖ UV cross-sections are coming from the new measurements from DLR

Detailed evaluations against laboratory and atmospheric spectra carried out by Geoffrey Toon (JPL)

https://mark4sun.jpl.nasa.gov/report/O3_Spectroscopy_Eval_2021_07_14.pdf

Ozone (contd..) consistency in the IR bands

Effectively the intensities of bands in the MW, 5 and 10 μm regions are increased by **2.8-3.8%**. While different effective scaling factors are observed elsewhere.



Example: O₂

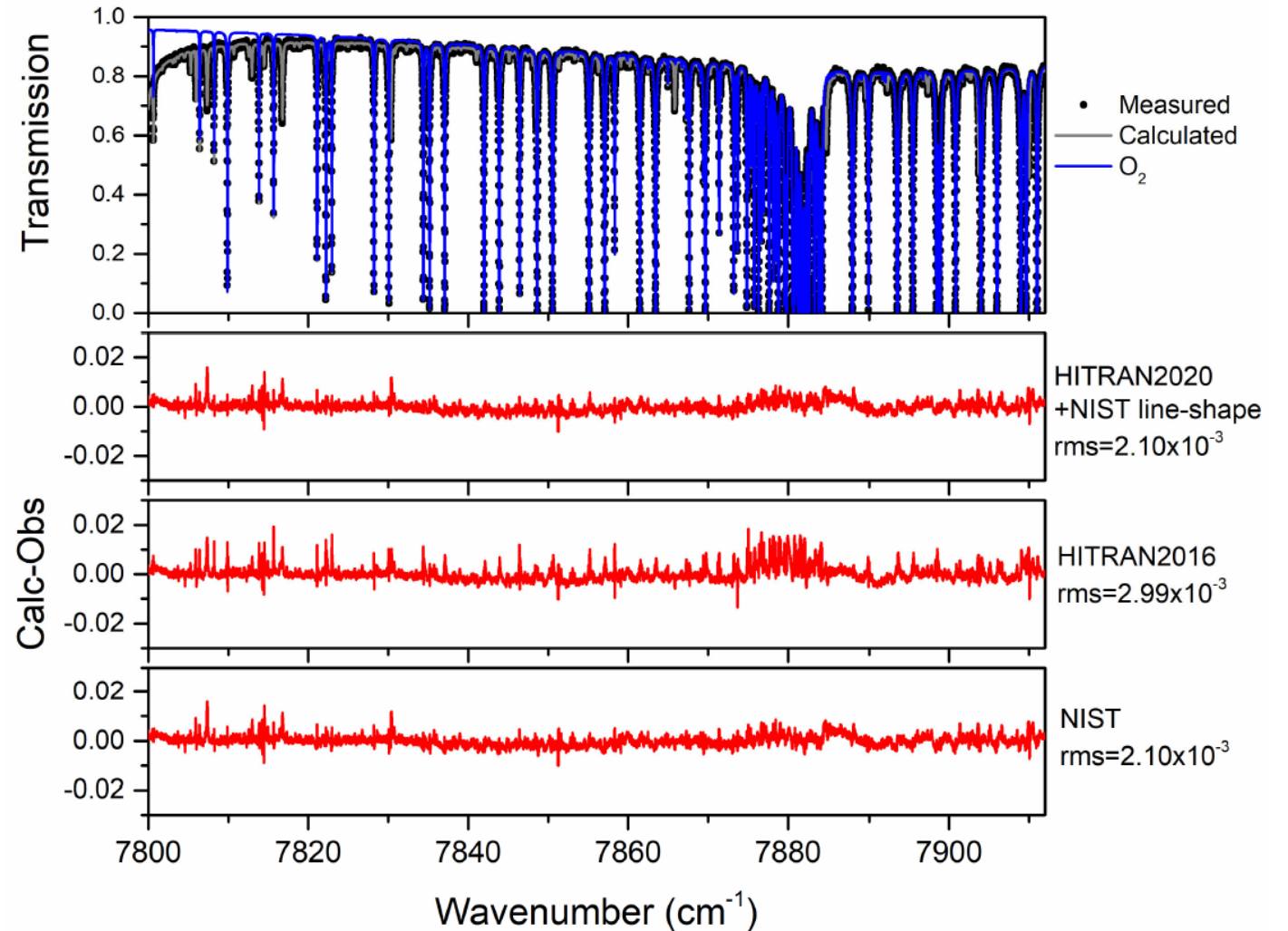
1.27 μm band

New model based on separation of magnetic dipole and electric quadrupole contributions thanks to recent data from Grenoble:

Konefał et al., JQSRT(2020) 241, 106653,
Tran et al., (2020) 240, 106673.

and NIST:

Fleurbaey ., JQSRT(2021) 261, 107495



Modern structure and interface at www.hitran.org

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The HITRAN Database

HITRAN is an acronym for the HITRAN database. HITRAN is a collection of computer codes used for the calculation of light in the atmosphere.

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Data Access

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mission molecular absorption spectroscopic parameters that a variety of the transmission and emission

News

- Oct 2021 | [The data on this page corresponds to the HITRAN2020 edition](#)
- Sep 2021 | [21000 users milestone](#)
- Apr 2021 | [History of HITRAN](#) **S. Rothman**
- Apr 2020 | [HITEMP now included](#)
- Jul 2015 | [All inquiries can be directed to HITRAN's support team at info@hitran.org](#)

Database Updates

- Oct 2021 | [The updates to the HITRAN2020 edition will be available in this section as they appear](#)

HAPI: The HITRAN Application Programming Interface

Introduction

The *HITRAN Application Programming Interface* (HAPI) [1] is a set of routines in Python which aims to provide remote access to functionality and data provided by *HITRANonline*. At the present time, the API can download, filter and process line-by-line transition data.

The main purpose of this API is to extend the functionality of the main site, in particular, for 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 of HAPI and user manual is available for download using the following links:

- [hapi.py V.1.1.1.0](#)
- [hapi_manual.pdf](#)

In addition, the HAPI project and version history are available on Github:

- <https://github.com/hitranonline/hapi>

HAPI is described in Ref. [1], and further suggestions and comments are welcome: please email rkochanov@cfa.harvard.edu.

Citation

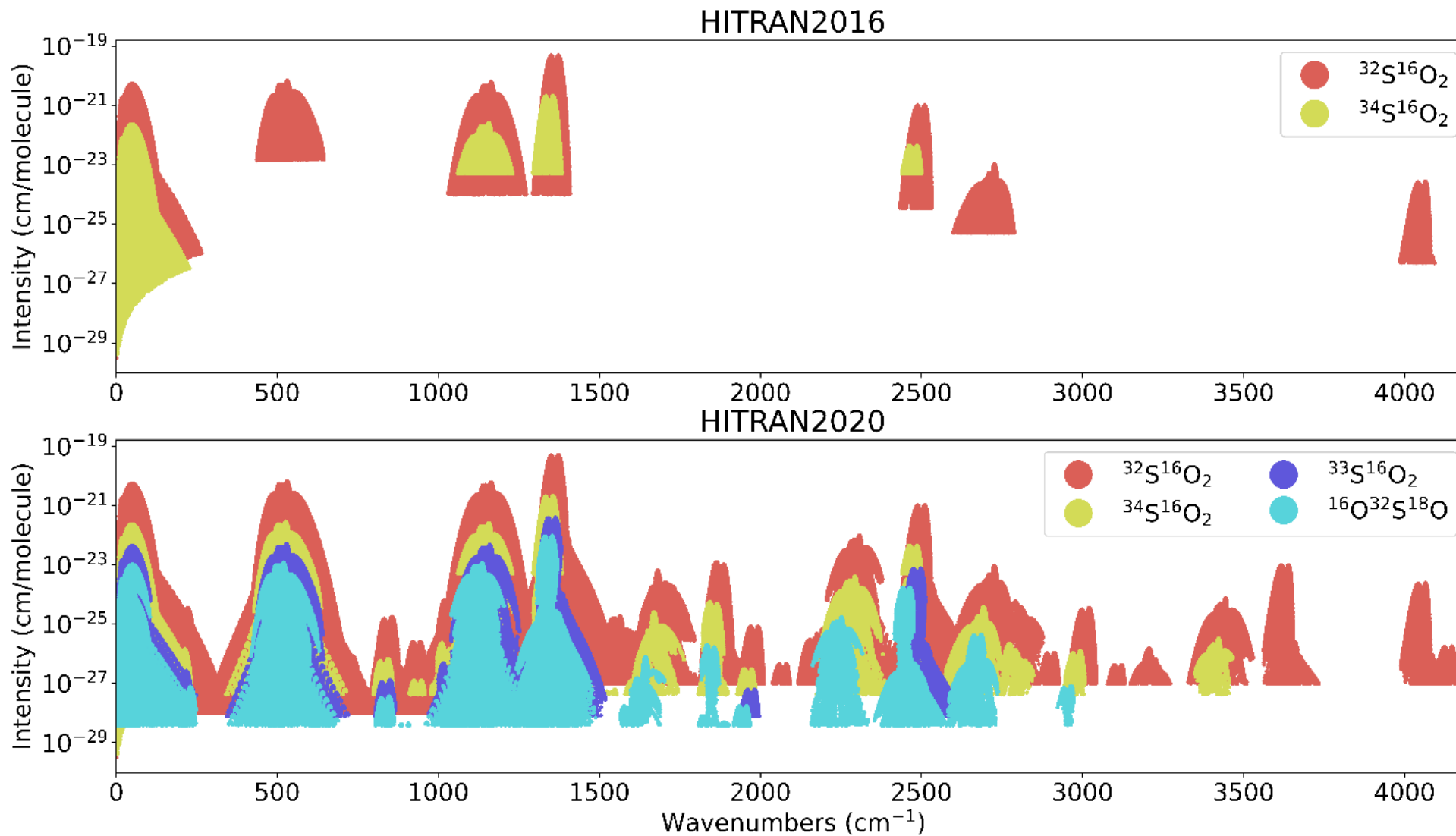
If you use HAPI in your research or software development, please cite it using the following reference:

- R.V. Kochanov, I.E. Gordon, L.S. Rothman, P. Wcislo, C. Hill, J.S. Wilzewski, HITRAN Application Programming Interface (HAPI): A comprehensive approach to working with spectroscopic data, *J. Quant. Spectrosc. Radiat. Transfer* **177**, 15-30 (2016) [[Link to article](#)] [[ADS](#)].

To make a reference to particular version of HAPI, use corresponding DOI from the [Zenodo](#) community in addition to the reference given above.

