CO_2 Spectroscopy Evaluation: 600 to 7000 cm^{-1}

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Various CO_2 linelists including HITRAN 2008, 2012, and 2016 (two versions), have been evaluated by fitting lab (mainly Kitt Peak) and atmospheric solar absorption (MkIV & TCCON) spectra.

The 600-7000 cm^{-1} region was divided into 40 windows, most encompassing at least one complete CO_2 absorption band or a sub-branch. Regions with no discernable CO_2 absorption were skipped.

RMS fitting residuals and retrieved CO_2 amounts for each of the 40 windows are compared among linelists.

Only the CO_2 linelist is changed. For all other gases ATM_2016 is used, after extracting all the CO_2 lines. So any difference in the RMS or the retrieved CO_2 amounts is entirely attributable to the CO_2 linelist.

A new “greatest hits” linelist (ATM18) was developed by merging the best predecessor linelists. Also some manual adjustments were performed to remove obvious position errors and inconsistencies.

The Linelists Evaluated

HITRAN 2008: 314,919 lines

HITRAN 2012: 471,847 lines

ATM 2016: 450,493 lines
Based mainly HITRAN 2012. Uses Toth (2009) for the 5740-6500 cm^{-1} region because it gave better fits (and still does). Empirical adjustments throughout.

HITRAN 2016a: 554,183 lines
Based on files the linelist that Iouli Gordon sent me June 27, 2017 (O2_hit16_first-9iso) and on June 30, 2017 (hit838corr). Before using, I fixed 19 lines with ABHW=0 and one with an intensity of zero.

HITRAN 2016b: 554,879 lines
Downloaded from HITRAN-Online website on Nov 28, 2017 (5a1de32a.par). Includes isotopologs 11 & 12. A format of "f5.3" had been enforced for SBHW, which has changed for some lines that were previously "f5.4", e.g.
25 3.681760 1.943E-33 1.457e-12.0865.1155 in HIT16a
became
25 3.681760 1.943E-33 1.457e-12.08650.116 in HIT16b

ATM 2018: 523,221 lines (new linelist)
Mostly HITRAN 2018b, except in regions where ATM 2016 or HITRAN 2008 were better.

Laboratory Spectra of CO_2

137 spectra from Kitt Peak and 13 from JPL (via Keeyoon Sung)

All at room temperature except for one at 235K.

Pressures from 0.1 to 700 Torr.

23 Kitt Peak spectra are enriched in ^{13}C, giving the lab spectra a much higher sensitivity to spectroscopic errors in isotopologs 2, 5, 6, 10, 11, 12, than atmospheric spectra.

Spectral coverage from 600 to 12,000 cm^{-1}, although we only investigate 600 to 7000 cm^{-1} in this evaluation.

Of the 6000 potential spectral fits (40 windows x 150 spectra), only 1813 (30.6%) could actually be performed due to the limited spectral coverage of the individual spectra.

This makes it difficult to compare intensities measured at low wavenumbers with those from high wavenumbers because these are never in the same spectrum.

Fitted Lab Windows

Table summarizes the 40 windows in which the lab spectra were fitted. Includes everywhere that there are discernable CO_2 lines, except for regions with unfittable artifacts. Collectively, these windows cover over 3000 cm^{-1}.

A particular window covers the range: Center-Width/2 to Center+Width/2

NCBF is the order of the polynomial fitted to the continuum level.

ISO_{bar} is the strength-weighted isotope number. A value of 1.0 means that the lines in the window are mainly $^{12}C^{16}O_2$. A value of 2.0 indicates $^{13}CO_2$ lines. A value of 3.0 indicates ^{18}OCO.

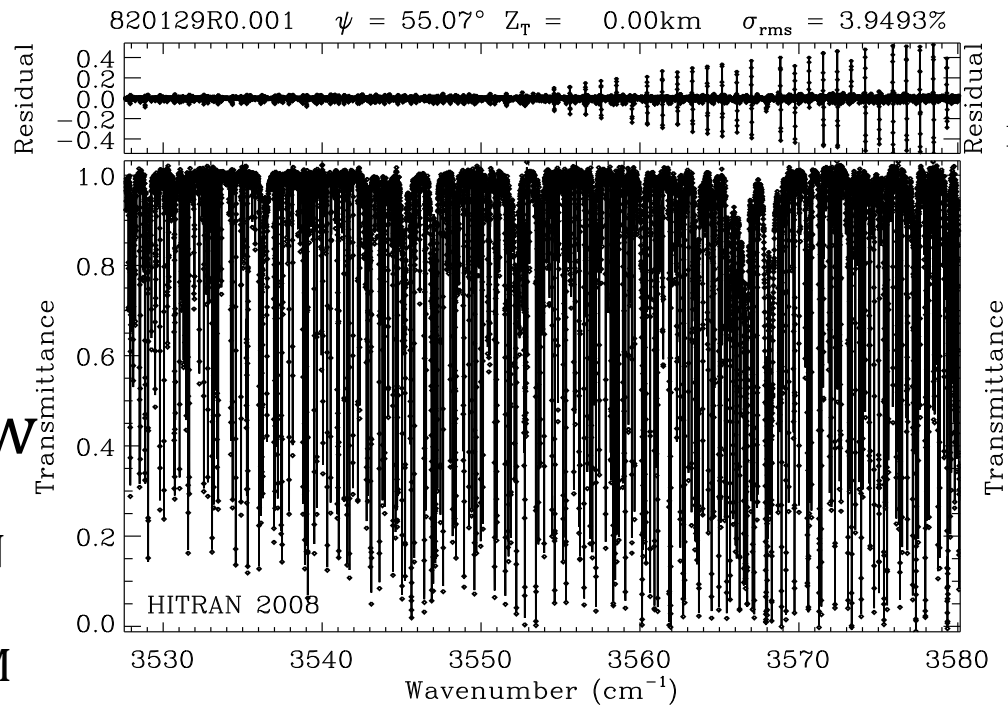
S_{max} is the largest CO_2 line strength.
S_{tot} is the sum of the CO_2 strengths
S_{bar} is the mean CO_2 line strength
$ABHW_{bar}$: mean (S-weighted) ABHW
E''_{bar} : mean (strength-weighted) E"

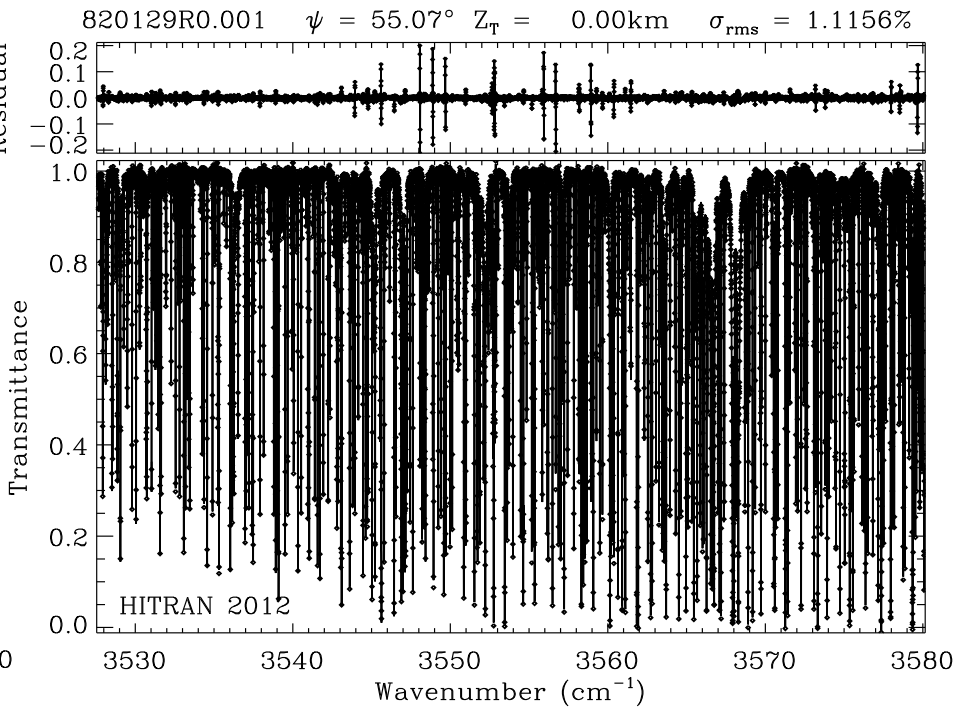
These properties depend only on the window, not the measured spectra.

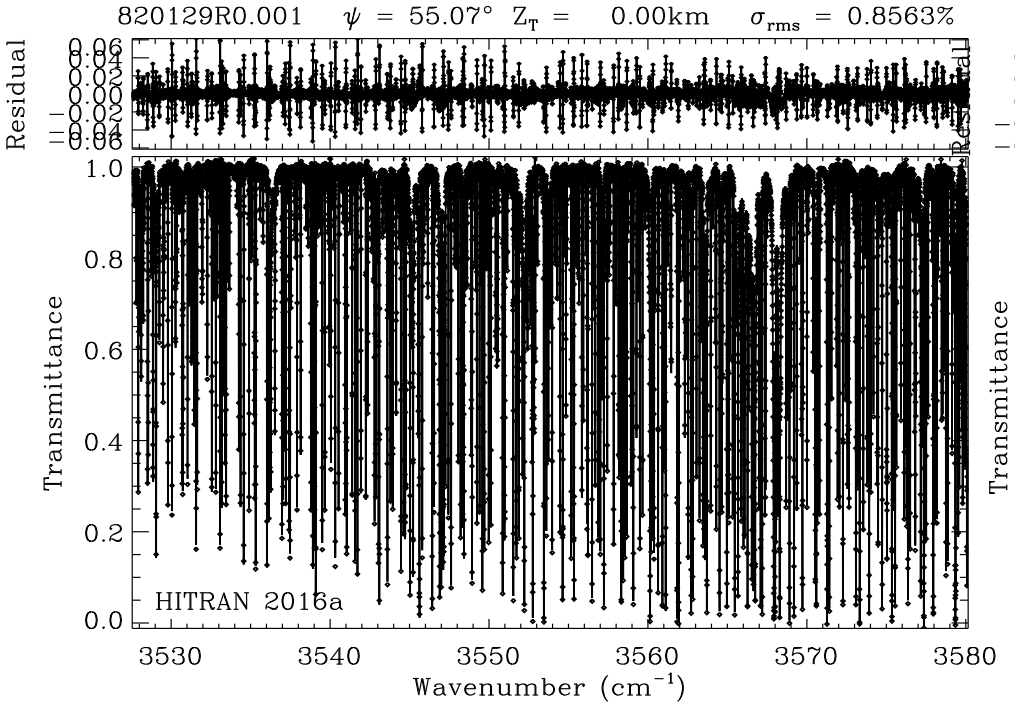
Center	Width	MIT A I F	NCBF	Gases to fit	Iso_{bar}	S_{max}	S_{tot}	S_{bar}	$ABHW_{bar}$	E''_{bar}
693.50	49.40	20 1 1 0	10 :	co2 h2o	1.01	1.707E-19	2.929E-18	1.051E-19	0.0740	335.3
754.50	65.50	20 1 1 0	10 :	co2 h2o	1.01	2.965E-21	4.756E-20	1.829E-21	0.0742	998.8
827.20	68.60	20 1 1 0	15 :	co2 h2o	1.01	1.570E-23	2.546E-22	9.940E-24	0.0743	1597.6
925.00	72.10	20 1 1 0	8 :	co2 h2o	1.03	2.147E-23	3.348E-22	1.336E-23	0.0745	1686.9
980.00	42.10	20 1 1 0	5 :	co2 h2o nh3	1.01	2.244E-23	3.086E-22	1.605E-23	0.0744	1586.3
1056.40	93.80	20 1 1 0	9 :	co2 h2o	1.02	3.461E-23	9.952E-22	2.225E-23	0.0745	1553.0
1239.50	40.60	20 1 1 0	5 :	co2 h2o	3.05	5.651E-25	1.801E-23	3.594E-25	0.0745	274.2
1280.60	39.80	20 1 1 0	5 :	co2 h2o ch4	3.07	5.996E-25	1.806E-23	4.081E-25	0.0741	216.9
1367.40	51.80	20 1 1 0	5 :	co2 h2o ch4	3.07	6.561E-25	3.536E-23	4.497E-25	0.0753	196.2
1857.40	16.50	20 1 1 0	4 :	co2 h2o	1.13	5.761E-25	6.328E-24	4.282E-25	0.0691	1101.4
1906.50	71.00	20 1 1 0	5 :	co2 h2o	1.02	2.789E-23	6.322E-22	1.539E-23	0.0726	359.6
1958.00	28.60	20 1 1 0	5 :	co2 h2o	1.01	3.045E-24	3.545E-23	2.205E-24	0.0685	595.2
1982.50	17.00	20 1 1 0	4 :	co2 h2o	1.13	9.520E-25	5.430E-24	4.171E-25	0.0673	1196.4
2082.00	178.00	20 1 1 0	5 :	co2 h2o co n2o	1.02	2.017E-22	6.184E-21	1.062E-22	0.0737	378.0
2299.00	202.00	20 1 1 0	5 :	co2 h2o n2o co ch4	1.02	3.542E-18	1.012E-16	2.294E-18	0.0749	261.1
2432.00	67.00	20 1 1 0	7 :	co2 n2o ch4	1.03	2.499E-24	6.402E-23	1.798E-24	0.0754	1469.9
2502.00	70.00	20 1 1 0	4 :	co2 n2o hdo ch4	2.95	2.547E-25	1.508E-23	1.653E-25	0.0744	304.7
2601.00	96.00	20 1 1 0	5 :	co2 n2o hdo ch4	3.05	4.210E-25	2.491E-23	2.698E-25	0.0745	250.8
2760.00	62.00	20 1 1 0	4 :	co2 h2o hdo n2o ch4	3.05	6.336E-26	3.579E-24	4.224E-26	0.0748	213.7
3155.00	42.00	20 1 1 0	5 :	co2 h2o n2o ch4	1.03	3.090E-25	5.115E-24	1.895E-25	0.0701	530.9
3207.00	50.00	20 1 1 0	5 :	co2 h2o n2o	1.00	5.059E-25	7.592E-24	3.531E-25	0.0704	419.7
3309.00	49.00	20 1 1 0	5 :	co2 h2o n2o	1.05	1.711E-24	2.793E-23	1.016E-24	0.0696	580.3
3364.00	52.00	20 1 1 0	5 :	co2 h2o n2o	1.00	4.951E-24	8.645E-23	3.016E-24	0.0713	422.2
3496.30	62.60	20 1 1 0	5 :	co2 h2o n2o	1.95	2.088E-22	4.161E-21	1.049E-22	0.0741	574.8
3548.85	42.50	20 1 1 0	5 :	co2 h2o n2o	1.21	2.200E-21	4.365E-20	8.405E-22	0.0718	925.2
3618.50	97.20	20 1 1 0	5 :	co2 h2o	1.03	3.835E-20	1.077E-18	2.525E-20	0.0750	242.1
3712.60	93.20	20 1 1 0	5 :	co2 h2o	1.01	5.851E-20	1.640E-18	3.828E-20	0.0751	259.1
3811.00	74.00	20 1 1 0	5 :	co2 h2o	1.03	2.299E-24	5.983E-23	1.589E-24	0.0753	1480.4
3872.00	32.00	20 1 1 0	5 :	co2 h2o	1.88	3.703E-26	1.858E-24	2.257E-26	0.0750	1310.5
3992.00	82.00	20 1 1 0	5 :	co2 h2o	1.22	2.389E-25	6.206E-24	1.145E-25	0.0712	1017.9
4622.00	83.00	20 1 1 0	5 :	co2 n2o	2.81	2.753E-25	1.867E-23	1.619E-25	0.0744	291.8
4812.00	184.00	20 1 1 0	6 :	co2 n2o	1.07	2.730E-22	8.292E-21	1.661E-22	0.0750	282.8
4962.00	116.00	20 1 1 0	6 :	co2 n2o	1.01	1.319E-21	3.708E-20	8.562E-22	0.0751	260.4
5096.00	152.00	20 1 1 0	6 :	co2 h2o n2o nh3	1.01	4.289E-22	1.216E-20	2.747E-22	0.0752	271.2
6072.00	98.00	20 1 1 0	5 :	co2	1.07	1.733E-24	5.046E-23	1.097E-24	0.0728	256.9
6211.00	128.00	20 1 1 0	6 :	co2	1.02	1.742E-23	4.966E-22	1.116E-23	0.0744	266.4
6338.00	124.00	20 1 1 0	6 :	co2	1.00	1.745E-23	4.844E-22	1.133E-23	0.0745	260.0
6506.00	124.00	20 1 1 0	6 :	co2	1.00	1.937E-24	5.783E-23	1.170E-24	0.0754	279.9
6769.00	82.00	20 1 1 0	6 :	co2 h2o	2.00	6.388E-25	1.762E-23	4.258E-25	0.0754	243.4
6940.00	120.00	20 1 1 0	8 :	co2 h2o	1.01	5.980E-23	1.688E-21	3.900E-23	0.0753	260.0