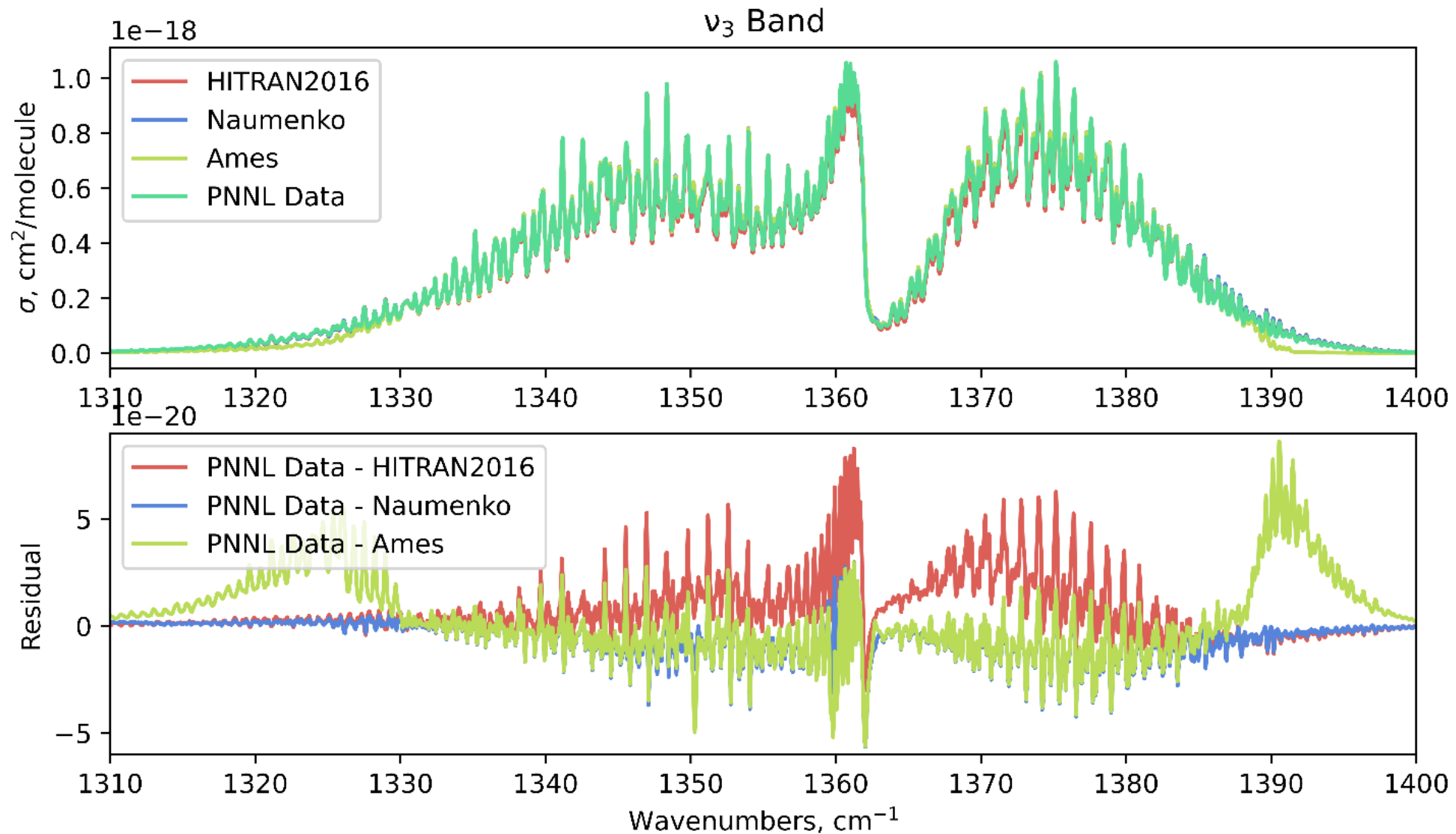
www.hitran.org/hapi

Improved parameters, new bands, isotopologues



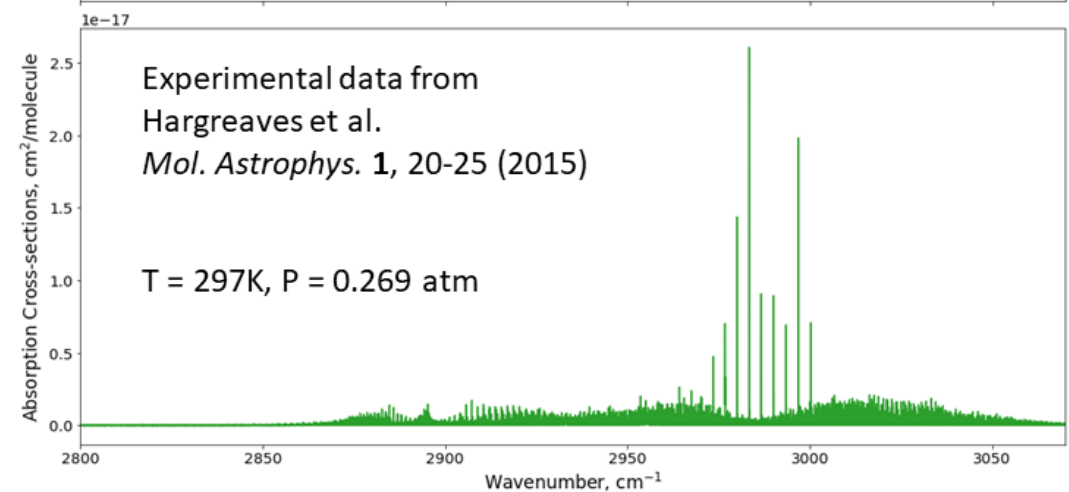
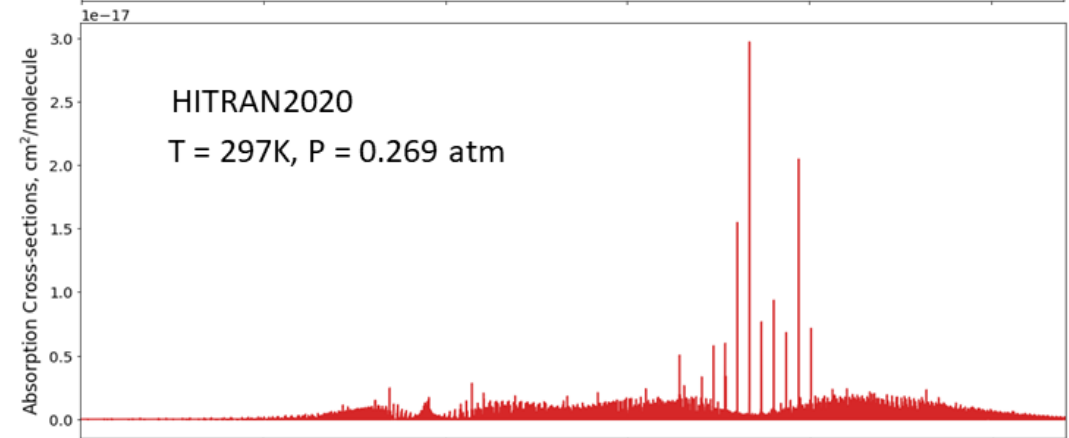
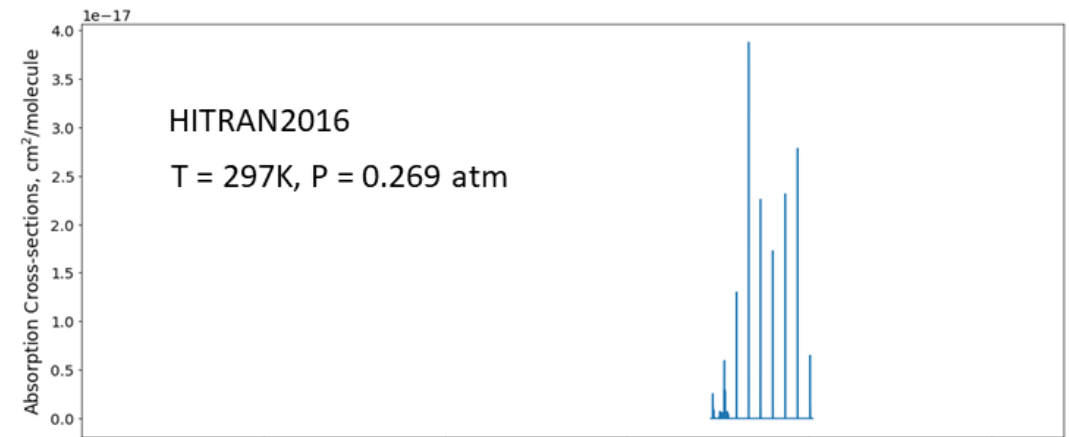
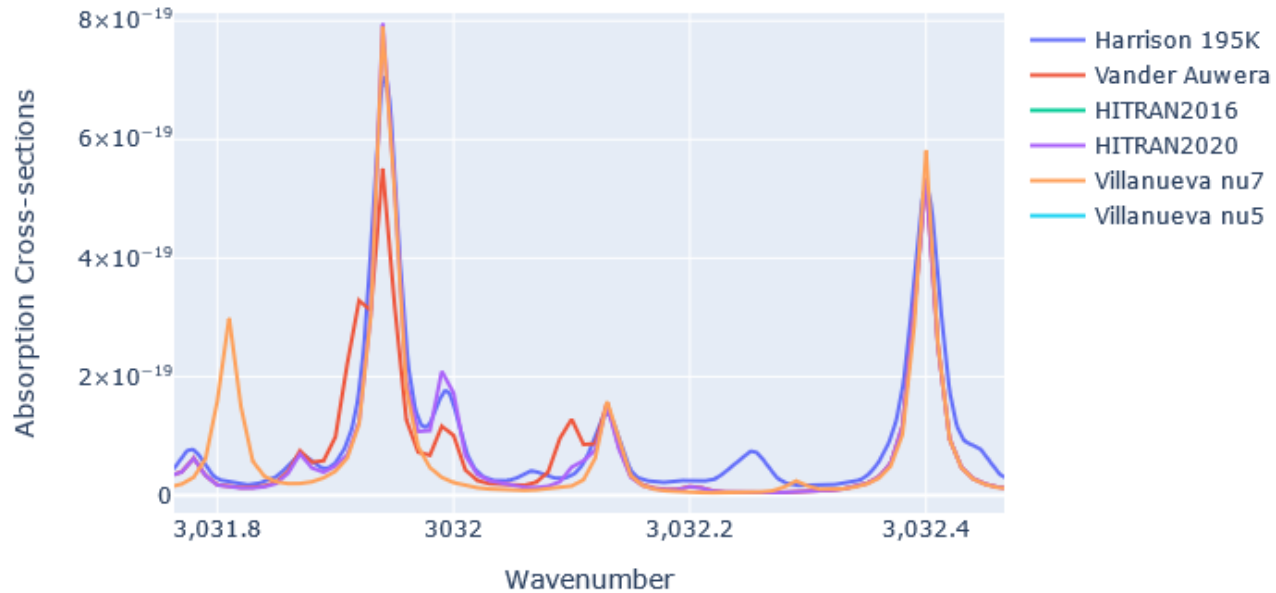
Other examples include NO, NO₂, OCS, HCN, HCOOH etc...

Improved parameters, new bands, isotopologues



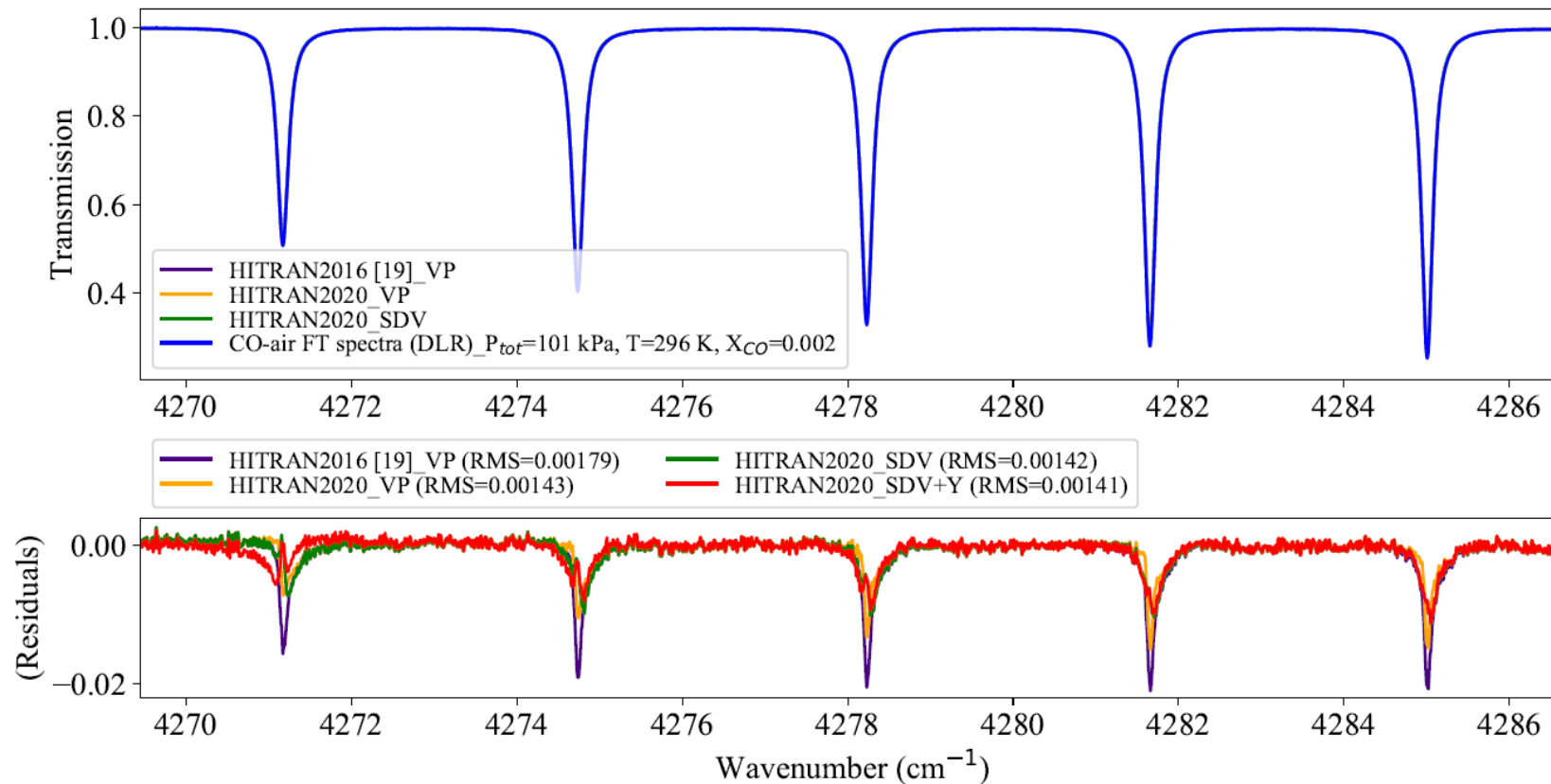
Improved parameters, new bands (e.g. C_2H_6)

Harrison 195K, 52 Torr



Non-Voigt line shapes

- Apart from Voigt HITRAN accommodates Hartman-Tran, SDV and Galatry profiles
- Example: every line of CO_2 , N_2O and CO now has speed-dependent Voigt and first order line mixing parameters.

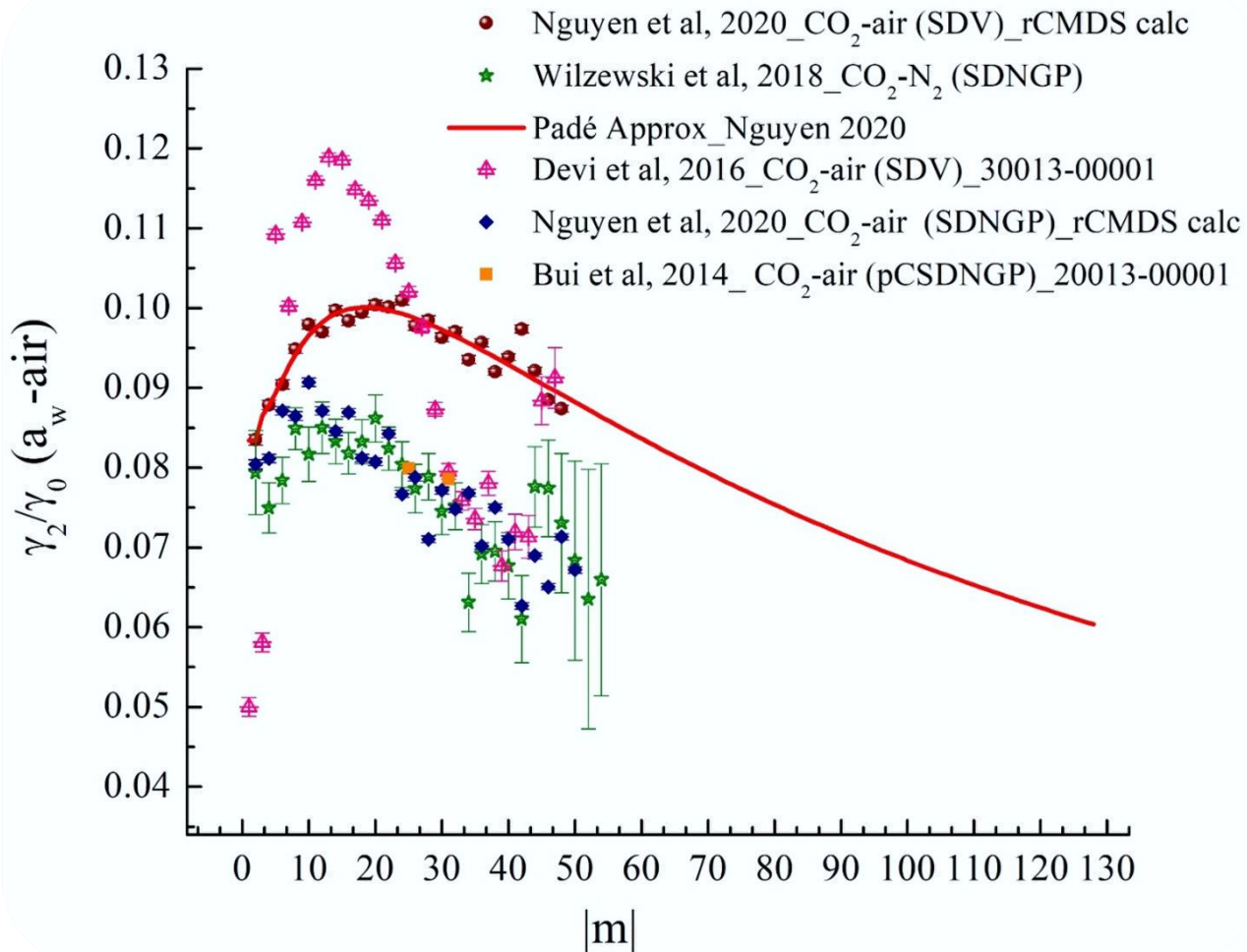


SDV parameters ^b	Common notation
Half-widths	γ_0 -air(SDV)
	γ_0 -self(SDV)
Temp. dep. half-widths	n_{γ_0} -air(SDV)
	n_{γ_0} -self(SDV)
Speed dep. half-widths	γ_2 -air(SDV)
	γ_2 -self(SDV)
Temp. dep. speed dep.	n_{γ_2} -air(SDV)
	n_{γ_2} -self(SDV)
Line shifts	δ_0 -air(SDV)
	δ_0 -self(SDV)
First-order line-mixing	Y_{air} (SDV)
	Y_{self} (SDV)
Temp. dep. first-order	n_Y -air(SDV)
line-mixing	n_Y -self(SDV)

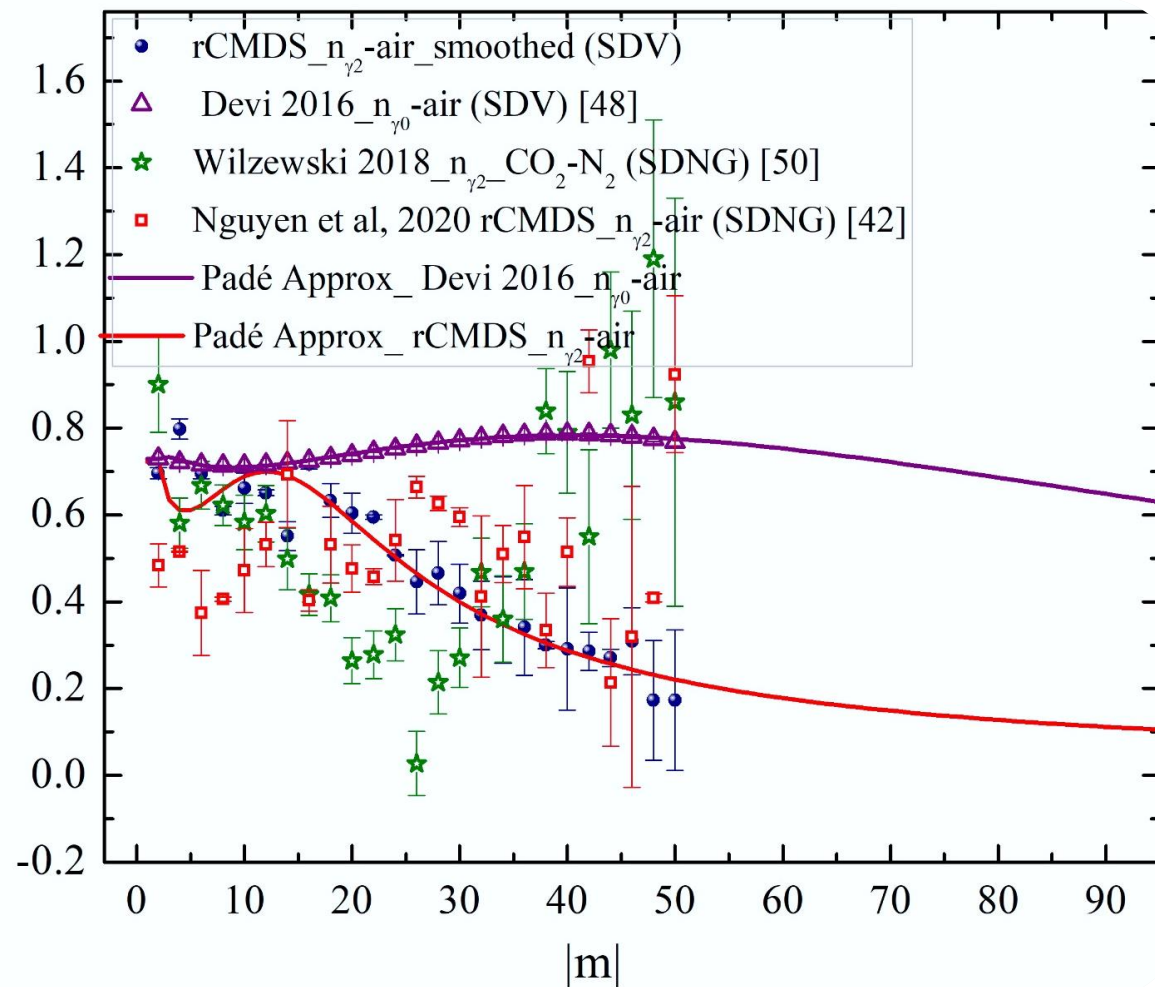
Hashemi et al., JQSRT(2020) 107283.

Hashemi et al., JQSRT(2021) 107735.

Non-Voigt line shapes (CO₂)



Nguyen et al, JQSRT, 242 (2020) 106729.
 Bui et al, JCP, 141 (17) (2014) 174301
 Devi et al, JQSRT, 177 (2016) 117-144 .