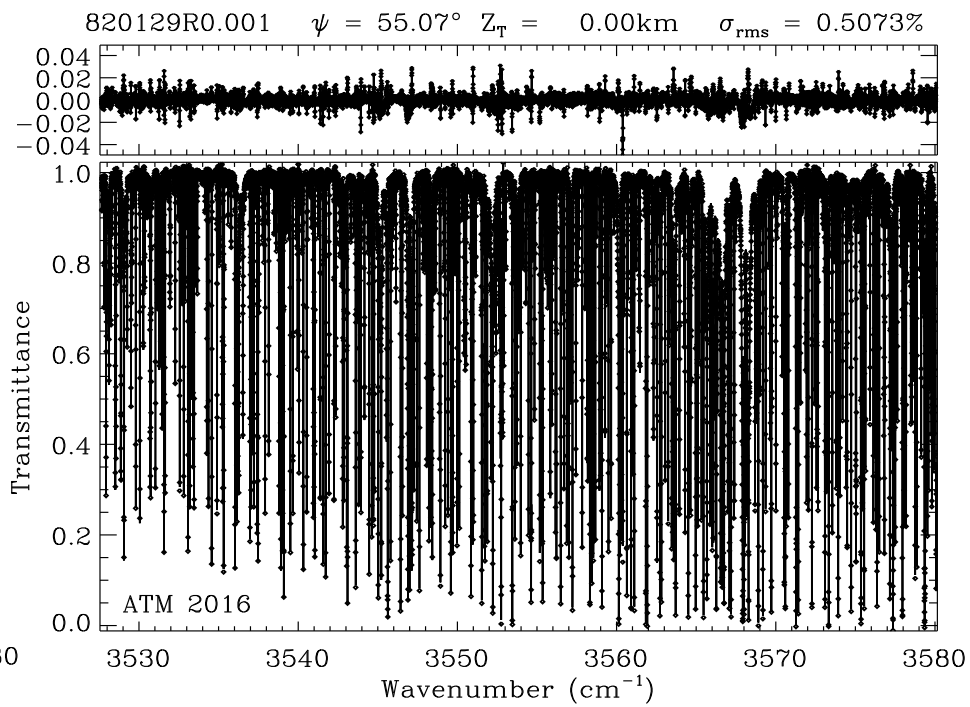
Examples of fits using various HITRAN linelist versions in the 3553 cm^{-1} window

In this window the HITRAN linelists show progressive improvements, but the ATM (based on empirical position improvements to HITRAN 2008 in this region) remains best of all.



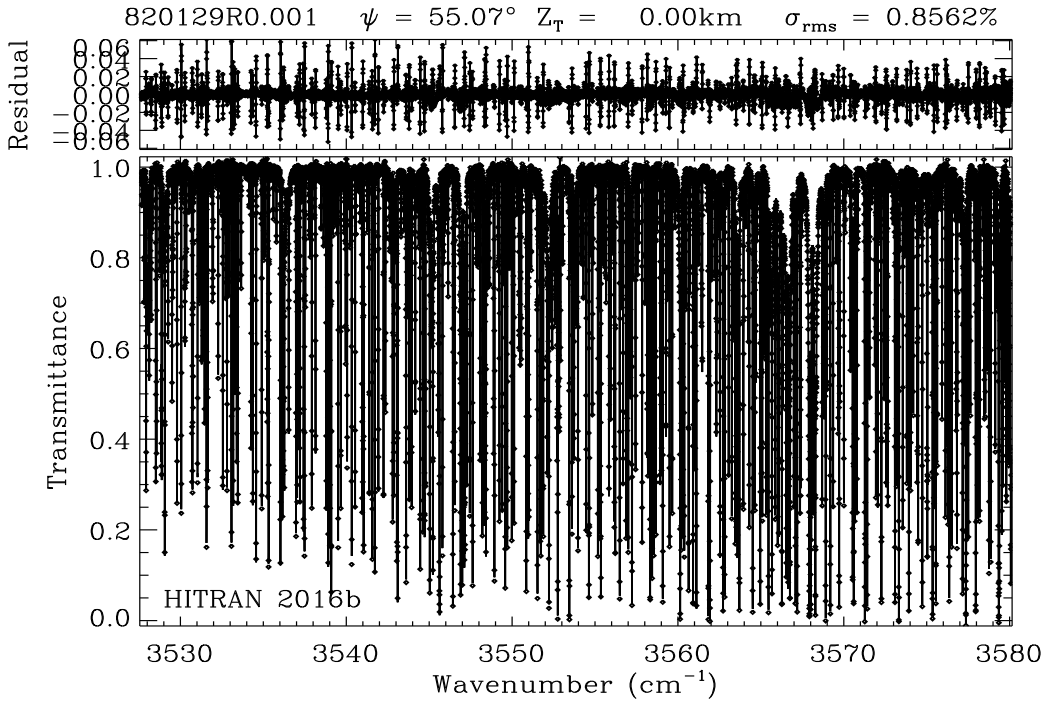


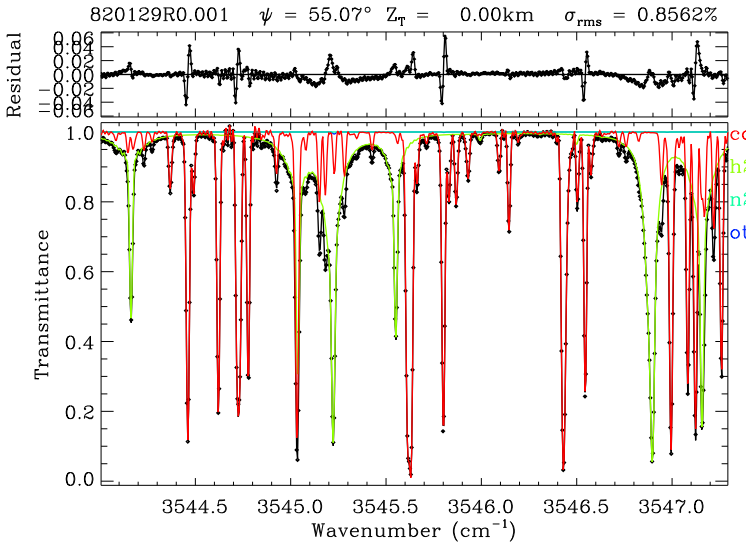


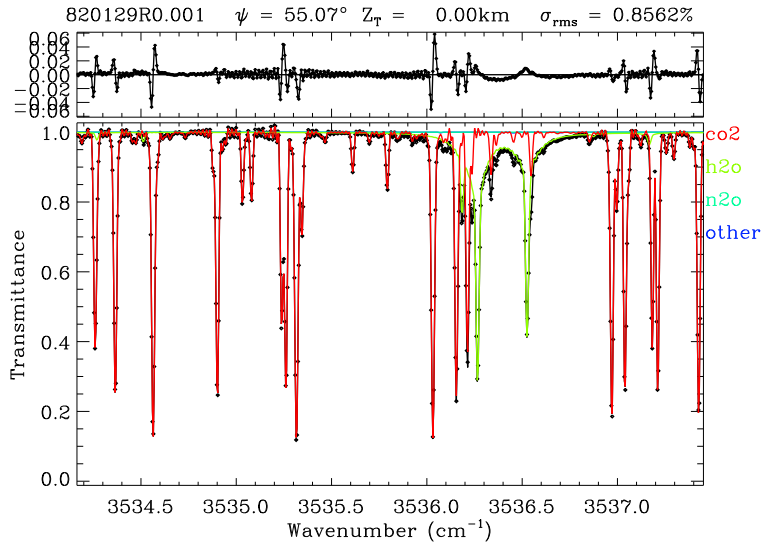


Examples of CO_2 fitting residuals in Kitt Peak lab spectra in the 3353 cm^{-1} window using the HITRAN 2016b linelist.

Lower panels zoom into some of the worst residuals and illustrate that they are due to position errors.







Average % RMS fitting residuals for Lab Spectra

148 spectra, 40 windows, 6 linelists

Each value in the table is an average rms spectral fitting residual for a particular window.

N_{used} shows the number of spectra fitted in each window, out of the 147 total.

Red values highlight the linelist(s) with the worst/largest RMS residuals.

Blue values highlight linelist(s) with the best/smallest RMS residuals.