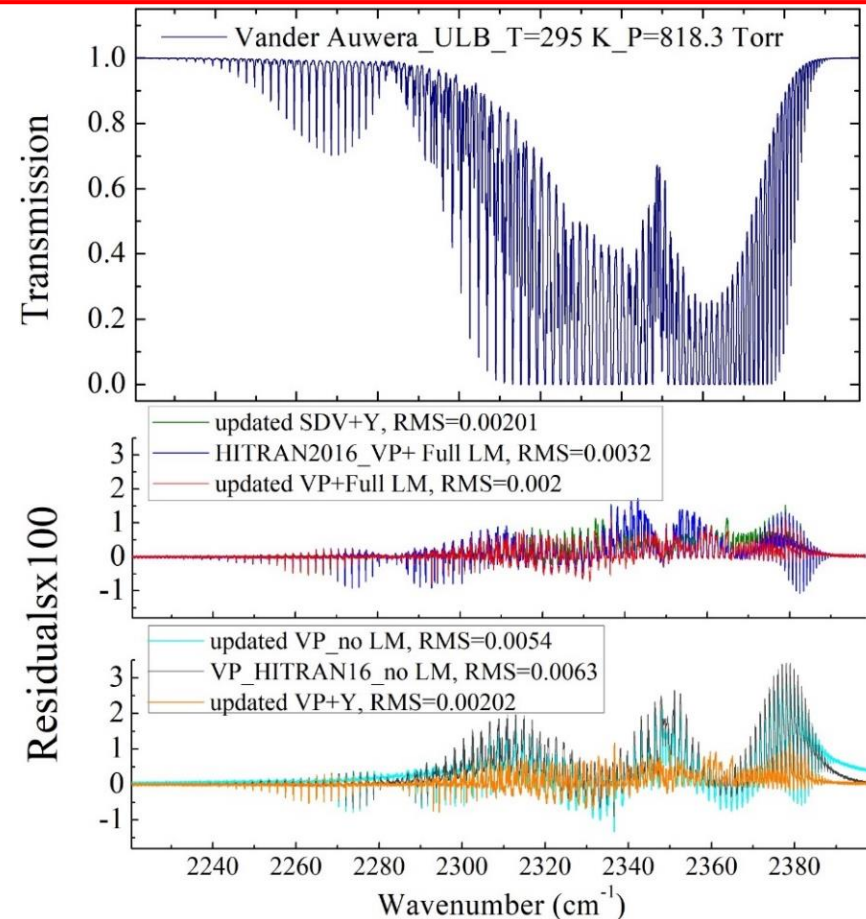
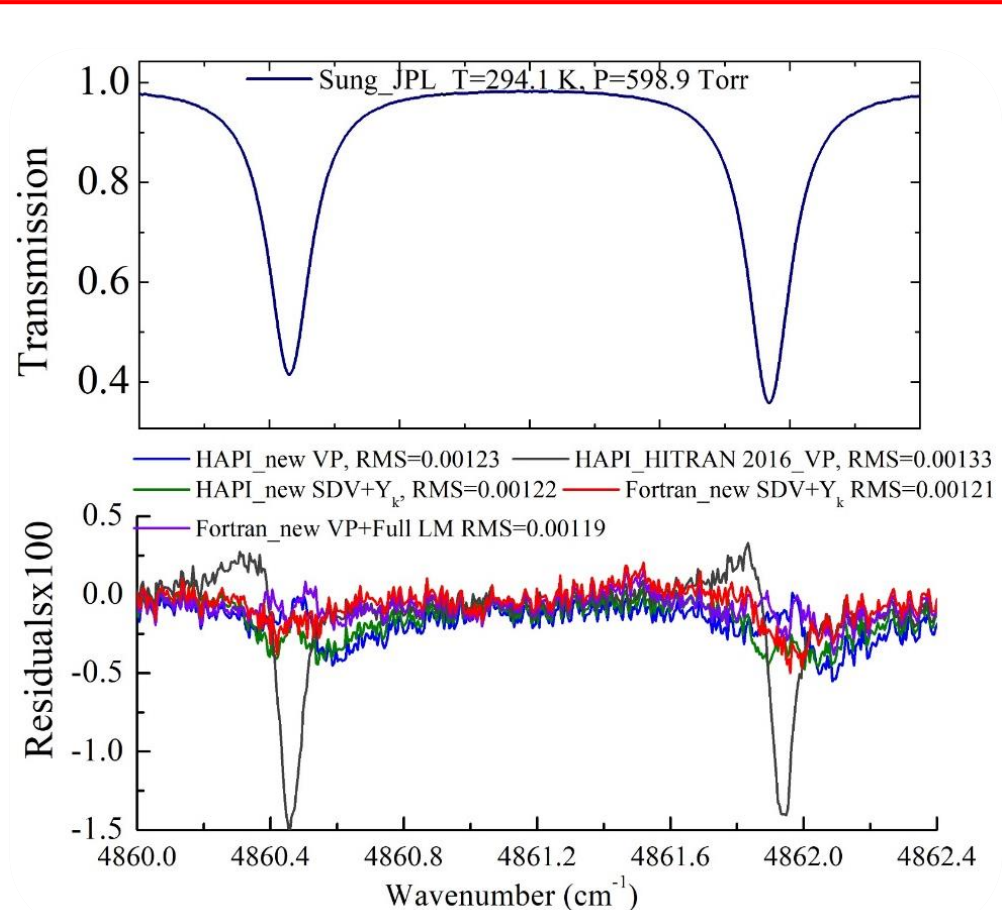
Wilzewski et al, JQSRT, 206 (2018) 296-305.
 Birk et al, 2021, JQSRT (2022)
 Daneshvar et al, JQSRT, 2014;149:258-74

Update of the CO₂ LM package

The line mixing package for CO₂ was updated. The approach by Lamouroux et al. (2015) is used for predicting the line-mixing effect in all the bands of CO₂ either accounting for the full line mixing (W) or the first-order approximation (Y):

- 1) VP+ first order LM
- 2) VP+ full LM
- 3) SDV+ first-order LM. This Fortran package is available at HITRANonline: <https://hitran.org/supplementary/>

Validation using laboratory spectra



Modern structure and interface at www.hitran.org

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Data Access menu:

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- Absorption Cross Sections**
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- Aerosol Properties
- HITEMP
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Absorption Cross Section Search

Select individual molecules below, then cross sections. [2. Get data >](#)
 (If you select fewer than six cross section data sets they will also appear in an interactive graph.)

Search for molecule by name:

News

- Oct 2021 | [The data on corresponds to the HITRAN](#)
- Sep 2021 | [21000 users mil](#)
- Apr 2021 | [History of HITRAN](#) [Supplemental folder](#)
- Apr 2020 | [HITEMP now in](#)
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HFC-152a: CH₃CHF₂

IR cross sections						
<input type="checkbox"/>	ν range /cm ⁻¹	T/K	p/Torr	Resolution	npts	Broadener
<input type="checkbox"/>	525.0 - 6500.0	323.15	760.0	0.112 cm ⁻¹	99147	N2
<input type="checkbox"/>	525.0 - 6500.0	298.15	760.0	0.112 cm ⁻¹	99147	N2
<input type="checkbox"/>	525.0 - 6500.0	278.15	760.0	0.112 cm ⁻¹	99147	N2
<input type="checkbox"/>	830.0 - 1500.0	253.0	0.0	0.03 cm ⁻¹	66706	
<input type="checkbox"/>	840.0 - 995.0	253.0	0.0	0.03 cm ⁻¹	18010	
<input type="checkbox"/>	840.0 - 994.9	270.0	0.0	0.03 cm ⁻¹	18000	
<input type="checkbox"/>	840.0 - 995.0	287.0	0.0	0.03 cm ⁻¹	18010	
<input type="checkbox"/>	1050.0 - 1205.0	253.0	0.0	0.03 cm ⁻¹	18010	
<input type="checkbox"/>	1050.0 - 1205.0	270.0	0.0	0.03 cm ⁻¹	18010	
<input type="checkbox"/>	1050.0 - 1205.0	287.0	0.0	0.03 cm ⁻¹	18010	
<input type="checkbox"/>	1319.9 - 1490.0	253.0	0.0	0.03 cm ⁻¹	19750	
<input type="checkbox"/>	1319.9 - 1490.1	270.0	0.0	0.03 cm ⁻¹	19760	
<input type="checkbox"/>	1319.9 - 1490.1	287.0	0.0	0.03 cm ⁻¹	19760	

www.hitran.org/xsc

Cross sections (.xsc)

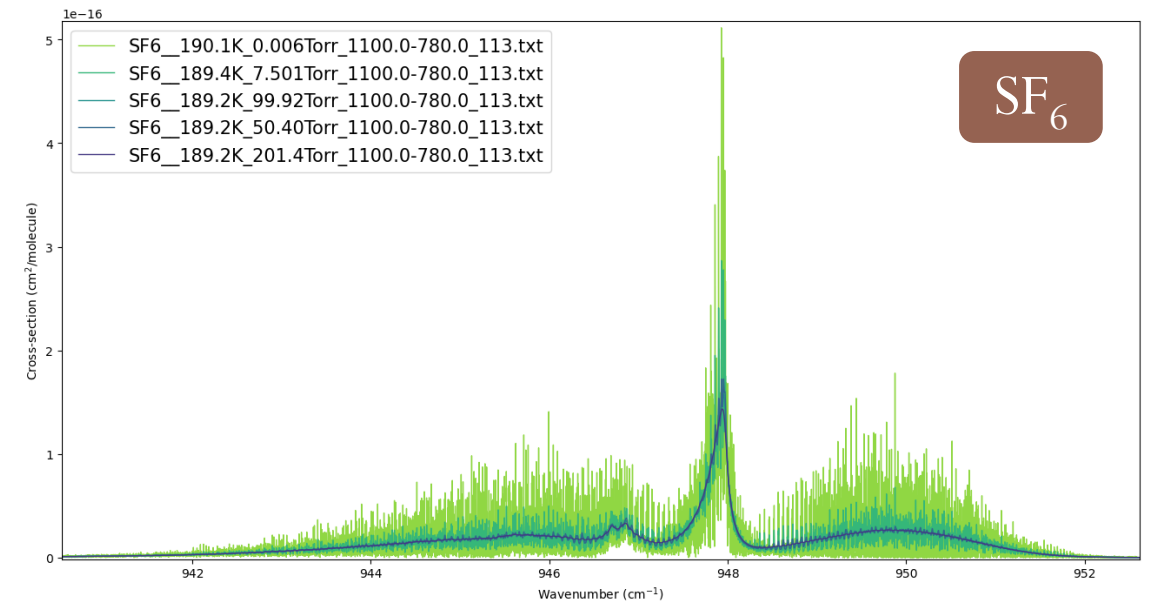
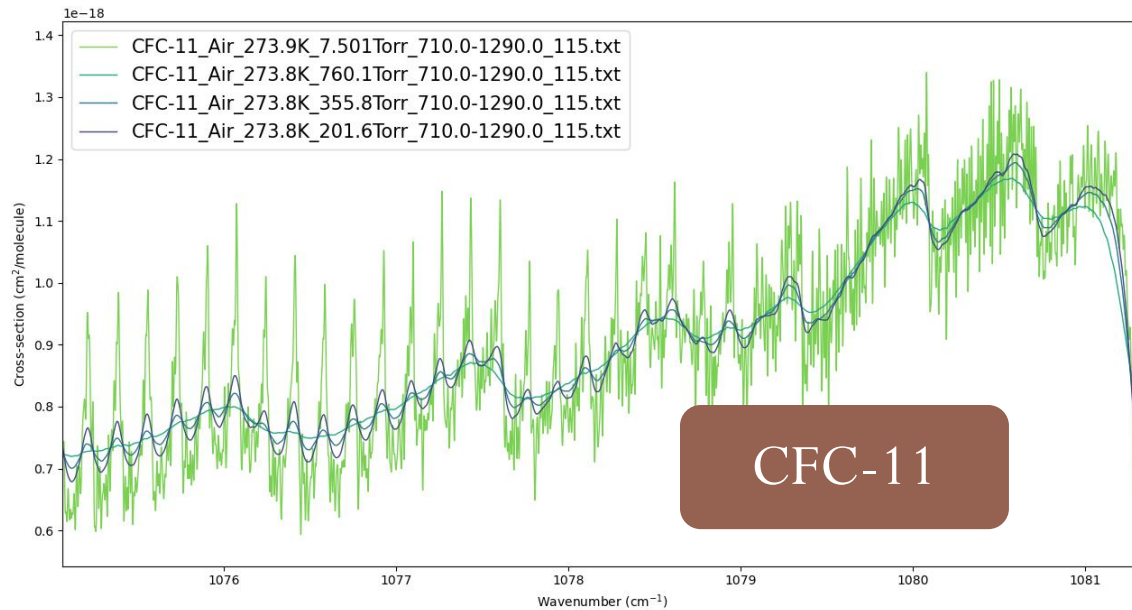
Molecule	Temperature range (K)	Pressure range (Torr)	Number of P,T sets	Spectral range (cm^{-1})
CCl_3F (CFC-11)	192 – 293	7.5 – 760	30	710 – 1290
$\text{CH}_3\text{CCl}_2\text{F}$ (HCFC-141b)	188 – 295	7.5 – 761	30	705 – 1280
SF_6	189 – 294	7.5 – 751	37	780 – 1100
CF_4 (CFC-14)	190 – 296	7.5 – 760	34	1190 – 1336

Harrison (2018), AMT 11, 5827-5836

Harrison (2019), JQSRT 238, 106489

Harrison (2020), JQSRT 254, 107202

Harrison (2021), JQSRT 260, 107432



- Also added UV and planetary relevant cross-sections

Modern structure and interface at www.hitran.org

The screenshot shows the HITRANonline website interface. The top navigation bar includes 'Home', 'Data Access', 'Documentation', 'Conferences', 'Links', and 'About'. The 'Data Access' menu is expanded, showing options like 'Line-by-line', 'Absorption Cross Sections', 'Collision Induced Absorption', 'Aerosol Properties', 'HITEMP', 'HAPI', and 'Supplemental'. The 'Collision Induced Absorption' page is displayed, featuring a 'News' section with recent updates and a table of available CIA data for various systems.

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The HITRAN Database

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News

- Oct 2021 | **Tutorials** corresponds to the new HITRAN2020 edition
- Sep 2021 | **2100** cm⁻¹ HITRAN2020
- Apr 2021 | **Historical** HITRAN2020
- Apr 2020 | **HITRAN2020** HITRAN2020
- Jul 2015 | **All in** HITRAN2020

Database Updates

- Oct 2021 | **Tutorials** HITRAN2020 edition

Collision Induced Absorption

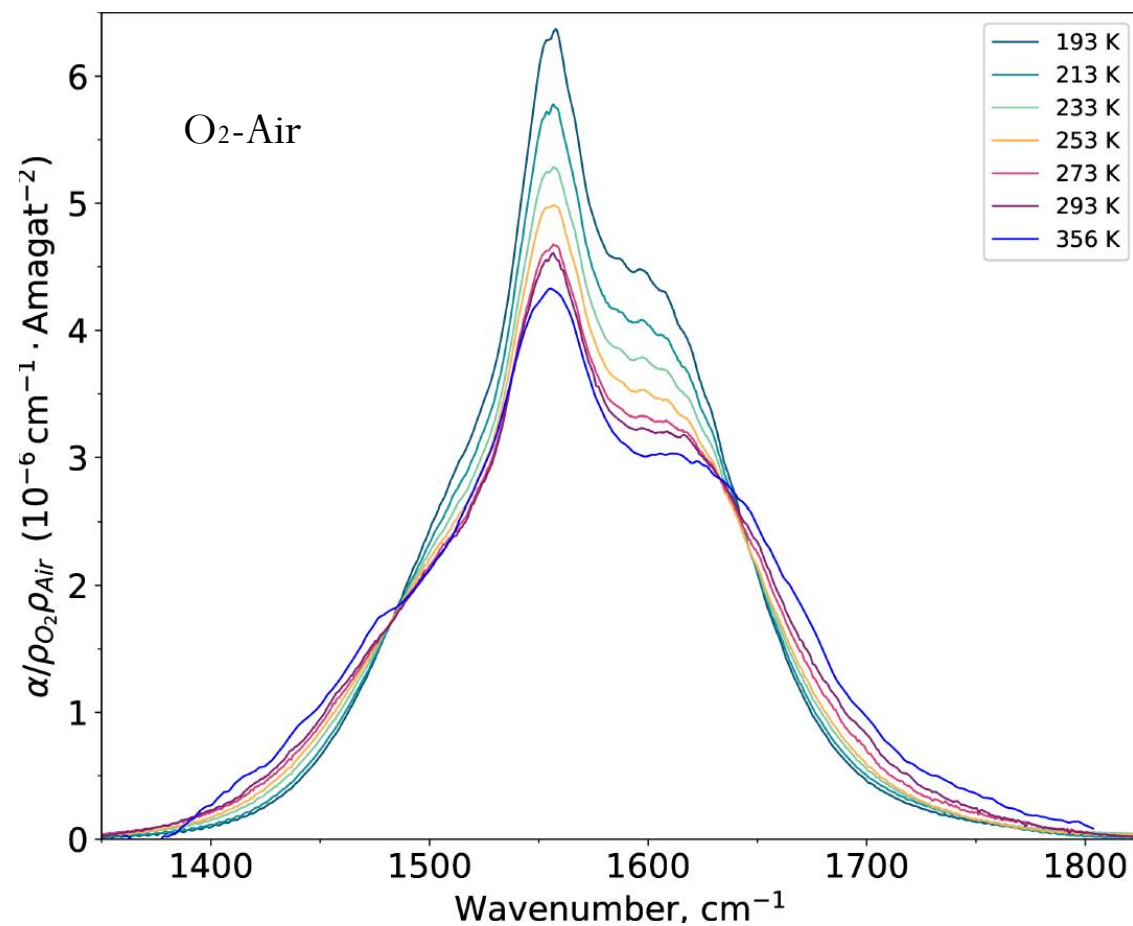
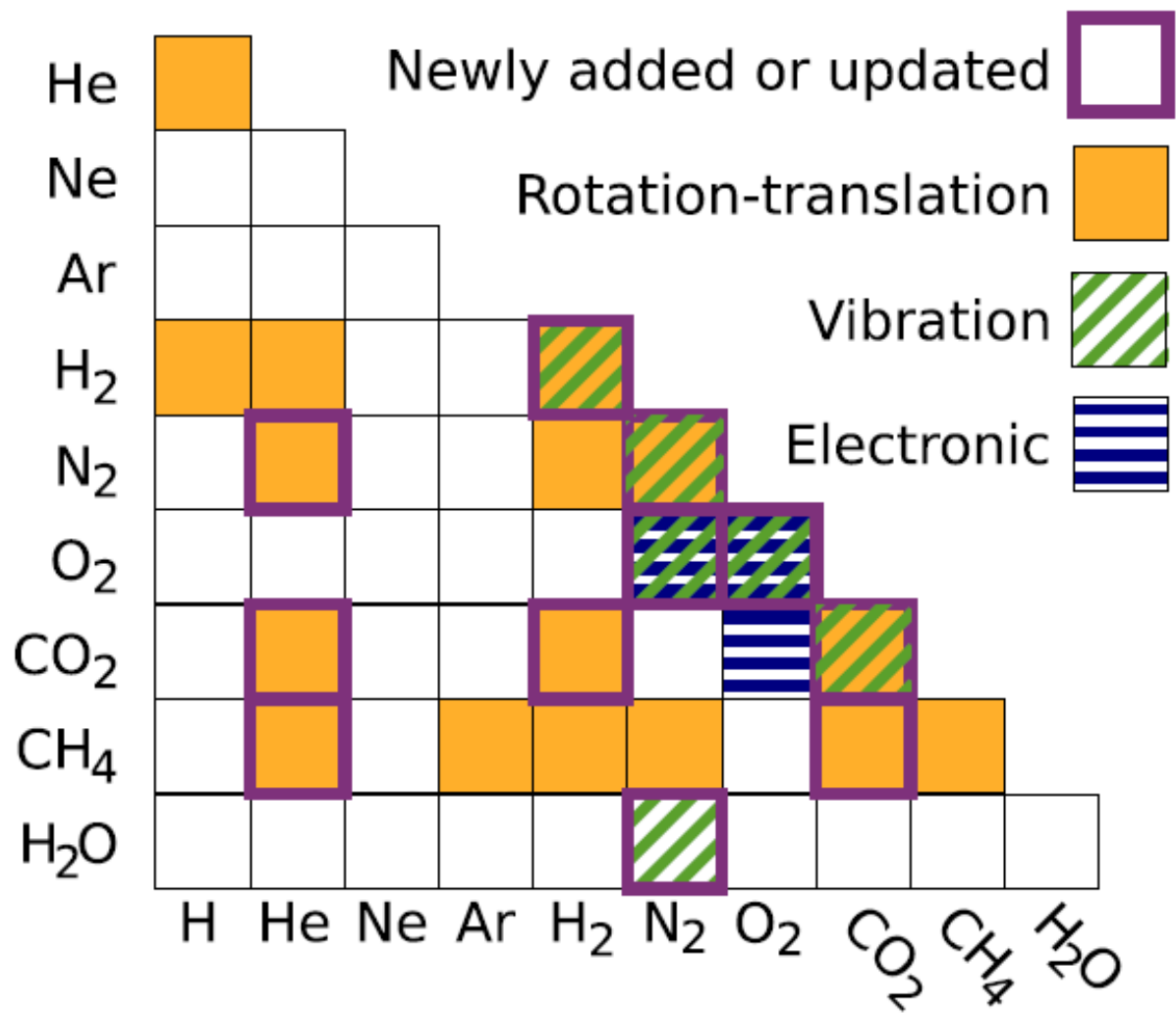
Details regarding the structure of the Collision Induced Absorption (CIA) data available through HITRANonline are given in Ref. [1]. Further descriptions of the content and format of the CIA files are described in the following readme document, with corresponding reference sources given in the reference document:

- [CIA_Readme.pdf](#)
- [CIA_References.pdf](#)

The following CIA data are available to download by clicking the appropriate download icon (↓), and selecting "Save File".

System	$\nu_{\min}/\text{cm}^{-1}$	$\nu_{\max}/\text{cm}^{-1}$	Filename	Download
H ₂ -CH ₄ (equilibrium)	0	1946	H2-CH4_eq_2011.cia	↓
H ₂ -CH ₄ (normal)	0	1946	H2-CH4_norm_2011.cia	↓
H ₂ -H ₂	20	10 000	H2-H2_2011.cia	↓
H ₂ -H	100	11 000	H2-H_2011.cia	↓
H ₂ -He	20	20 000	H2-He_2011.cia	↓
He-H	50	11 000	He-H_2011.cia	↓
N ₂ -H ₂	0	1 886	N2-H2_2011.cia	↓
N ₂ -He	1	1 000	N2-He_2018.cia	↓
N ₂ -N ₂	0	5 000	N2-N2_2018.cia	↓

Update of the CIA section



Update to update

Karman, *et al.*, "Update of the HITRAN collision-induced absorption section", *Icarus* 328 (2019) 160-175.

Referencing the original sources

Open Access Editor's Choice Article

Referencing Sources of Molecular Spectroscopic Data in the Era of Data Science: Application to the HITRAN and AMBDAS Databases