Rectangles show the linelist adopted for ATM18

Bold in the right-hand column indicates that the rms is better than any predecessor due to manual adjustment of best predecessor.

iwin	f_{cen}	Width	N_{used}	N_{tot}	hit08	hit12	atm16	hit16a	hit16b	atm18
1	693.50	24.70	45	148	0.7401	0.7184	0.7184	0.7167	0.7166	0.7166
2	754.50	32.75	45	148	0.5754	0.5645	0.5645	0.5637	0.5638	0.5638
3	828.35	33.15	65	148	0.8157	0.8019	0.8019	0.8017	0.8017	0.8017
4	925.00	36.05	67	148	0.4319	0.4318	0.4318	0.4313	0.4313	0.4313
5	980.00	21.05	69	148	0.3195	0.3194	0.3194	0.3191	0.3191	0.3191
6	1056.40	46.90	69	148	0.4023	0.4008	0.4008	0.4001	0.4002	0.4002
7	1239.50	20.30	69	148	0.5242	0.5216	0.5216	0.5128	0.5129	0.5129
8	1280.60	19.90	69	148	0.8701	0.8702	0.8702	0.8670	0.8669	0.8669
9	1367.40	25.90	69	148	0.7757	0.7759	0.7759	0.7752	0.7752	0.7752
10	1857.40	8.25	40	148	0.1688	0.1691	0.1691	0.1565	0.1566	0.1566
11	1906.50	35.50	40	148	0.2260	0.2254	0.2254	0.2233	0.2233	**0.2226**
12	1958.00	14.30	40	148	0.1806	0.1788	0.1788	0.1753	0.1753	**0.1747**
13	1982.50	8.50	40	148	0.1411	0.1381	0.1381	0.1314	0.1315	0.1315
14	2082.00	89.00	40	148	0.2543	0.2485	0.2485	0.2437	0.2436	**0.2423**
15	2299.00	111.00	41	148	0.6661	0.5675	0.5665	0.5118	0.4958	**0.4766**
16	2432.00	33.50	43	148	0.1337	0.1337	0.1337	0.1323	0.1323	**0.1312**
17	2502.00	35.00	43	148	0.1194	0.1195	0.1195	0.1182	0.1182	**0.1140**
18	2601.00	48.00	43	148	0.1219	0.1220	0.1220	0.1192	0.1192	0.1192
19	2760.00	31.00	51	148	0.2735	0.2666	0.2666	0.2646	0.2645	0.2645
20	3155.00	21.00	42	148	0.2980	0.2981	0.2981	0.2980	0.2980	0.2980
21	3207.00	25.00	42	148	0.2717	0.2711	0.2711	0.2706	0.2706	0.2706
22	3309.00	24.50	42	148	0.2455	0.2463	0.2448	0.2440	0.2440	0.2440
23	3364.00	26.00	42	148	0.2729	0.2755	0.2714	0.2611	0.2611	0.2611
24	3496.30	31.30	42	148	0.8499	0.7988	0.6412	0.7042	0.7037	0.6101
25	3548.85	21.25	45	148	0.8323	0.6133	0.5794	0.6471	0.6472	**0.5475**
26	3618.40	48.60	45	148	1.0633	0.7627	0.7037	0.7178	0.7175	**0.6925**
27	3712.60	46.60	45	148	0.8219	0.6090	0.6066	0.6150	0.6140	**0.6063**
28	3811.00	37.00	45	148	0.2896	0.2891	0.2891	0.2891	0.2891	0.2891
29	3872.00	16.00	46	148	0.2776	0.2767	0.2767	0.2907	0.2907	0.2767
30	3991.00	42.00	43	148	0.1585	0.1566	0.1566	0.1565	0.1565	0.1565
31	4622.00	41.50	43	148	0.1576	0.1521	0.1521	0.1527	0.1527	**0.1512**
32	4812.00	92.00	37	148	0.1818	0.1829	0.1807	0.1893	0.1894	**0.1796**
33	4962.00	58.00	37	148	0.2962	0.2886	0.2860	0.2845	0.2849	**0.2796**
34	5096.00	76.00	37	148	0.2144	0.2156	0.2147	0.2127	0.2130	**0.2120**
35	6072.00	49.00	36	148	0.0899	0.0902	0.0894	0.0900	0.0901	**0.0887**
36	6211.00	64.00	35	148	0.1302	0.1289	0.1236	0.1281	0.1282	0.1236
37	6338.00	62.00	36	148	0.1374	0.1359	0.1299	0.1352	0.1354	0.1299
38	6506.00	62.00	31	148	0.1278	0.1280	0.1278	0.1281	0.1281	0.1278
39	6769.00	41.00	32	148	0.1820	0.1825	0.1825	0.1821	0.1822	0.1820
40	6940.00	60.00	32	148	0.2816	0.2819	0.2819	0.2833	0.2835	0.2816
Average over all windows:					**0.3730**	0.3489	**0.3420**	0.3436	0.3432	**0.3357**

RMS Residuals from fits to lab spectra – plotted versus cm^{-1}

The plot shows the RMS spectral fits averaged over the 150 lab spectra.

Upper panel shows absolute RMS values. Lower panel shows differences from HITRAN 2012 values.

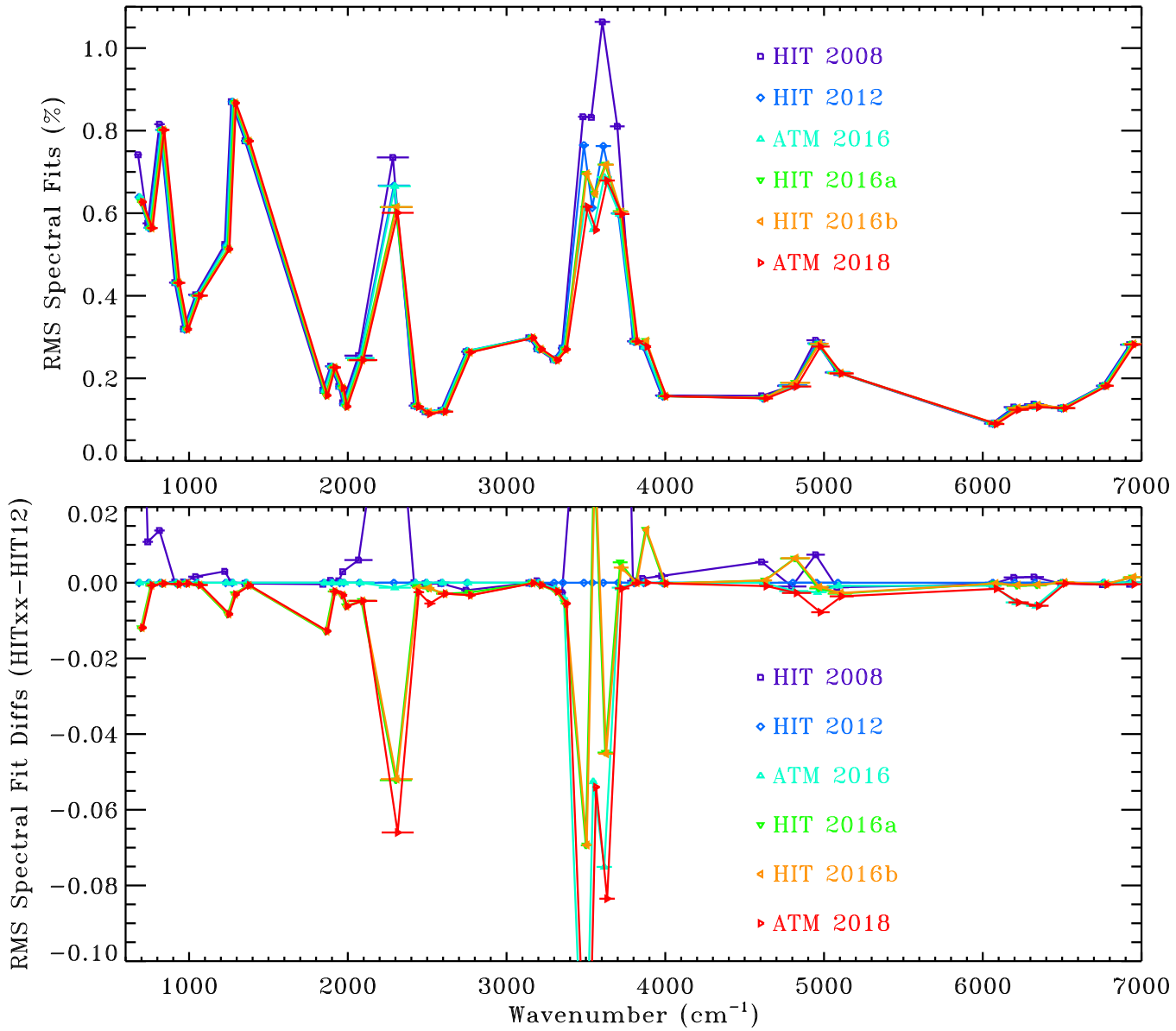
The absolute value of the RMS fit is unimportant. This is generally dominated by instrumental issues and interfering absorptions (e.g. H_2O).

Variation of RMS from linelist to linelist is entirely due to the CO_2 spectroscopy, since everything else is unchanged.

Big improvements are apparent for HITRAN16a,b in the 2300 cm^{-1} and the 3600 cm^{-1} regions.

HITRAN 2016a and b produce similar results. Differences can only be seen at 2300 and 3600 cm^{-1}.

ATM18 linelist provides the lowest RMS, or equal lowest, in every window. If it wasn't, the culpable lines would be replaced with those from whatever linelist was better.

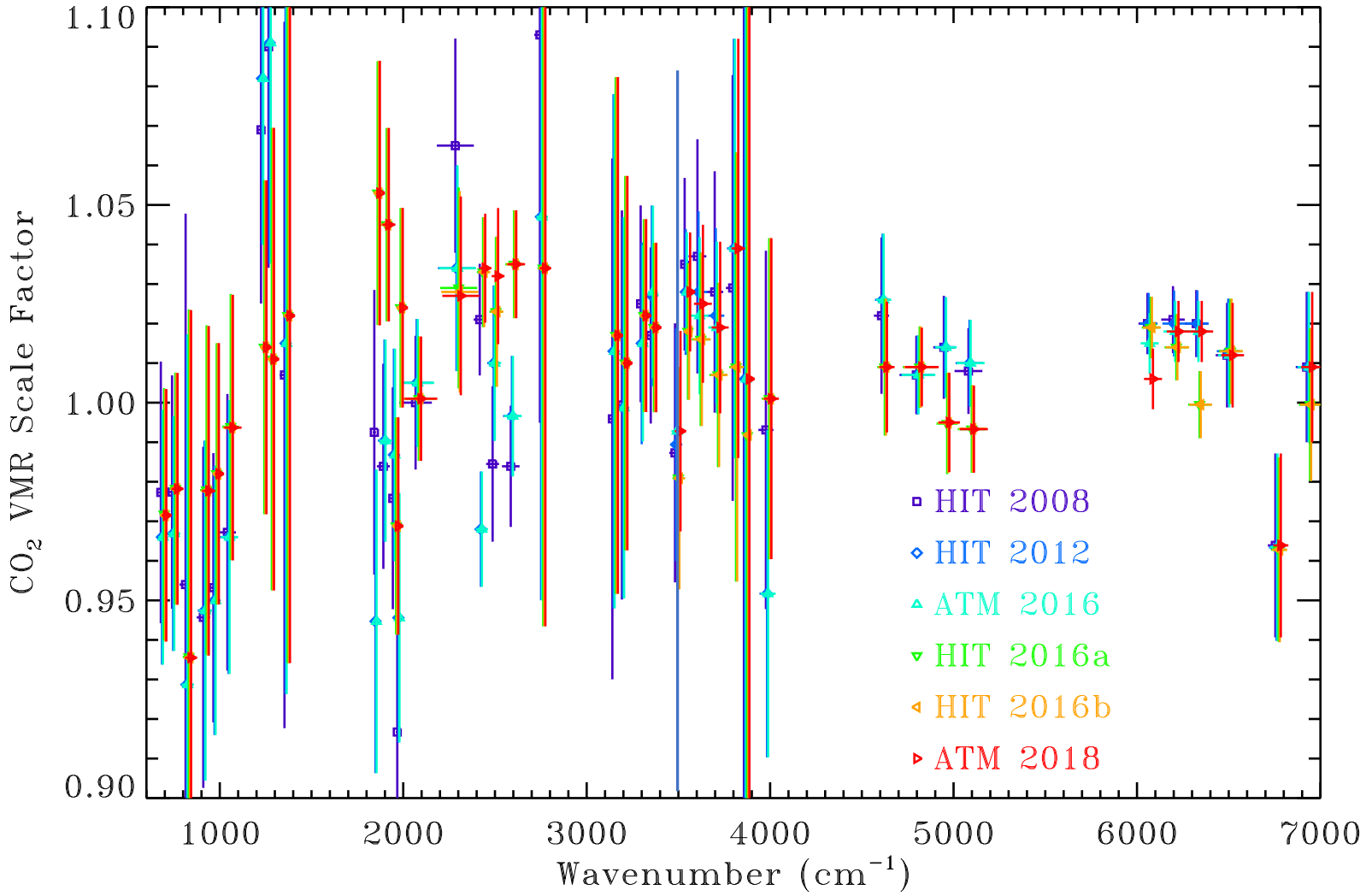


CO_2 VMR Scale Factors retrieved from lab spectra

The VSF is the retrieved CO_2 amount divided by the expected CO_2 amount. In a perfect world, the VSFs (y-values) would all be 1.00.

VSF values greater than 1 mean that the line intensities, or the absorber amounts, need to be multiplied by the VSF value.

Width and line position errors can also contribute to an incorrect retrieved CO_2 amount, but in this case the relationship between the VSF value and the width/position error is more complicated.



RMS Residuals from fits to lab spectra - Discussion

HITRAN 2008 is clearly the worst overall. But in 2/3 of the highest wavenumber windows, it is the best of all 5 linelists. ATM16 is the best overall.

Comparing HITRAN 16a and 16b, they produce very similar results but small differences due to truncation of SBHW to "f5.3" format in pure CO2 spectra and due to addition of isotopologs 11 and 12:

- In 15 windows HIT16a is slightly better
- In 18 windows they produce the same rms fit
- In 7 windows HIT16b is slightly better

The improvement in HIT16b over HIT16a due to the addition of isotopologs 11 & 12 is most notable in strong bands (2299, 3618, 3712 cm^{-1}) in ^{13}C-enriched spectra CO_2.

Comparing HITRAN 2012 with ATM 2016, they produce similar results

- In 14 windows ATM 2016 is better
- In 26 windows they produce equally good fits
- In 0 windows HITRAN 2012 is better

It is no surprise that HITRAN 2012 is nowhere better than ATM 2016. If it had been, I would have replaced the offending lines in ATM 2016 with those from HITRAN 2016. Additionally, empirical adjustments have been performed to the ATM linelist to fix obvious deficiencies (e.g., position errors).

Since only 1/148 lab spectra used here was below 290K, these results don't really validate the T-dependent parameters.

RMS Spectral Fitting Residuals: MkIV Balloon

MkIV instrument observes direct sunlight from balloon, covering the entire 650-5650 cm^{-1} region simultaneously at 0.01 cm^{-1} resolution (60 cm OPD)

Table shows % rms fitting residuals for each window, averaged over N_{row}= 19 spectra covering tangent altitudes from 9 to 38 km

34 windows, 6 linelists, 19 spectra, = 3876 fits

HITRAN 2012 is better than HITRAN 2008
HITRAN 2016 is better than HITRAN 2012

ATM16 is the best of the pre-2018 linelists, mainly due to the fact that line position errors in the 3480-3570 cm^{-1} region were fixed manually.

iwin	fcen	Width	Nrow	Npp	hit08	hit12	atm16	hit16a	hit16b	atm18
1	694.60	23.60	19	19	0.6794	0.6588	0.6588	0.6542	0.6542	0.6542
2	754.50	32.75	19	19	0.8275	0.7693	0.7693	0.7658	0.7658	0.7658
3	827.20	34.30	19	19	0.3490	0.3417	0.3417	0.3416	0.3416	0.3416
4	925.00	36.05	19	19	0.2931	0.2927	0.2927	0.2926	0.2926	0.2926
5	980.00	21.05	19	19	0.4609	0.4600	0.4600	0.4598	0.4598	0.4598
6	1056.40	46.90	19	19	0.4218	0.4223	0.4223	0.4217	0.4217	0.4217
7	1239.50	20.30	19	19	0.2529	0.2526	0.2526	0.2526	0.2526	0.2526
8	1280.60	19.90	19	19	0.4311	0.4308	0.4308	0.4308	0.4308	0.4308
9	1367.40	25.90	19	19	1.1333	1.1333	1.1333	1.1331	1.1331	1.1331
10	1857.90	7.65	19	19	0.5769	0.5770	0.5770	0.5756	0.5756	0.5756
11	1906.50	35.50	19	19	0.7017	0.7026	0.7026	0.7035	0.7035	**0.7013**
12	1958.00	14.30	19	19	0.5468	0.5440	0.5440	0.5498	0.5498	0.5440
13	1982.50	8.50	19	19	0.4958	0.4884	0.4884	0.4879	0.4879	0.4879
14	2082.50	88.50	19	19	0.7599	0.7532	0.7529	0.7519	0.7519	0.7519
15	2299.30	125.15	19	19	0.5408	0.5182	0.5182	0.4848	0.4845	**0.4799**
16	2430.60	32.10	19	19	0.1633	0.1628	0.1628	0.1628	0.1628	0.1628
17	2501.90	34.80	19	19	0.2067	0.2062	0.2062	0.2066	0.2066	0.2065
18	2601.00	48.00	19	19	0.2565	0.2559	0.2559	0.2560	0.2560	0.2560
19	2760.00	31.00	19	19	0.2641	0.2630	0.2630	0.2629	0.2629	0.2629
20	3155.00	19.00	19	19	0.5235	0.5229	0.5229	0.5222	0.5222	0.5222
21	3206.75	20.25	19	19	0.2183	0.2156	0.2156	0.2126	0.2126	0.2126
22	3309.00	24.50	19	19	0.2037	0.1913	0.1893	0.1877	0.1877	0.1877
23	3364.00	26.00	19	19	0.2434	0.2194	0.2112	0.2109	0.2109	0.2109
24	3496.30	31.30	19	19	1.5538	1.2227	0.4524	0.7021	0.7022	0.4524
25	3548.80	21.20	19	19	1.4078	0.8453	0.6375	0.7253	0.7253	0.6375
26	3618.50	48.60	19	19	0.7788	0.5241	0.4970	0.4685	0.4685	0.4685
27	3713.50	41.55	19	19	0.6196	0.4006	0.4003	0.4899	0.4899	0.4003
28	3811.20	37.00	19	19	0.9404	0.9044	0.9044	0.9039	0.9039	0.9044
29	3871.90	15.80	19	19	1.1193	1.0621	1.0621	1.0620	1.0620	1.0621
30	3991.00	42.00	19	19	0.4540	0.4535	0.4535	0.4535	0.4535	0.4535
31	4622.10	41.40	19	19	0.2915	0.2797	0.2797	0.2792	0.2792	**0.2784**
32	4812.00	92.00	19	19	0.4900	0.4924	0.4899	0.5324	0.5324	**0.4892**
33	4962.00	58.00	19	19	0.5876	0.5702	0.5680	0.5682	0.5682	**0.5561**
34	5096.00	76.00	19	19	0.5278	0.5282	0.5269	0.5213	0.5213	**0.5190**
Average over all windows:					**0.5682**	**0.5196**	**0.4895**	**0.5010**	**0.5010**	**0.4866**

MkIV Balloon Spectral Fitting Residuals

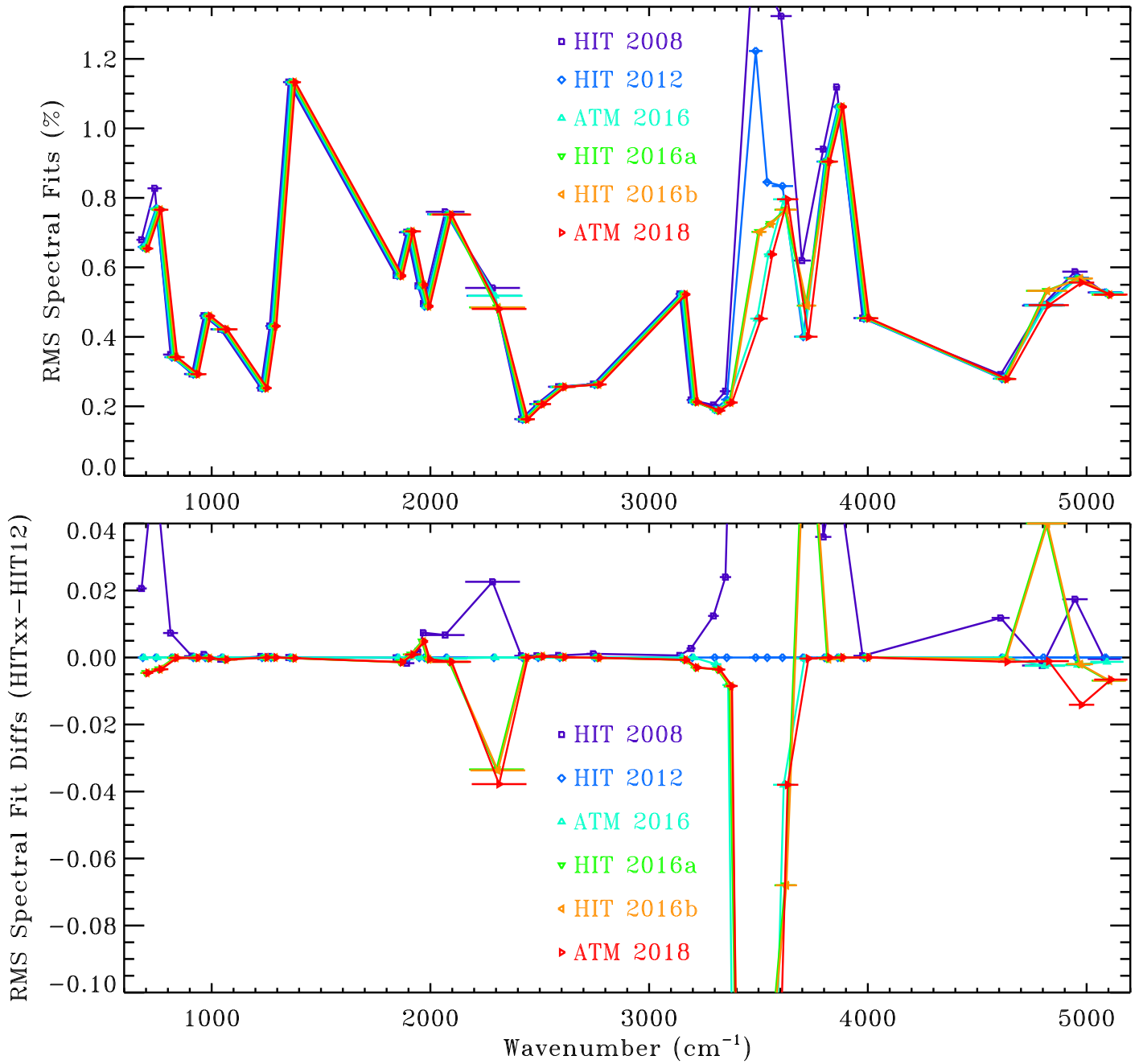
Top Panel: RMS fitting residuals for 34 windows using 5 different linelists. The absolute fitting residuals are dominated by interfering atmospheric absorptions, especially H_2O.

Bottom Panel: Differences from HIT12.

Difference between HIT16a and HIT16b are tiny because isotopologs 11 & 12 are not discernable in atmospheric spectra and because the rounding of the SBHW values doesn't matter in air-broadened spectra.

HIT16 shows improvements below 900 cm^{-1}, and in windows centered at 2290, 3623, and 5096 cm^{-1}.

HIT16 worst of all linelists in 4812 cm^{-1} window.