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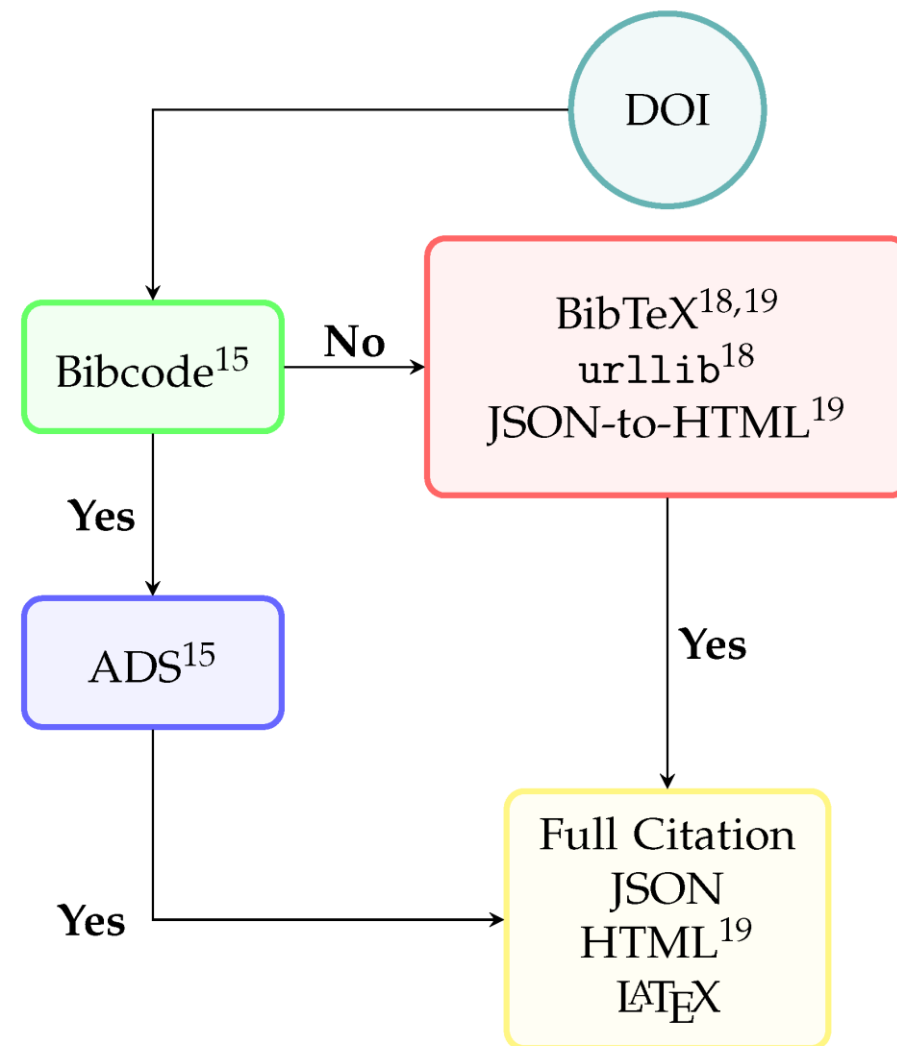
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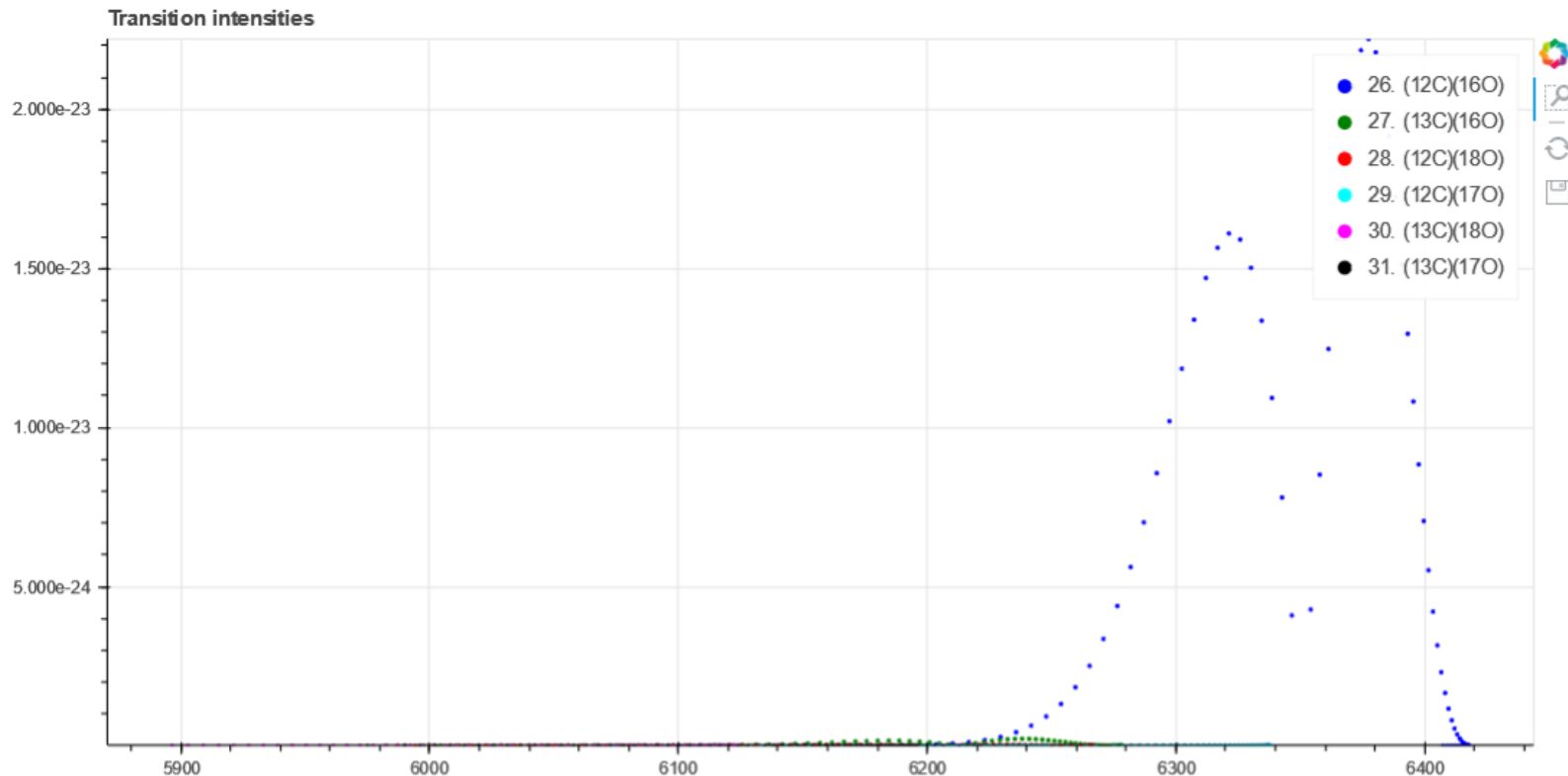
Search Results

708 transitions written in 4.02 secs (query time: 0.05 secs).

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3 output files were generated using the output format *.par* (160 chars).

6167df73.par	[112.0 KB]	view in browser	Output transitions data (160-character .par format)
6167df73.bib.html	[8.9 KB]	view in browser	List of sources (html format)
6167df73.bib	[4.8 KB]	view in browser	List of sources (BibTeX format)



Hover the mouse pointer over parameters below for citation and notes.

Isotopologue	ν	S	A	γ_{air}	γ_{self}	E''	n_{air}	δ_{air}	J'	J''
$^{13}\text{C}^{18}\text{O}$	5896.4479	1.219e-31	0.003468	0.0432	0.046	1953.1202	0.67	-0.009	32	33
$^{13}\text{C}^{18}\text{O}$	5902.7851	2.084e-31	0.003514	0.0438	0.046	1838.582	0.67	-0.009	31	32
$^{13}\text{C}^{18}\text{O}$	5909.0354	3.501e-31	0.00356	0.0443	0.047	1727.4728	0.67	-0.009	30	31

Referencing Multiple Sources

¹² C ¹⁸ O	6140.6839	1.337e-26	0.005193	0.0553	0.059	384.2612	0.72	-0.007	13	14
¹² C ¹⁷ O	6141.6383	4.729e-29	0.004659	0.0471	0.05	1312.6581	0.67	-0.008	25	26
¹³ C ¹⁷ O	6141.6494	4.207e-29	0.005023	0.0712	0.077	10.7362	0.74	-0.005	3	2
¹³ C ¹⁶ O	6141.8175	4.83e-26	0.005089	0.0538	0.058	499.5146	0.7	-0.008	15	16
¹² C ¹⁸ O	6141.9807	5.238e-30	0.02402	0.0651	0.071	2128.4137	0.74	-0.006	5	4
¹² C ¹⁷ O	6143.0759	5.324e-31	0.02364	0.0569	0.062	2405.8643	0.74	-0.007	11	12
¹³ C ¹⁶ O	6143.5520	1.317e-29	0.02055	0.0757	0.081	2099.7101	0.75	-0.005	2	1
¹² C ¹⁶ O	6144.8286	2.448e-29	0.02102	0.0477	0.051	3378.9537	0.67	-0.008	24	25
¹³ C ¹⁷ O	6144.8503	5.389e-29	0.00528	0.0677	0.074	21.472	0.74	-0.006	4	3
¹² C ¹⁶ O	6144.8924									
¹² C ¹⁸ O	6145.0227									
¹² C ¹⁸ O	6145.6023									
¹³ C ¹⁶ O	6146.9004									
¹³ C ¹⁶ O	6146.9495									
¹² C ¹⁶ O	6147.0017									
¹² C ¹⁷ O	6147.8670									
¹² C ¹⁷ O	6147.8924									
¹³ C ¹⁷ O	6147.9565									
¹² C ¹⁸ O	6147.9662									
¹² C ¹⁶ O	6149.7093									
¹³ C ¹⁶ O	6150.1502									
¹² C ¹⁸ O	6150.4248									
¹² C ¹⁸ O	6150.8113									
¹³ C ¹⁷ O	6150.9677									
¹² C ¹⁶ O	6151.1146	3.767e-29	0.02131	0.0483	0.051	3284.0846	0.67	-0.008	23	24
¹³ C ¹⁶ O	6151.9853	7.522e-26	0.005251	0.0553	0.059	385.7275	0.72	-0.007	13	14
¹² C ¹⁷ O	6152.6093	6.876e-31	0.02448	0.0586	0.064	2320.5079	0.75	-0.007	9	10
¹³ C ¹⁶ O	6153.3014	2.911e-29	0.0243	0.0651	0.071	2132.4969	0.74	-0.006	5	4
¹² C ¹⁸ O	6153.5578	6.259e-30	0.02638	0.0595	0.065	2222.7523	0.75	-0.006	9	8

1326. I.E. Gordon (2020). Intensities of the bands with $\Delta v=3$ from Ref. [1326a] were multiplied by a factor 1.026 based on the experimental works from Ref. [1326b] and Ref. [1326c]..

- 1326a. G. Li, I.E. Gordon, L.S. Rothman, Y. Tan, S.-M. Hu, S. Kassi, A. Campargue, E.S. Medvedev, "Rovibrational Line Lists for Nine Isotopologues of the CO Molecule in the $X^1\Sigma^+$ Ground Electronic State", *The Astrophysical Journal Supplement Series* **21615** (2015). [[link to article](#)] [ADS]
- 1326b. A. Cygan, P. Wcisło, S. Wójtewicz, G. Kowzan, M. Zaborowski, D. Charczun, K. Bielska, R. S. Trawiński, R. Ciuryło, P. Masłowski, D. Lisak, "High-accuracy and wide dynamic range frequency-based dispersion spectroscopy in an optical cavity", *Optics Express* **27**21810 (2019). [[link to article](#)] [ADS]
- 1326c. Y. Borkov, A. Solodov, A. Solodov, T. Petrova, E. Karlovets, V. Perevalov, "Fourier transform CO spectra near 1.6 μm ", *Journal of Quantitative Spectroscopy and Radiative Transfer* **253**107064 (2020). [[link to article](#)] [ADS]

Future Updates

- Adding continuum absorption by water vapor. Working with Eli Mlawer's group at AER on parametrizing both self and foreign continuum to be included in HITRAN
- New trace species. More isotopologues for existing molecules
- More bands for trace gases, especially in the FIR/TIR
- More lines with sophisticated line shapes. The new requirements for spectral uncertainties have been reduced to 0.1%!
- More CIA and laboratory cross-sections (got permission to get the rest of PNNL). Wider temperature regimes
- Increase user engagement

Acknowledgments:



We would like to thank all the contributors and collaborators who have worked towards the HITRAN2020 edition and validated the data. It was not easy in the times of pandemic.

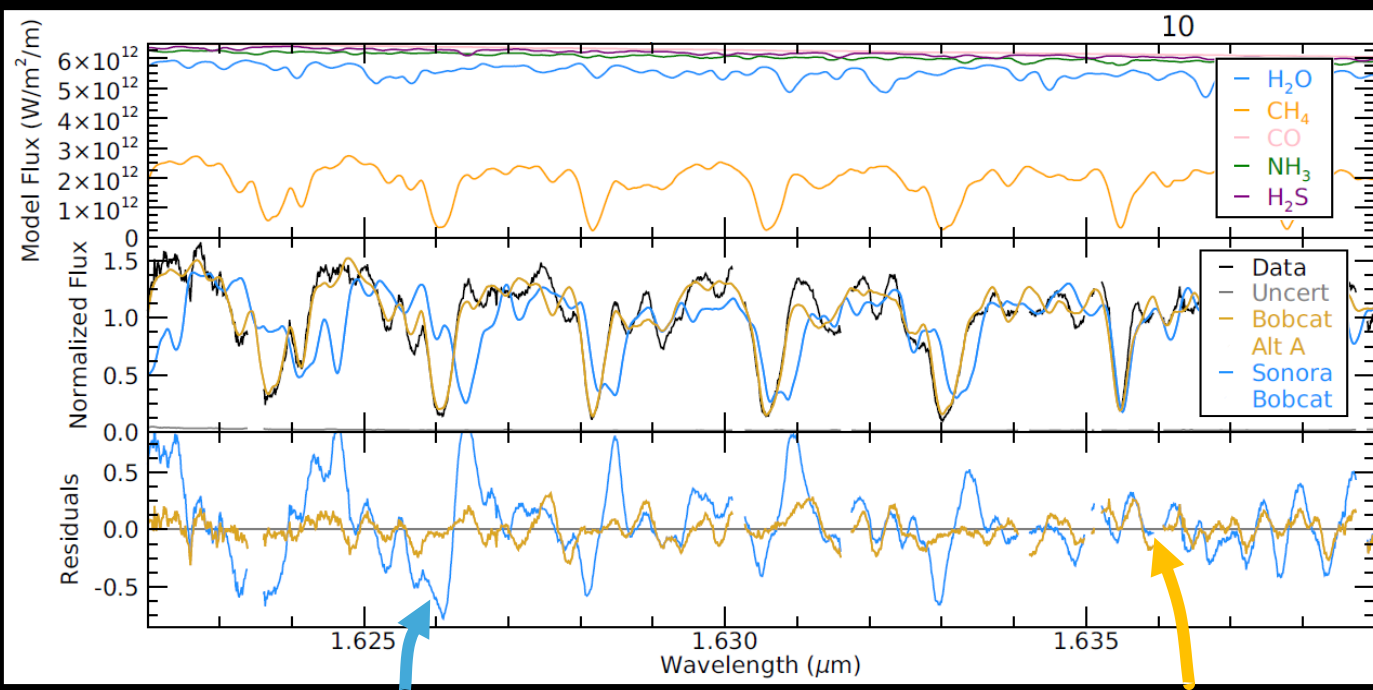
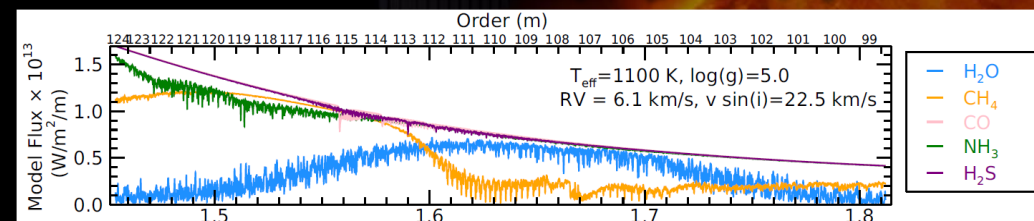