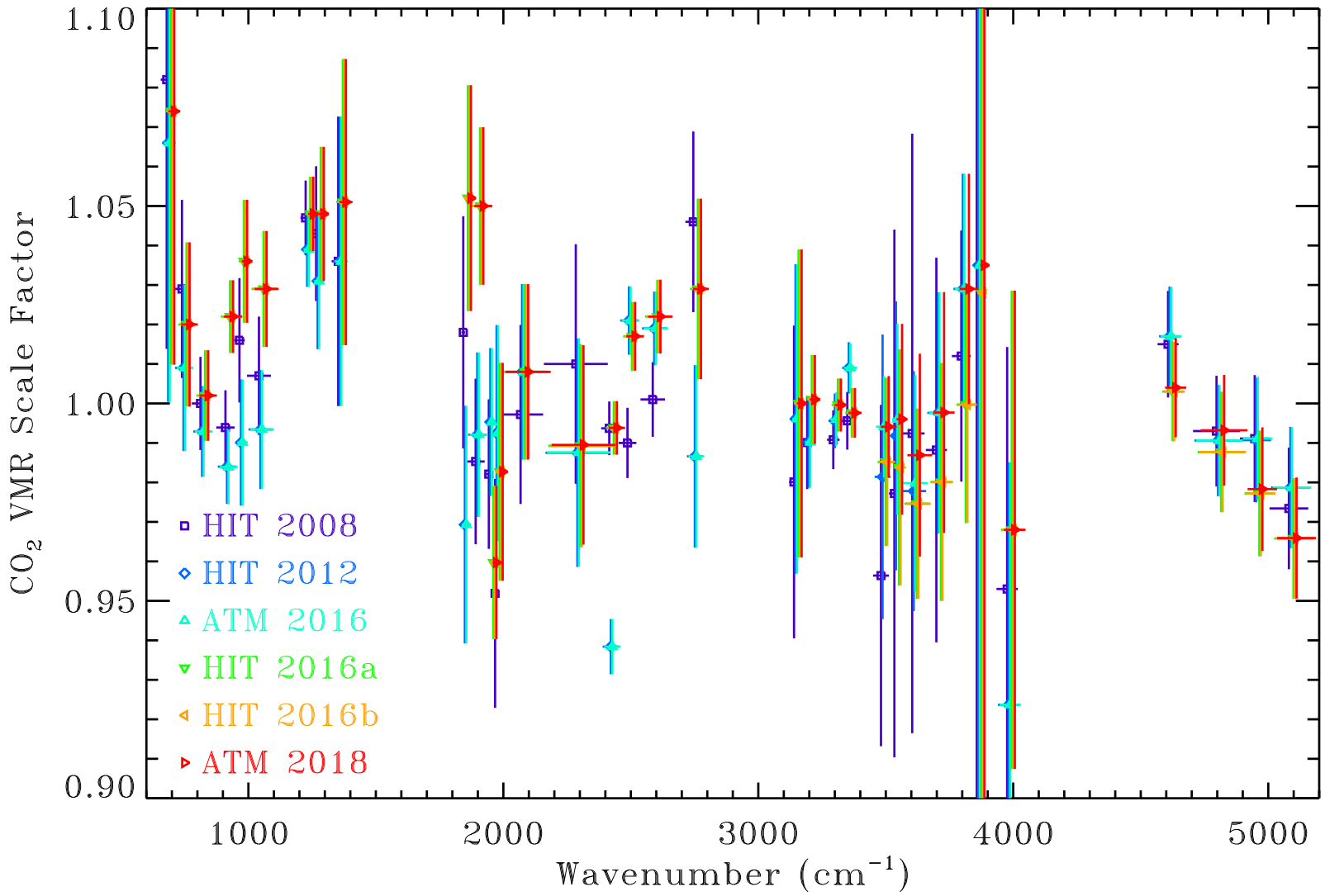
MkIV Balloon: Retrieved CO_2 VMR Scale Factors

The VSF represents the retrieved CO_2 amount divided by the expected amount. Ideally, these values would all be 1.0.

HIT12 points mostly buried under the ATM16 points, except around 3600 cm^{-1}.

HIT16a points mostly buried beneath HIT16b points. X-values offset for clarity.

MkIV instrument records 600-5650 cm^{-1} simultaneously, so derived VSFs should be accurate.



The effect of neglecting Line Mixing

For speed of computation we have ignored LM.

To test the likely impact of this, we have included the effect of LM for one window and compared the results with the non-LM case.

fcen	Width	Nrow	Npp	hit08	hit12	atm16	hit16a	hit16b	hit16c
6211.00	64.00	35	148	0.1301	0.1287	0.1235	0.1279	0.1280	0.1280
6211.00 LM	64.00	35	148	0.1417	0.1401	0.1347	0.1392	0.1393	0.1393
6338.00	62.00	36	148	0.1372	0.1357	0.1296	0.1350	0.1352	0.1352
6338.00 LM	62.00	36	148	0.1503	0.1487	0.1427	0.1480	0.1481	0.1481

We conclude that although LM has a significant effect on the rms and the VSF for spectral measured at higher pressures, it doesn’t affect the relative ranking of the linelists.

MkIV Ground-Based Spectral Fitting Residuals

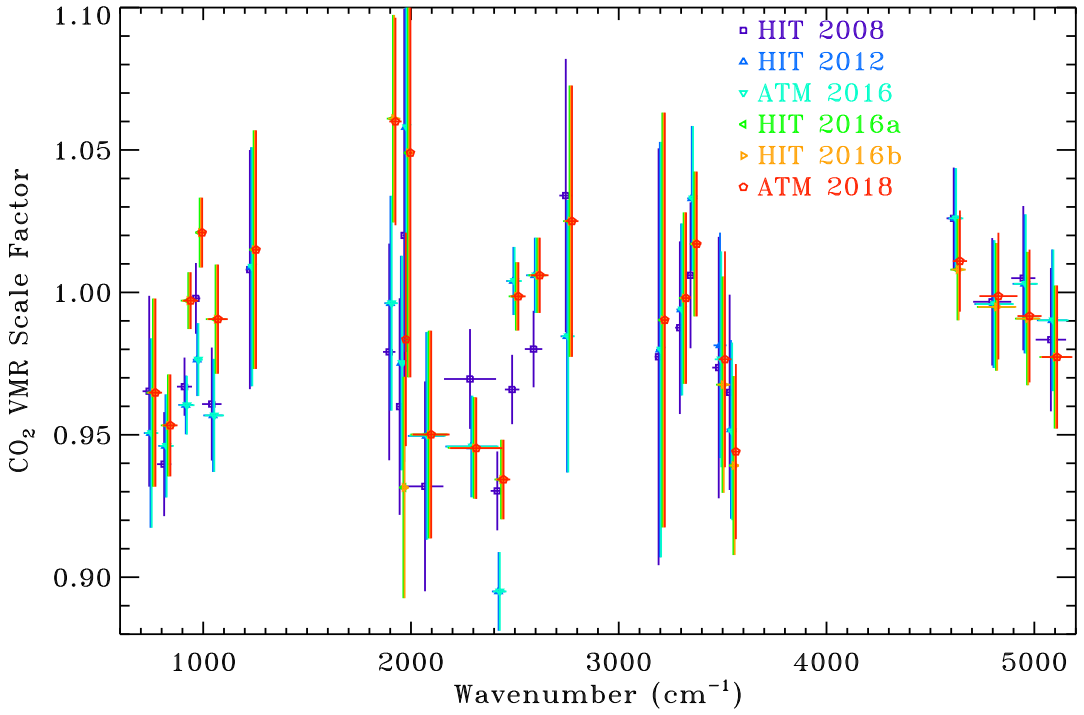
33 windows, 125 spectra = 4125 spectral fits (100% completion).

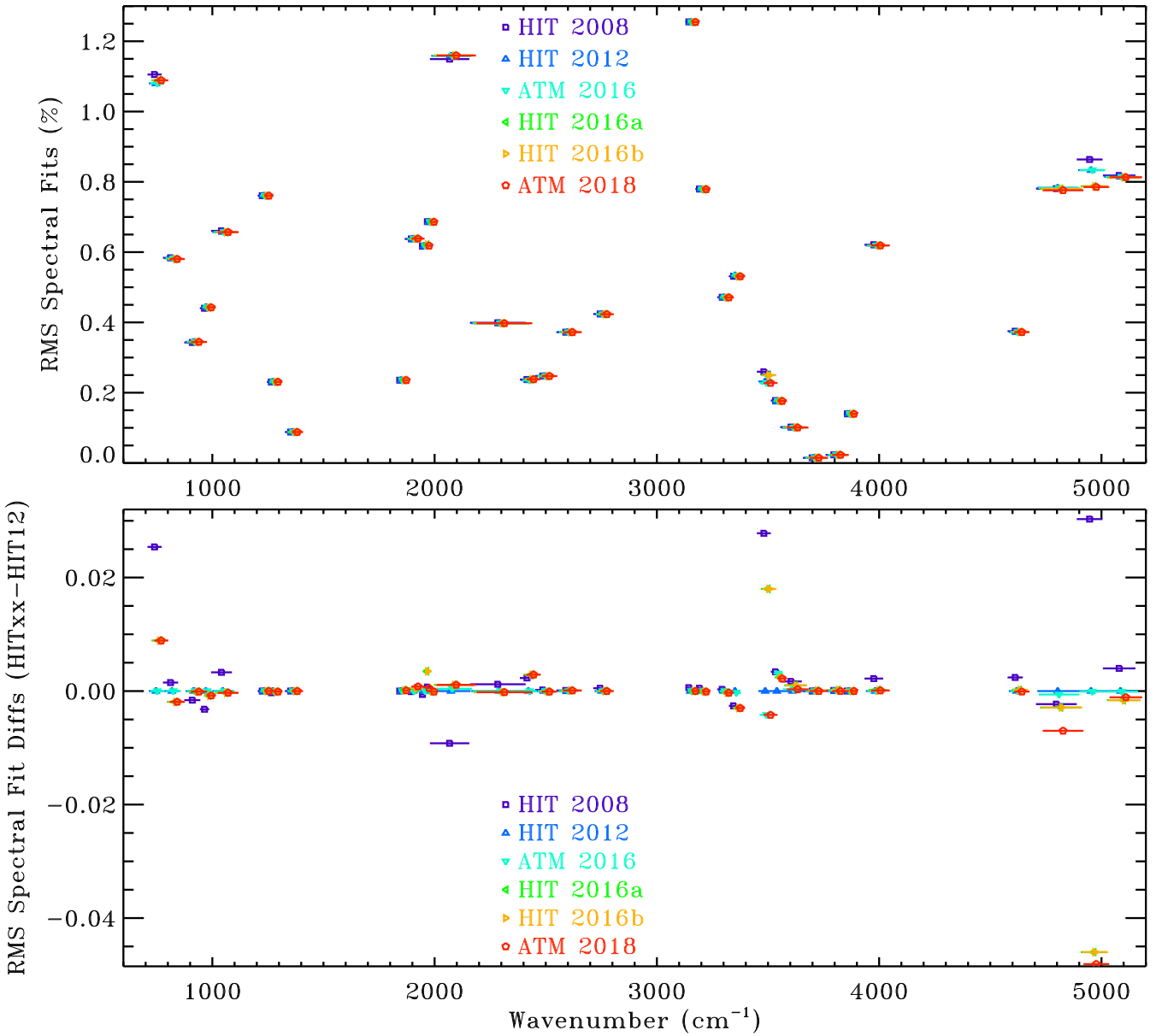
Selected a subset of 125 MkIV spectra, each cover 650-5650 cm^{-1} simultaneously.

Spectra cover surface temperatures of -35C to +35C, and 0 to 3.8 km altitude (650 to 1000 mbar).

iwin	Fcen	HWidth	Nrow	Npp	hit08	hit12	atm16	hit16a	hit16b	atm18
1	755.20	32.05	125	125	1.1054	1.0800	1.0800	1.0889	1.0889	1.0889
2	827.20	34.30	125	125	0.5838	0.5823	0.5823	0.5804	0.5804	0.5804
3	925.00	36.05	125	125	0.3430	0.3446	0.3446	0.3445	0.3445	0.3445
4	980.00	21.05	125	125	0.4403	0.4435	0.4435	0.4427	0.4427	0.4427
5	1056.40	46.90	125	125	0.6605	0.6572	0.6572	0.6569	0.6569	0.6569
6	1239.50	20.30	125	125	0.7606	0.7606	0.7606	0.7606	0.7606	0.7606
7	1280.60	19.90	125	125	0.2306	0.2309	0.2309	0.2308	0.2308	0.2308
8	1367.40	25.90	125	125	0.0881	0.0881	0.0881	0.0881	0.0881	0.0881
9	1857.90	7.65	125	125	0.2356	0.2356	0.2356	0.2358	0.2357	0.2357
10	1910.30	29.70	125	125	0.6376	0.6377	0.6377	0.6382	0.6382	0.6382
11	1960.45	11.85	125	125	0.6171	0.6177	0.6177	0.6212	0.6212	0.6180
12	1982.50	8.50	125	125	0.6867	0.6860	0.6860	0.6859	0.6859	0.6859
13	2082.50	88.50	125	125	1.1493	1.1585	1.1589	1.1596	1.1596	1.1596
14	2299.30	125.15	125	125	0.3990	0.3978	0.3978	0.3976	0.3976	0.3976
15	2430.60	32.10	125	125	0.2376	0.2353	0.2353	0.2382	0.2382	0.2382
16	2501.90	34.80	125	125	0.2476	0.2474	0.2474	0.2473	0.2473	0.2473
17	2605.00	42.00	125	125	0.3723	0.3722	0.3722	0.3723	0.3723	0.3723
18	2760.00	31.00	125	125	0.4239	0.4234	0.4234	0.4234	0.4234	0.4234
19	3159.00	15.20	125	125	1.2551	1.2545	1.2545	1.2545	1.2545	1.2545
20	3206.75	18.50	125	125	0.7795	0.7790	0.7790	0.7789	0.7789	0.7789
21	3309.00	22.50	125	125	0.4716	0.4713	0.4713	0.4710	0.4710	0.4710
22	3360.50	22.00	125	125	0.5314	0.5340	0.5337	0.5310	0.5310	0.5310
23	3496.30	31.30	125	125	0.2597	0.2319	0.2277	0.2499	0.2499	0.2277
24	3548.80	21.20	125	125	0.1777	0.1743	0.1774	0.1767	0.1767	0.1765
25	3618.50	48.60	125	125	0.1022	0.1005	0.1008	0.1015	0.1015	0.1008
26	3713.50	41.55	125	125	0.0147	0.0147	0.0147	0.0148	0.0148	0.0147
27	3811.20	37.00	125	125	0.0232	0.0231	0.0232	0.0233	0.0233	0.0231
28	3871.90	15.80	125	125	0.1398	0.1398	0.1398	0.1398	0.1398	0.1398
29	3991.00	42.00	125	125	0.6211	0.6189	0.6189	0.6191	0.6190	0.6190
30	4627.00	34.40	125	125	0.3750	0.3726	0.3726	0.3728	0.3728	**0.3725**
31	4812.35	91.65	125	125	0.7807	0.7830	0.7824	0.7801	0.7801	**0.7760**
32	4962.00	58.00	125	125	0.8637	0.8334	0.8333	0.7874	0.7874	**0.7853**
33	5094.75	73.25	125	125	0.8182	0.8142	0.8141	0.8126	0.8126	0.8131
Average over all windows:					**0.4980**	**0.4953**	**0.4952**	**0.4947**	**0.4947**	**0.4940**

MkIV ground-based:
RMS Fitting residuals (right)
VMR Scale Factors (below)





TCCON Ground-Based RMS Spectral Fitting Residuals

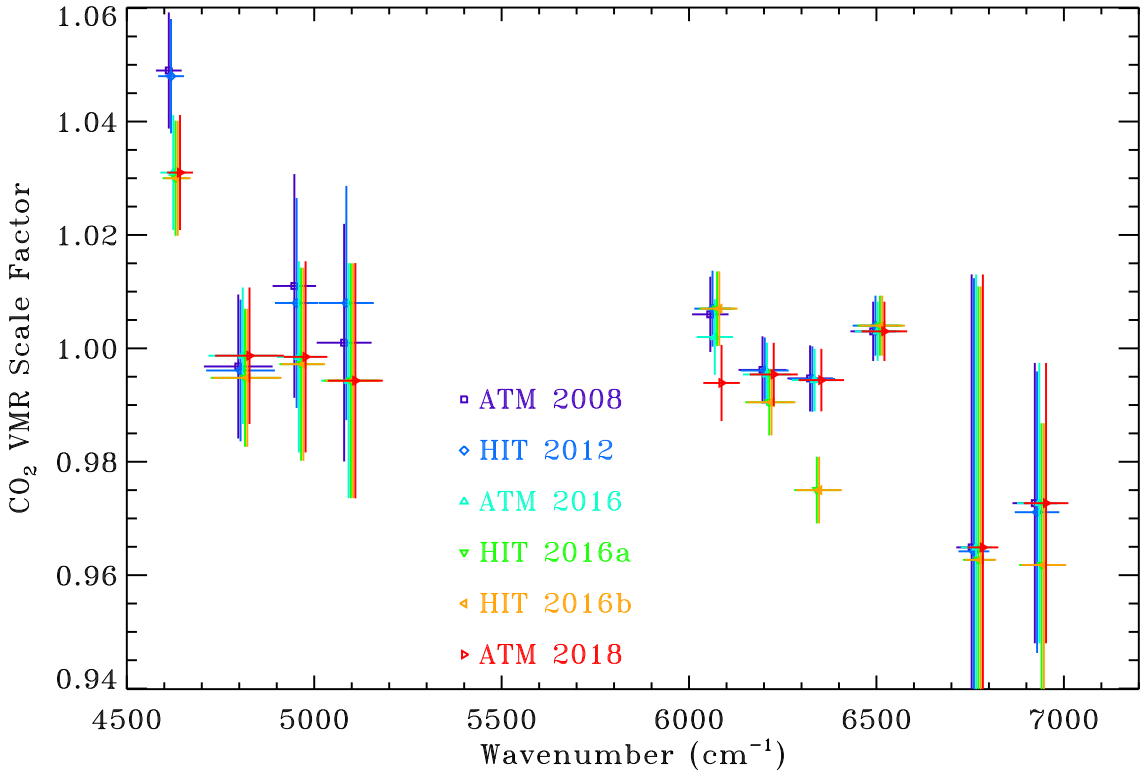
iwin	Fcen	Width	Nrow	Npp	hit08	hit12	atm16	hit16a	hit16b	atm18
1	4627.00	34.40	25	25	0.2619	0.2577	0.2577	0.2581	0.2581	0.2579
2	4812.35	91.65	25	25	0.4388	0.4341	0.4238	0.4246	0.4246	0.4238
3	4962.00	58.00	25	25	0.6748	0.6345	0.5703	0.5744	0.5744	**0.5703**
4	5094.75	73.25	25	25	0.7025	0.6976	0.6932	0.6931	0.6931	0.6932
5	6071.70	48.70	25	25	0.2215	0.2245	0.2218	0.2198	0.2198	**0.2154**
6	6211.00	64.00	25	25	0.2045	0.2019	0.1934	0.2015	0.2015	0.1934
7	6338.00	60.55	25	25	0.2012	0.1993	0.1909	0.1991	0.1992	0.1909
8	6506.25	60.75	25	25	0.1780	0.1802	0.1780	0.1804	0.1804	0.1780
9	6769.00	41.10	25	25	0.8307	0.8309	0.8307	0.8308	0.8308	0.8307
10	6937.50	59.50	25	25	0.6651	0.6680	0.6651	0.6663	0.6663	0.6651
Average over all windows:					**0.4379**	**0.4329**	**0.4225**	**0.4248**	**0.4248**	**0.4225**

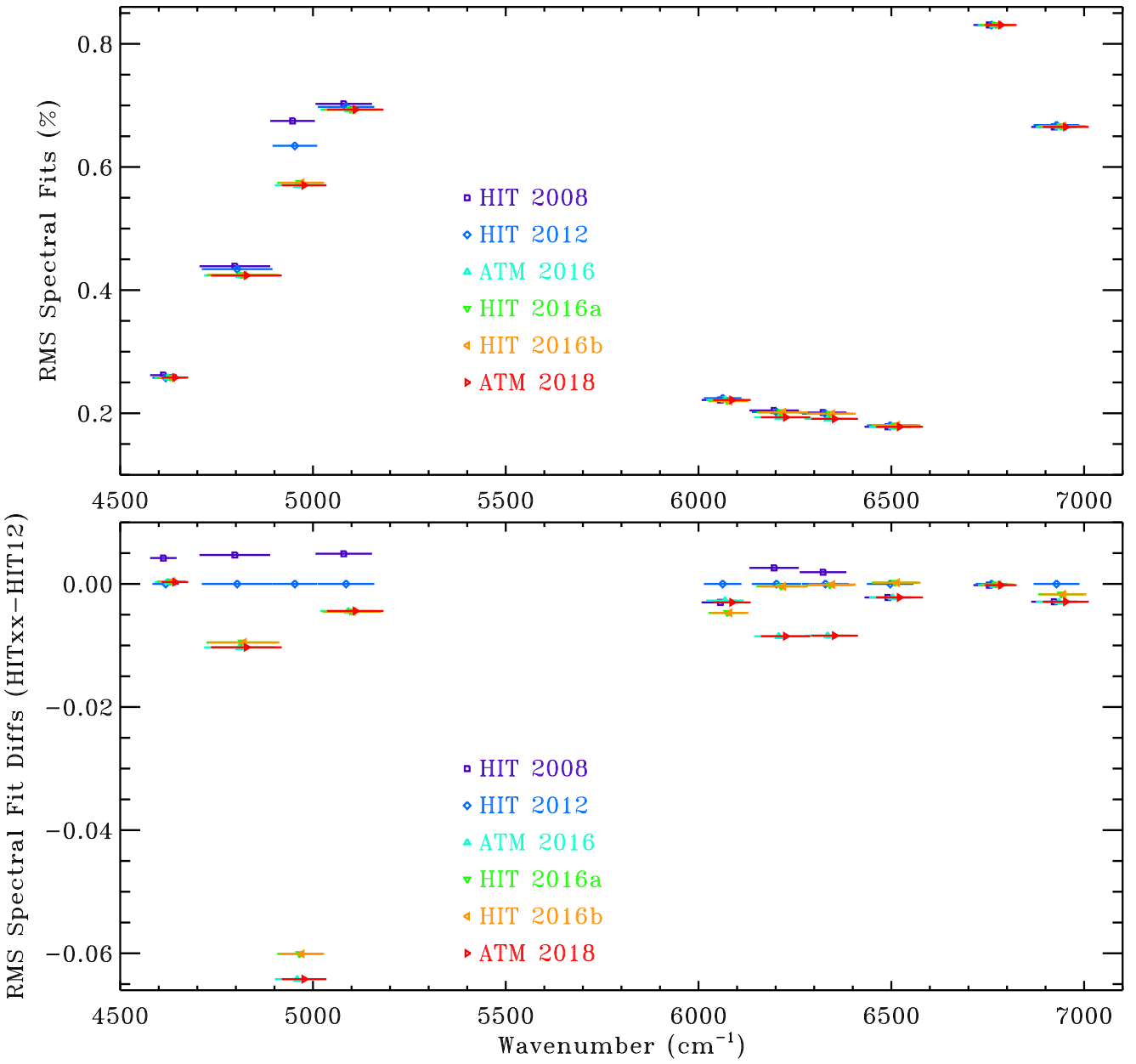
The Total Column Carbon Observing Network (TCCON) covers the 3900 to 9500 cm^{-1} region with an InGaAs detector at 45 cm OPD (0.02 cm^{-1} resolution).

TCCON measures CO2 using the two near-identical CO_2 bands at 6220 and 6338 cm^{-1}

The OCO-2 and GOSAT satellite instruments also use the strongr CO_2 band at 4812 cm^{-1}.

TCCON Ground-Based RMS fitting residuals (right) VMR Scale Factors (below)

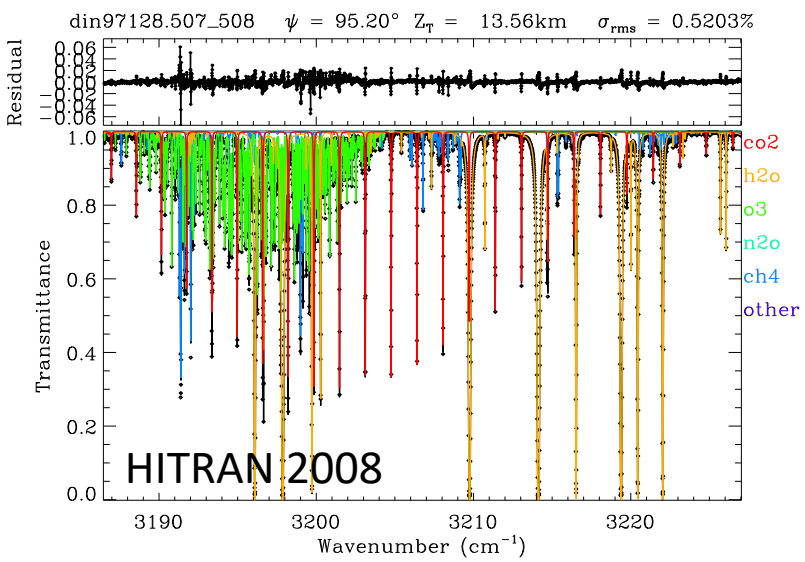


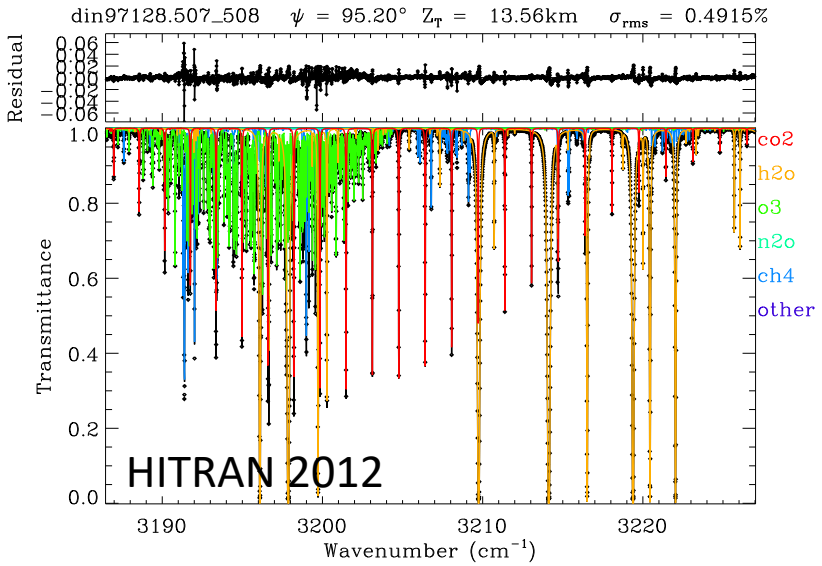


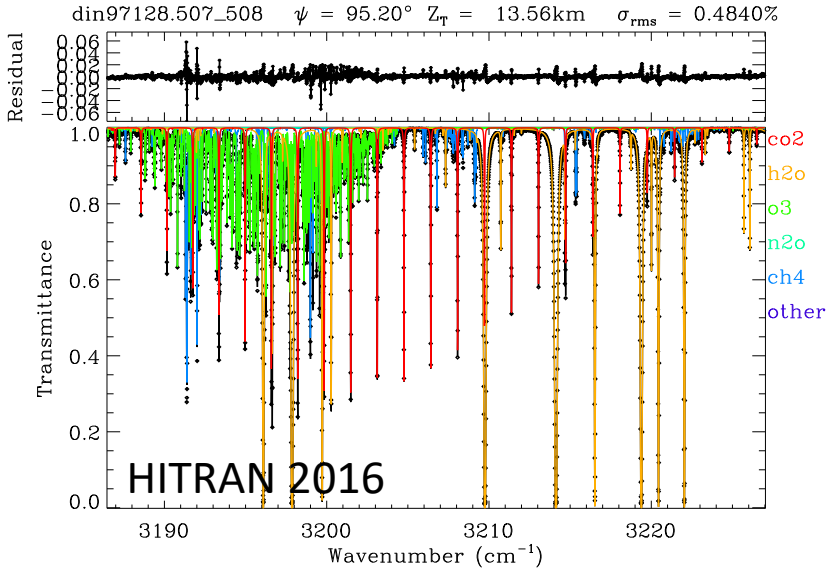
Types of Spectra and their Pros and Cons for Spectroscopy Evaluation