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HITEMP FOR BROWN DWARFS

- T-class brown-dwarfs often referred to as “methane” dwarfs due to onset of CH₄ absorption
- *H* and *K* spectral bands used for classification

▼ H band overview from Tannock et al. (2022), MNRAS, *in press*



Model with ExoMol CH₄

Model with HITEMP CH₄

- Tannock et al. (2022), *in press*
- 1.46–2.48 μm measurements
 - T6 (1060 K)
 - $R=45,000$ (Gemini South/IGRINS)
- **CH₄ HITEMP** list provides clear improvement for brown dwarfs models
 - “Bobcat Alt A” model

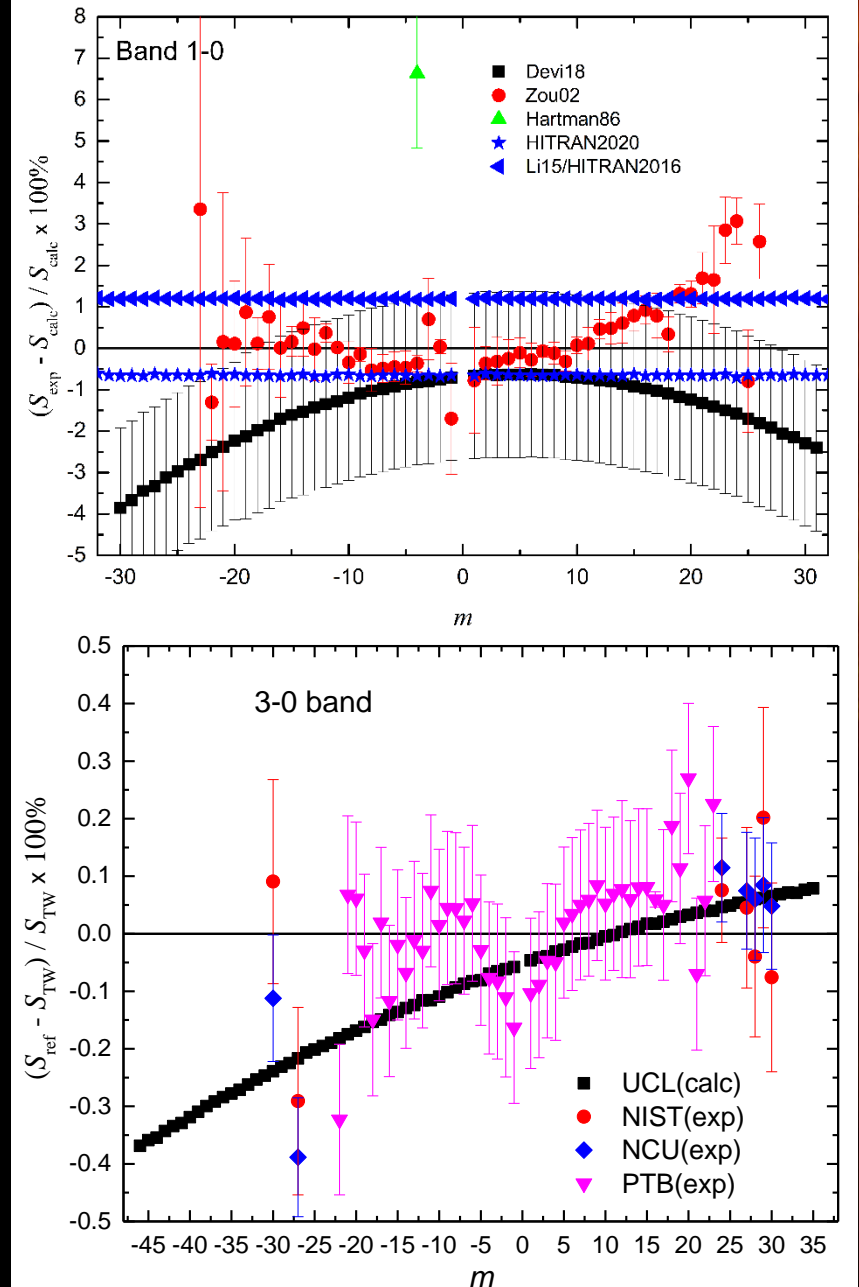
▼ from Tannock et al. (2022), MNRAS, *in press*



CO IMPROVEMENTS

- CO in HITEMP originates from Li et al. (2015)
- HITRAN2020 contained intensity scaling for some bands to make more consistent with modern observations
 - Not carried over to HITEMP
- New *ab initio* data from Meshkov, et al. (2022), *JQSRT* 280,108090
 - Positions and intensities can be used for updating HITRAN and HITEMP
 - Improvements shown for 1-0 and 3-0 bands
 - The 3-0 band comparison with very highly accurate experiments from Bielsja et al. (2022) *Phys Rev Letters*

▼ From Meshkov et al. (2022)



Access to different broadeners

HITRANonline Logged in as louli Gordon | [Logout](#)

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

Line-by-Line Search ⚙️ ⌚ 👤

New Output Format

Edit this output format by dragging (or double-clicking) parameters. Reorder them by dragging rows within the table.

[Save and Return to Data Search](#) [Cancel](#)

Output Format Name:

Description:

Here we select broadening and shifting parameters due to the pressure of H₂ and He along with their uncertainty codes and references.

Field separator: Fixed width format ⓘ

Line endings: Output header line

HDF5 output

New Output Format

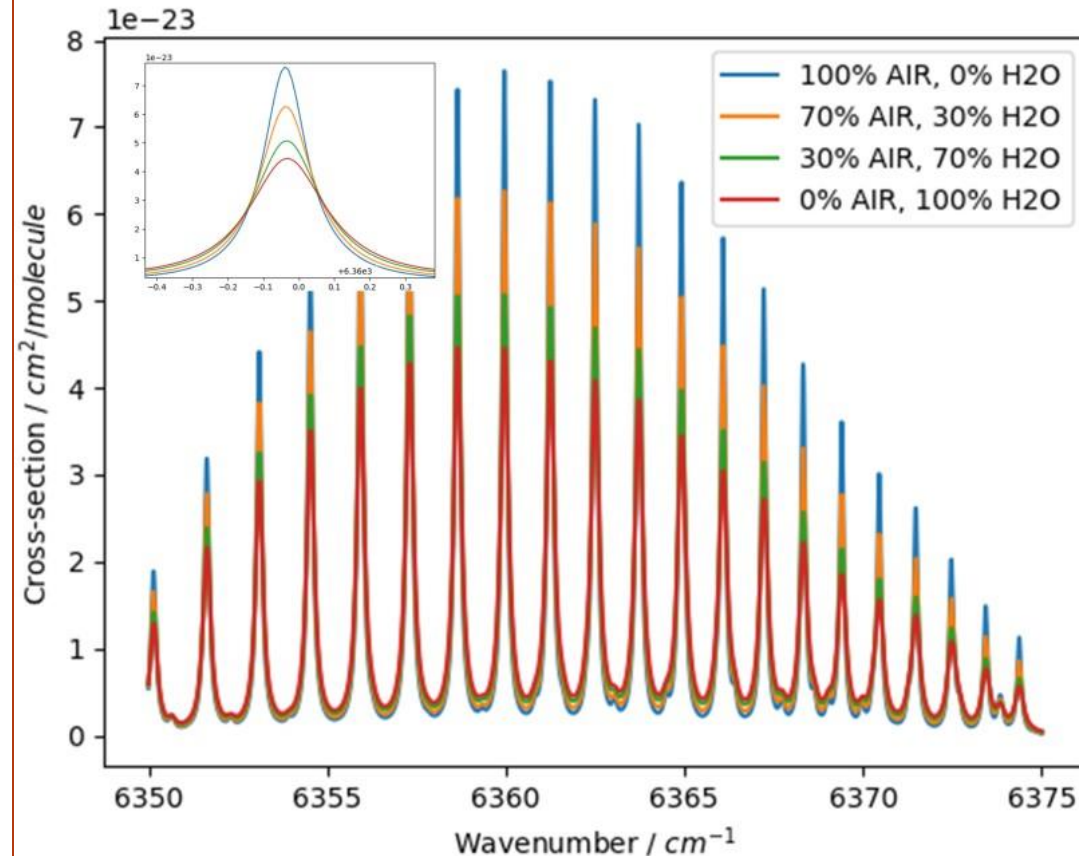
Parameter	Units	Fortran Format	Err	Ref
ⓘ Molecule ID		I2		
ⓘ Isotopologue ID		I1		
ⓘ ν	cm ⁻¹	F12.6	☑	☑
ⓘ ν_{H_2}	cm ⁻¹ ·atm ⁻¹	F6.4	☑	☑
ⓘ ν_{H_2}		F7.4	☑	☑
ⓘ δ_{H_2}	cm ⁻¹ ·atm ⁻¹	F9.6	☑	☑
ⓘ ν_{He}	cm ⁻¹ ·atm ⁻¹	F6.4	☑	☑
ⓘ ν_{He}		F7.4	☑	☑
ⓘ δ_{He}	cm ⁻¹ ·atm ⁻¹	F9.6	☑	☑

Available Parameters

Parameter	
ⓘ Y_{air}	E10.3
ⓘ qns'	A256
ⓘ qns''	A256
ⓘ $\beta_{G, self}$	F9.6
ⓘ Transition ID	I12
ⓘ .par line	A160
ⓘ δ'_{H_2}	E10.3
ⓘ ν_{CO_2}	F6.4
ⓘ ν_{CO_2}	F7.4
ⓘ δ_{CO_2}	F9.6

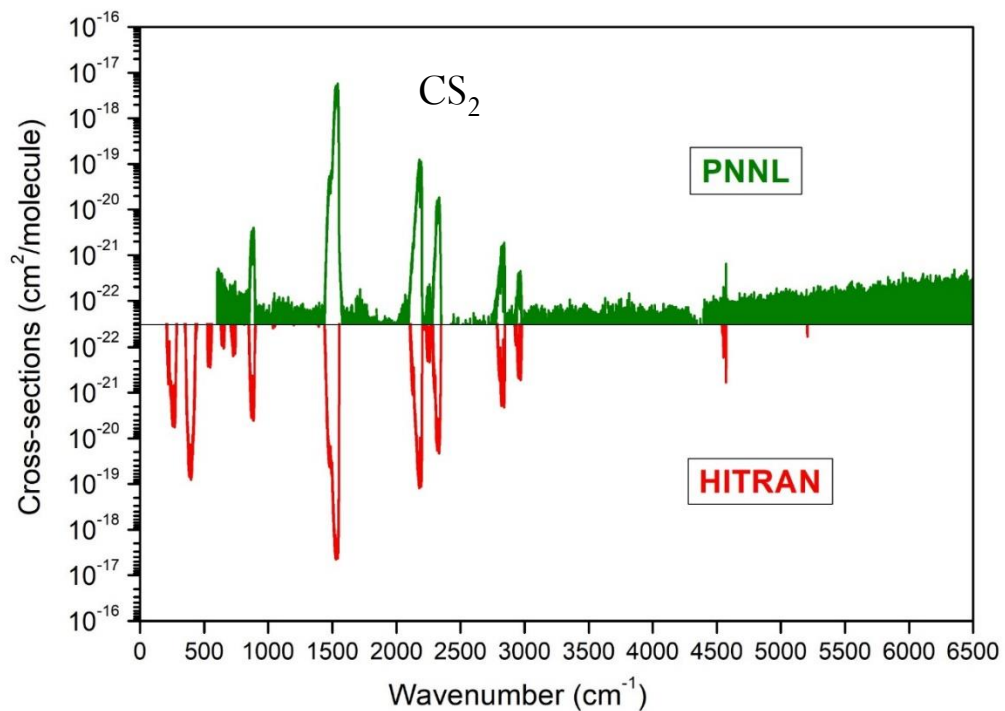
Broadening by H₂O added for the first time

```
16 h.fetch('co2', 2, 1, 6350.0, 6375.0,  
17       ParameterGroups=('voigt_h2o',))  
18  
19 mix = [  
20     {'air':1.0, 'h2o':0.0},  
21     {'air':0.7, 'h2o':0.3},  
22     {'air':0.3, 'h2o':0.7},  
23     {'air':0.0, 'h2o':1.0},  
24 ]  
25  
26 leg = []  
27 for d in mix:  
28     leg.append(make_legend(d))  
29 nu, xsc = h.absorptionCrossSection(  
30     SourceTables='co2',  
31     Diluent=d,  
32     profile='Voigt',  
33     WavenumberRange=[NUMIN, NUMAX],  
34 )  
35 pl.plot(nu, xsc)
```

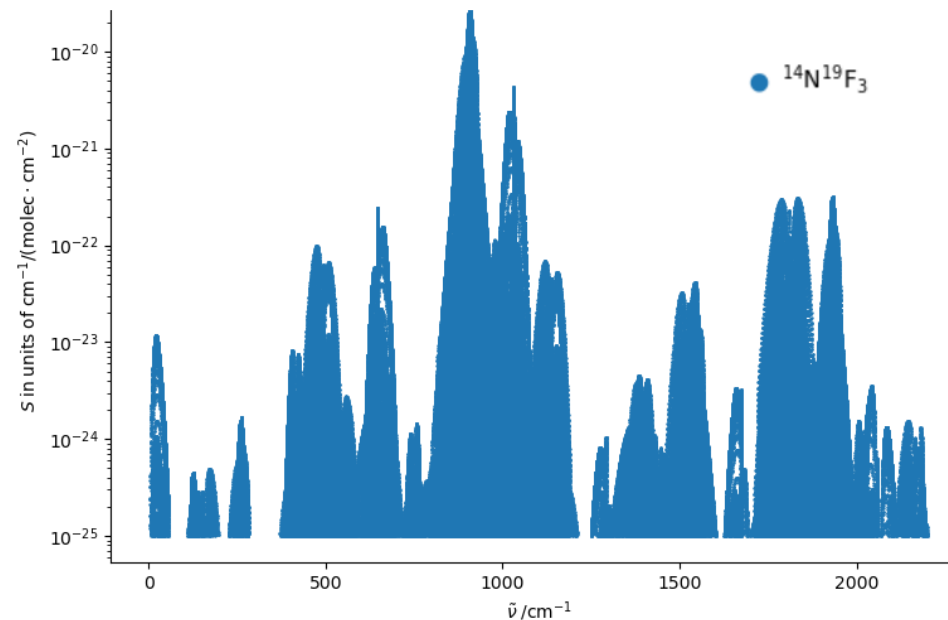
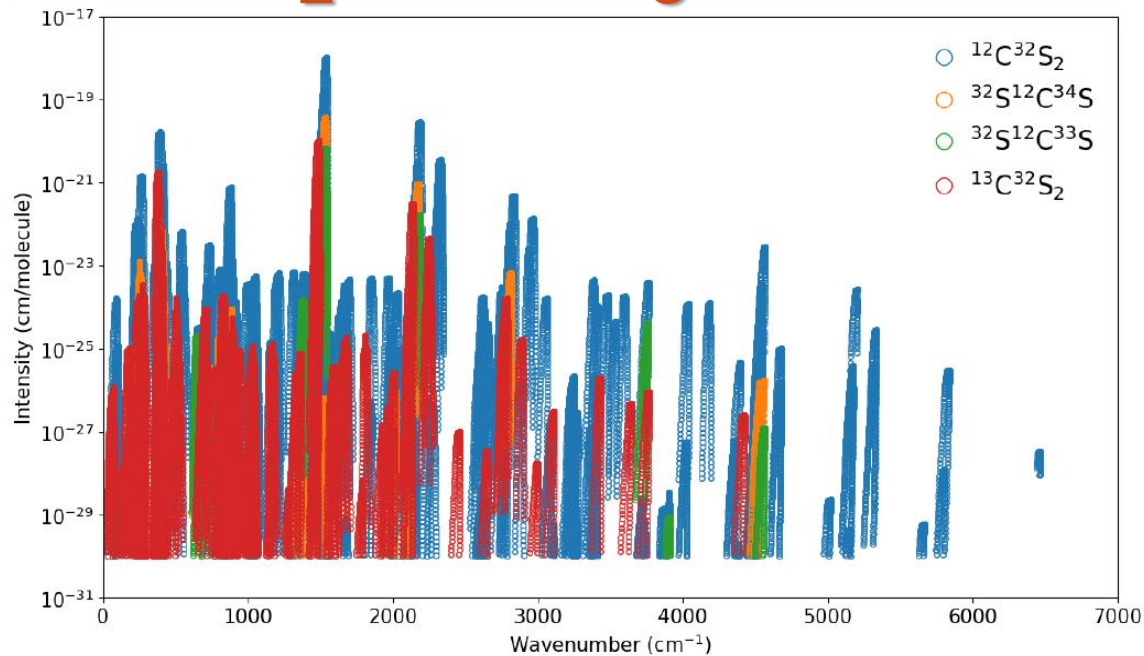


Already available: CO₂, N₂O, CO, CH₄, O₂, NH₃, and H₂S broadened by water.
Tan, et al., J. Geophys. Res. Atmos. 33 (2019) 2019JD030929

New molecules (examples CS₂ and NF₃)

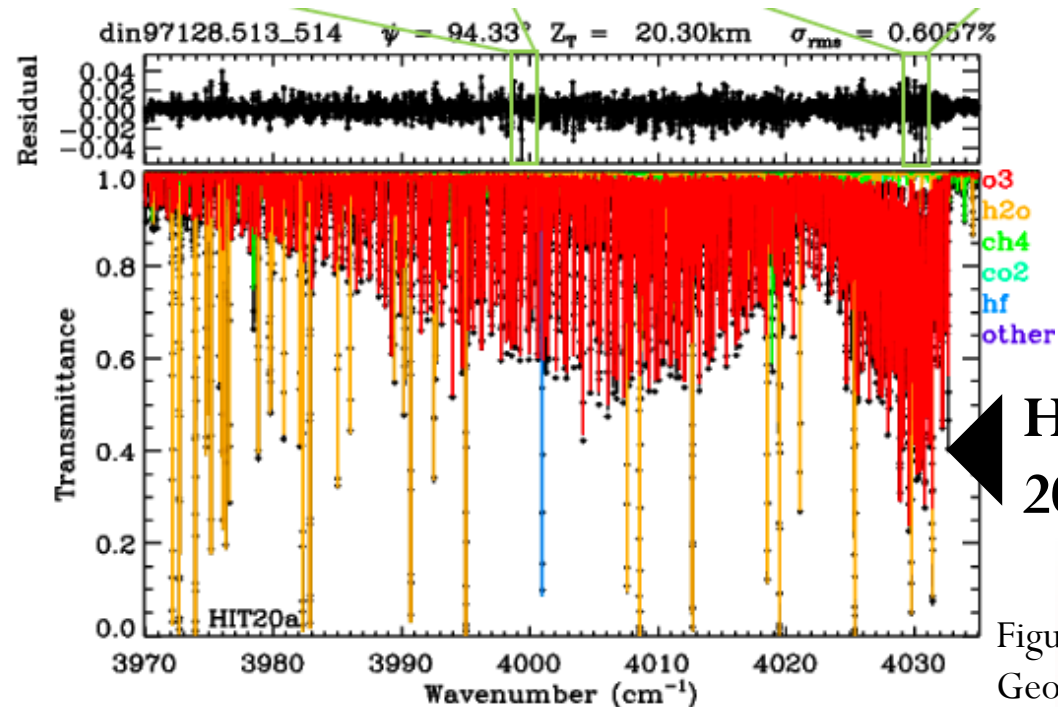
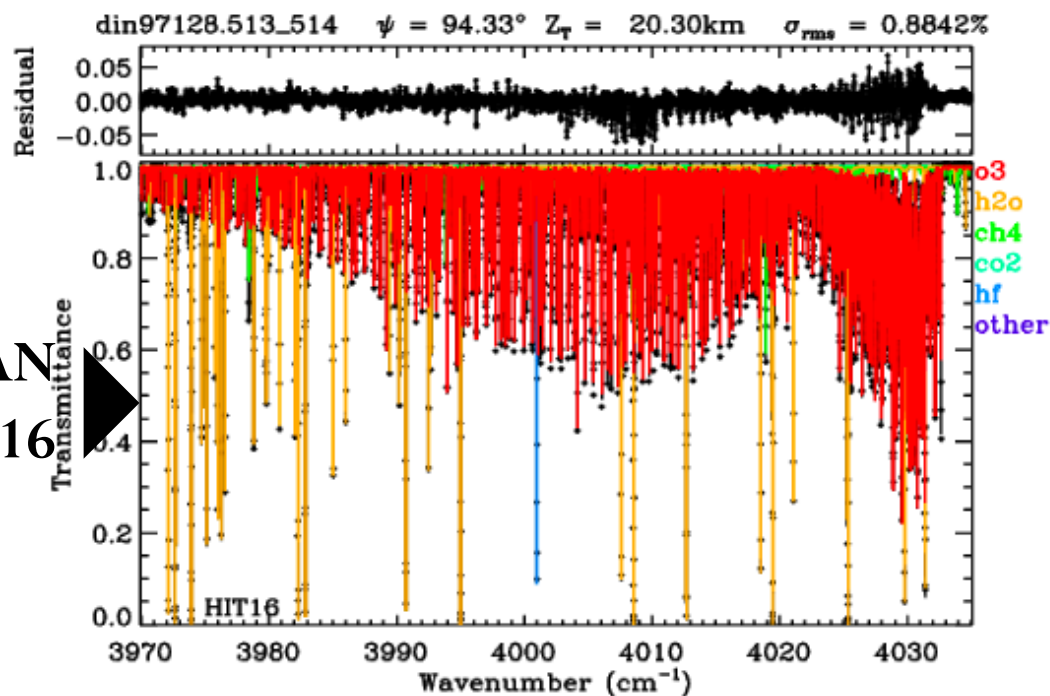


- CS₂ line list is based on Karlovets et al. (2020) JQSRT 258, 107275
- NF₃ line list is based on Egorov et al., JQSRT(2019) 239, 106668



Ozone (contd..) overall reduction of RMS

- The RMS values are reduced throughout the spectral regions. In particular, line positions are much improved. See validation with a balloon spectra below.



HITRAN
2016

HITRAN
2020

Figure credit:
Geoff Toon (JPL)

Accessing HITRAN with HAPI

○ HAPI (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

Many more options to include
additional parameters, filtering
etc.

Upcoming:

- HAPI v2.0
 - Kochanov et al. (2021), *in prep*
- HAPIEST
 - Karns et al. (2021), *in prep*