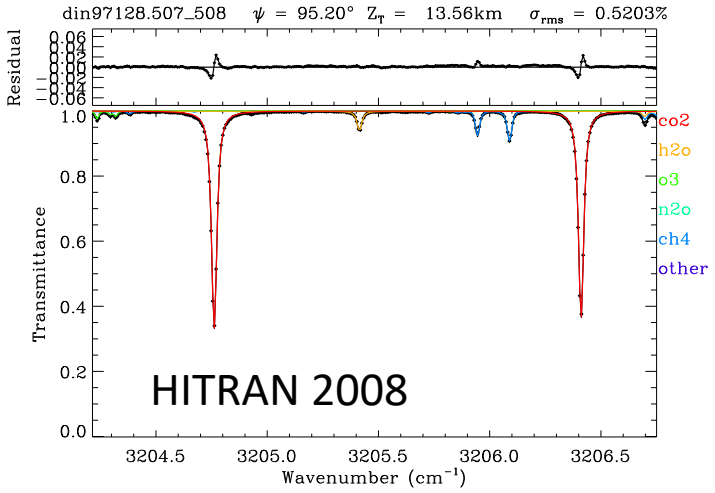
Type	Pros	Cons
Laboratory	- Well-known cell conditions (L, T, P, VMR) - Large isotopic enrichments possible	Dim Source, so narrow spectral coverage and/or poor SNR
Occultation MkIV Balloon	- Bright source (sun) allows simultaneous coverage 650-5650 cm^{-1} at high resolution - Wide range of P/T conditions - Solar and instrumental features removed - Long path lengths (~400 km)	• Inhomogenous atmospheric path • No control over P/T conditions • Interferences from other gases • Unknown VMRs and isotopic fractionations (except CO_2, N_2, O_2)
Ground-based MkIV	- Bright Source (sun) - Simultaneous coverage 650-5650 cm^{-1} - Long path lengths (~100 km) - Sensitive to lineshape (e.g. width, shifts, LM)	Inhomogeneous atmospheric path Wide regions blacked out: • H_2O (1350-1900; 3350-4000 cm^{-1}) • CO_2 (650-700; 2280-2390 cm^{-1})
Ground-based TCCON	- Bright Source (sun) - Simultaneous coverage 4000-14800 cm^{-1} - Long path lengths (~100 km) - Sensitive to lineshape (e.g. width, shifts, LM)	Inhomogeneous atmospheric path Regions strongly contaminated by: • H_2O (7000-7200) • CO_2 (4800-5000 cm-1)

Fits to MkIV balloon spectra at 14 km tangent altitude in the 3200 cm^{-1} region

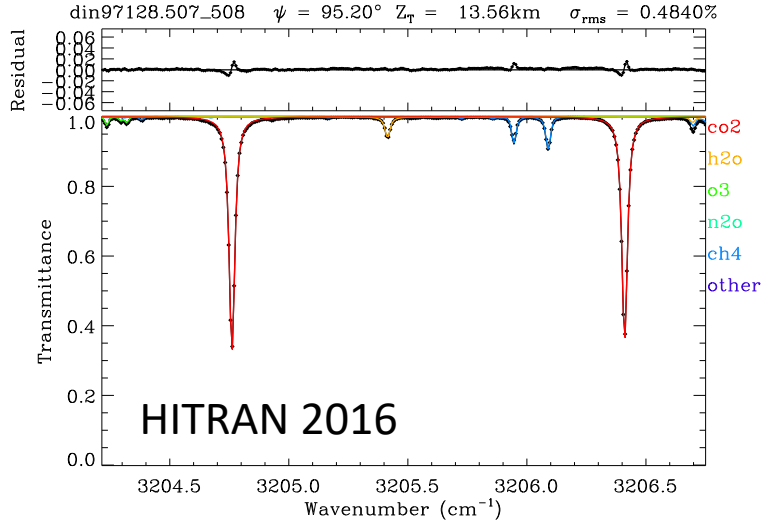








Illustrating the progressive improvement in the spectral fits from HITRAN 2008 to HITRAN 2016. Residuals are mainly due to H_2O, O_3 and CH_4, but these linelists were unchanged, so improvement in rms fitting residuals is due solely to CO_2. HITRAN 2016 still not perfect, but better than its predecessors.



Summary & Conclusions

Four spectral datasets (Kitt Peak lab, MkIV balloon, MKIV ground, and TCCON ground) have been used to evaluate six different linelists (HITRAN 2008, 12, 16a, 16b and ATM 16 & 18) over the 650 to 7000 cm^{-1} region.

Spectral fitting was performed with the GFIT code and the linelists were evaluated in terms of: the rms fitting residuals and the window-to-window consistency of the retrieved gas amounts. There was no analysis of separate isotopologs. They were all lumped together as CO_2 which makes it important to know the fractionation. For CO_2 this is probably better known in the atmosphere than in the laboratory.

Results show progressive overall improvements in each HITRAN version, but there have been some regions where the HITRAN 2016 fits have regressed, particularly above 3400 cm^{-1}. Also in the 6200-6400 cm^{-1} region used by TCCON to measure atmospheric CO_2 the consistency of the retrievals has degraded.

Merged available linelists to make new linelist (ATM18), based primarily on HITRAN 2016b, except for:

- Replaced the 3419 - 3923 cm^{-1} and 5750 - 6598 cm^{-1} sections with ATM 2016.
- Replaced the 6715 - 7000 cm^{-1} section with HITRAN 2008
- For isotopologues 10,11,12, use HIT16b throughout.

Future Work

HITRAN 2016 linelists provide improved window-to-window consistency below 5200 cm^{-1}. But the consistency of the 6211 and 6338 cm^{-1} windows, used by TCCON, is poorer using HIT16a,b than previously. This is a serious problem because anything that degrades the uncertainties of one window, but not the other, will affect the weighted average. I therefore plan to recommend the ATM18 CO_2 for TCCON.

In future, obtain additional low-T lab spectra (preferably air-broadened) to test T-dependence of ABHW.

HITRAN 2016 Paper (Gordon et al., 2017) CO_2 Section

2.2. CO_2 (molecule 2)

Accurate and comprehensive line lists for all naturally abundant isotopologues of carbon dioxide are required by remote-sensing missions dedicated to monitor the concentration of carbon dioxide in Earth's atmosphere. The recently launched OCO-2 mission [64–66], together with several other space and ground based projects (GOSAT [67], AIRS [68], ASCENDS [69], TCCON [32], NDACC [70]) are dedicated to explicitly monitor the atmospheric

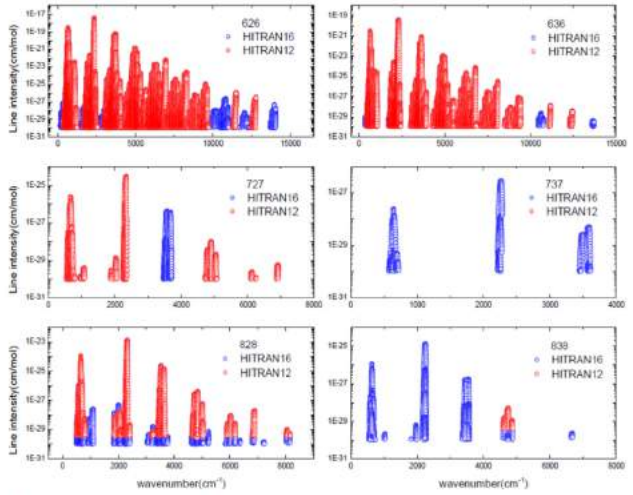


Fig. 5. Overview of the line lists of stable symmetric isotopologues of carbon dioxide in HITRAN2012 and HITRAN2016.

CO_2 content. These experiments aim not only to look at overall CO_2 concentration and its variation, but also wish to pinpoint where CO_2 is being produced (sources) and where it is absorbed (sinks). This activity is clearly vital to monitoring and essential for eventually controlling the CO_2 content of the atmosphere [71]. A successful retrieval of CO_2 concentration requires validated line lists with transition intensities given at sub-percent accuracy, line positions accurate to 0.0001 cm^{-1} or better, and beyond-Voigt-profile line-shape models [65,72,73].

Determination of isotopic ratios of carbon in Earth's samples and astrophysical objects remains crucial for modeling geophysical processes. For example, quantification of ^{14}C in fossil fuels can provide information about the sources of human-related contribution to the total CO_2 concentration in the terrestrial atmosphere. This can be done with recently developed cavity-enhanced laser spectroscopic techniques in the IR [74–76]. However, these measurements require a priori simultaneous knowledge of reliable line intensities of many isotopologues. Precise determination of $^{13}C/^{12}C$ and $^{16}O/^{17}O/^{18}O$ ratios is also vital, for instance, in understanding processes of formation of radiation fields in the Martian atmosphere, which is 96% rich in carbon dioxide [77].

A summary of the carbon dioxide line list in the HITRAN2012 database and comparison to HITRAN2016 is given in Table 4. The HITRAN2012 database was considerably improved with respect to its previous 2008 edition. However, several issues related to spectral completeness, inconsistency of multiple data sources, and insufficient accuracy of line intensities, still remained unsolved. The majority of entries in the 2012 version of the HITRAN database were taken from the effective Hamiltonian calculations included in the 2008 edition of the CDSD-296 database [78].

For less abundant isotopologues, obtaining high-quality experimental data is not trivial. Therefore fits of the effective Hamiltonian or the effective dipole moment [78], were based on only four major isotopologues $^{12}C^{16}O_2$, $^{13}C^{16}O_2$, $^{16}O^{12}C^{18}O$ and

Table 4
Comparison of HITRAN2016 and HITRAN2012 line lists for isotopologues of carbon dioxide.

ISO/abundance	HITRAN2012			HITRAN2016		
	Number of lines	Spectral region (cm^{-1})	Q(296 K)	Number of lines	Spectral region (cm^{-1})	Q(296 K)
626/0.984204	169,292	345.936–12,784.056	286.94	173,024	158.301–14,075.298	286.094
636/1.1057 × 10^{-2}	70,611	406.834–12,462.046	578.41	70,577	332.649–13,734.963	576.644
628/3.9470 × 10^{-3}	116,482	0.736–9557.398	609.48	127,850	1.472–12,677.181	607.713
627/7.3399 × 10^{-4}	72,525	0.757–9599.317	3552.70	77,941	0.757–12,726.562	3542.610
638/4.4345 × 10^{-5}	26,737	489.678–6744.158	1229.10	43,782	2.945–9212.609	1225.270
637/8.2462 × 10^{-6}	2953	583.593–6768.643	7162.90	25,175	9.086–8061.741	7140.024
828/3.9556 × 10^{-6}	7118	491.688–8160.439	324.21	10,522	482.813–8162.743	323.424
728/1.4718 × 10^{-6}	821	626.438–5046.875	3776.40	15,878	491.181–8193.172	3766.044
727/1.3685 × 10^{-7}	5187	535.384–6932.980	11,002.00	6518	535.383–6932.693	10,971.91
838/4.4440 × 10^{-8}	121	4599.239–4887.290	653.50	2916	2245.898–4750.068	652.242
837/1.653 × 10^{-8}	N/A	N/A	7615.20	4190	549.472–4914.496	7593.900
737/1.5375 × 10^{-9}	N/A	N/A	N/A	1501	575.852–3614.084	22,129.96
646/radioactive	N/A	N/A	N/A	41,610	426.445–7928.788	2033.353

Note: ISO is the AFGL shorthand notation for the isotopologue, abundance is the terrestrial value assumed by HITRAN, and Q(296) is the partition sum at 296 K.

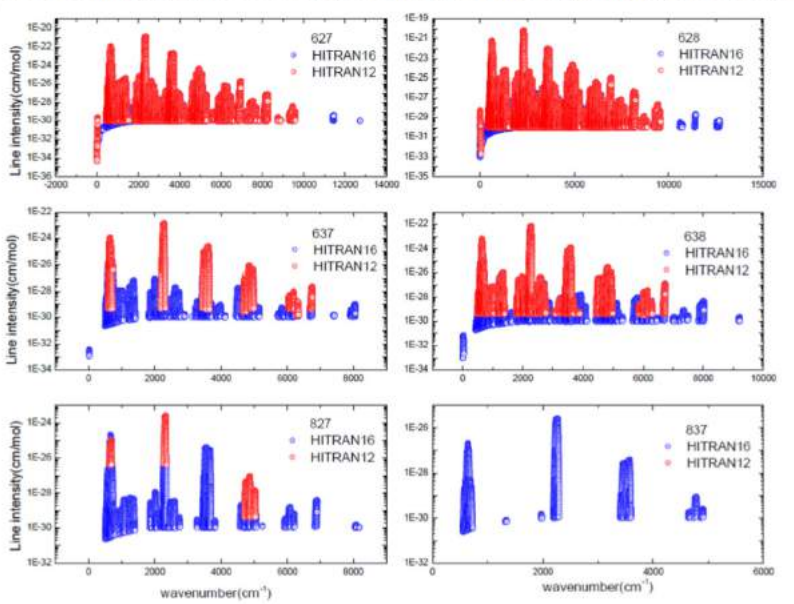


Fig. 6. Overview of the line lists of stable asymmetric isotopologues of carbon dioxide in HITRAN2012 and HITRAN2016.

$^{16}O^{12}C^{17}O$, for which measured spectroscopic parameters were available. As a result, several spectral gaps were present in HITRAN2012 (see for instance discussion in Refs. [79,80]) which represent regions where experimental data were unavailable. For similar reasons, no entries were included in the database for the $^{18}O^{13}C^{17}O$, $^{17}O^{13}C^{17}O$, and $^{16}O^{14}C^{16}O$ isotopologues (837, 737, and 646 in old AFGL notation). An overview of this problem is displayed in Figs. 5 and 6, where CO_2 ro-vibrational spectra from HITRAN2012 and HITRAN2016 are compared for different isotopologues.

Wherever possible, the effective Hamiltonian fits were extrapolated to the trace isotopologues, using a method of isotopic substitution [81]. In the 2012 edition, multiple data sources caused sporadic discontinuities in intensity patterns of ro-vibrational lines [82–84]. Furthermore, a high percentage of line intensities in HITRAN2012 have stated uncertainty of 20% or worse (HITRAN uncertainty index equal to 3). Although this assessment has been proven to be overly pessimistic in many cases [82,83,85–87], the uncertainty budget, especially for the Effective Hamiltonian calculations, was still too high for precise measurements of atmospheric CO_2 concentration. The most accurate entries in HITRAN2012 were taken from NASA JPL measurements by Toth et al. [88–90] and covered the 1.6-μm and 2.06-μm spectral regions, which are used in remote-sensing measurements. The stated 1–5% accuracy of these experimental line intensities (HITRAN uncertainty index equal to 7 and 6), has been confirmed by a number of comparisons [82,83,91]; nonetheless the rigorous requirements for part-per-million resolution in measurements of CO_2 atmospheric concentration were not achieved.

Since the 2012 release of the HITRAN database, a large number of experimental and theoretical studies have been devoted to improve the knowledge of line positions, line intensities and line shapes of CO_2 isotopologues. For a comprehensive review of measurements and theoretical models see Ref [92]. and references therein.

Theoretical line lists (denoted as "Ames") for 12 stable and one radioactive (646) isotopologue of CO_2 were published by Huang et al. in the 0–20,000 cm^{-1} spectral region and for temperature below 1500 K [79,93,94]. Room-temperature line lists (denoted a "UCL-IAO") for 13 CO_2 isotopologues were also calculated by Za et al. [82,83,85,91] in the 0–8000 cm^{-1} spectral region. Both c these latter studies contained intensities computed with *ab initi* dipole moment surfaces and semi-empirical line positions, base on a fitted potential energy surface for the Ames effort and on th effective Hamiltonian calculations for UCL-IAO. A major advantag of the variational approach used in the Ames and UCL-IAO line list is that it should give similar accuracy for all isotopologues. Thi allows coverage of spectral regions currently not probed by ex periments for rare isotopologues. UCL-IAO also provides un certainty estimates of line intensities, based on a purely theoretic methodology [17]. Such a reliable analysis allows for the detectio of ro-vibrational resonance interactions, which significantly lowe the accuracy of theoretical line positions and intensities. Using thi method, the lines identified as unreliable have been replaced wit the data from CDSD-296 [92] and, in several cases of interpolya resonance interactions (asymmetric isotopologues), with th

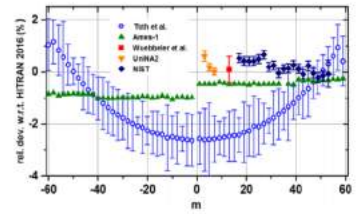


Fig. 7. Comparison of line intensities between HITRAN2016, HITRAN2012 (Tot et al. [88]), and other accurate experimental and theoretical sources for the 20012 00001 band (2-μm band) of $^{12}C^{16}O_2$: measurements Wübbeler et al. [102], NIS [104] and UniNA2 [103], and theory Ames-1 [79]. The zero relative deviation lir corresponds to HITRAN2016 line intensities (in this case from Zak et al. [82]). Th running index m equals -J, J, and J + 1 for the P, Q, and R branches, respectively.

experimental data from Lyulin et al. [95], Karlovets et al. [96,97] and Campargue et al. [98].

Recently, there have been a number of high-precision near-IR spectroscopic measurements which provide rigorous tests of theoretical line intensities based on effective dipole moment surface and ab initio calculations [84–87,99]. Particularly, in the 1.6-μm and 2.0-μm spectral regions, the UCL-IAO line lists have been experimentally verified as accurate to the sub-percent level. Fig. 7 compares the UCL-IAO and Ames line lists to HITRAN2012 (Toth et al. blue open circles [100, 101]) for the 20012 − 00001 band and to state-of-the-art experiments including advanced high-resolution laser measurements [101–104]. A number of comparisons here suggest that the UCL-IAO study models line intensities more accurately than the Ames study. Note that more recent results from Ames, which are available from their website (www.huang.seti.org), give closer agreement with UCL-IAO. From Fig. 7 it is clear that there is a 1–3% average difference in line intensities between the new and the previous version of HITRAN for this band. The independent experiments from the National Institute of Standards and Technology [104], and the University of Naples II [103] confirm, however, a conservative 0.5% accuracy of line intensities for this band in HITRAN2016. This level of accuracy could potentially satisfy even the most stringent requirements of current remote-sensing missions. Interestingly, although line intensities for this band and the 20013 − 00001 and 30013 − 00001 bands probed by OCO-2 originate from the same source (Toth et al. [100]), the agreement between UCL-IAO and HITRAN2012 is substantially better for the OCO-2 bands.

For wavenumbers greater than 8000 cm^{-1}, the majority of the line parameters were taken from CDSD-296 [92]. As we have already mentioned above, both HITRAN2012 and CDSD-296 have several spectral gaps, in particular in the wavenumber region greater than 8000 cm^{-1}. Recently, several experimental studies of the carbon dioxide spectra in the high-frequency region have been performed [105–108]. The measured line intensities allowed determining the absent effective dipole moment parameters for several series of transitions. Using these effective dipole moment parameters and an effective Hamiltonian from Ref. [109], the line positions and intensities for the principal isotopologue were generated and included into HITRAN2016 covering the 9800–10,500 cm^{-1} and 11,600–12,400 cm^{-1} wavenumber gaps.

Line positions were updated with respect to the previous version of the database. The majority of lines come from the effective Hamiltonian calculations included in UCL-IAO line lists, which are based on the fits to the observed line positions collected from the literature and published in the latest, 2015 release of the CDSD-296 database [92]. These fits were completed and updated with recent, accurate measurements performed on isotopically-enriched samples of CO_2. Uncertainties in the fitted line positions depend on the quality of the experimental data and vary from 0.001 cm^{-1} to 10^{-9} cm^{-1}. For asymmetric isotopologues, a number of bands are affected by strong interpolyad anharmonic resonance interactions. The effective Hamiltonian model does not include this type of interaction for the asymmetric isotopologues. Hence in such cases, line positions were taken directly from measurements [80,95–98,110,111].

The uncertainty codes for the line positions were transferred from CDSD-296 to HITRAN2016. The uncertainty code 3 (0.001–0.01 cm^{-1}) was given for the line positions in the 9800–10,500 cm^{-1} and 11,600–12,400 cm^{-1} wavenumber regions. Partition functions in the current release of the database are based on the direct summations taken from the variational calculations of Huang et al. [79]. On average, the new partition functions agree excellently with those of CDSD-296 [83]; however they do not agree perfectly with those in HITRAN2012 (from TIPS [112]) and three previous editions of the database and differ at 296 K by about −0.3%. Although this difference is marginal, it could have an effect in the applications where sub-percent accuracy is required.

As stated above, the radioactive isotopologue $^{14}CO_2$, 646, has been added to the database. This is the first edition of HITRAN where radioactive species have been incorporated (also for CO, see Section 2.5). All lines of the 646 isotopologue were taken from the UCL line lists given in Ref. [83]. Due to issues with what constitutes a so-called natural terrestrial abundance of radioactive species (which is part of the traditional definition of intensities in HITRAN, see Eq. (1) of the Definitions and Units documentation in HITRAN*online*), line intensities for these type of species are given for unit abundance; a 10^{-27} $cm^{-1}/(molecule \cdot cm^{-2})$ cut-off value for the intensity has been applied. This cut-off produced 41,610 lines in the J range 0 to 114. Vibrational assignments for the 646 isotopologue were based on isotopic shifts of energy levels and respective assignments for the 626 and 636 isotopologues, and hence should be regarded as provisional. An abundance-scaled intensity cut-off of 10^{-30} $cm^{-1}/(molecule \cdot cm^{-2})$ is used for all stable isotopologues. Note that, for the time being, data for the radioactive isotopologues are provided as static files rather than through the HITRAN*online* interface.

Uncertainties of line intensities were informed by theoretical error analysis, which classified lines as reliable, intermediate, or unreliable. Bands with reliable lines stronger than 10^{-23} $cm^{-1}/(molecule \cdot cm^{-2})$ (for unit abundance) were assigned HITRAN uncertainty code 8 (i.e. accuracy of 1% or better). Line intensities of reliable parallel bands weaker than 10^{-23} $cm^{-1}/(molecule \cdot cm^{-2})$ were given an uncertainty code 7 (i.e. accuracy 1-2%). Reliable perpendicular bands weaker than 10^{-23} $cm^{-1}/(molecule \cdot cm^{-2})$ and intermediate lines were marked with HITRAN uncertainty code 6 (i.e. accuracy 2-5%). So-called unreliable lines were taken from the effective dipole moment calculations [92] and experiments. Typical intensity uncertainties for these entries range between 5 and 20%.

It is important to point out that an intensive study of the 1.6-μm and 2.06-μm bands that includes non-Voigt lineshapes and line mixing has been published by the OCO-2 spectroscopy support group ABSCO (ABSorption COefficient tables for the OCO-2 mission) [84,86]. The data were fit using a multi spectrum fit procedure which, among other things, enables retrieval of the lineshape parameters using the speed-dependent Voigt (SDV) profile as well as line mixing. These are very good experiments and it is debatable whether to use them for the strong and weak bands in place of UCL-IAO parameters described above. Indeed the ABSCO team have validated (using TCCON spectra) the cross-sections generated using results of Refs. [84,86] and found them to be the most efficient [113]. However, achieving high-precision results in nuanced correlations, with line mixing and model assumptions that can create discontinuities in inter-band comparisons, is difficult. At the moment, HITRAN cannot provide users with tools that can be used to generate cross-sections from the works of Devi et al. [84] and Benner et al. [86]. The usable products of the ABSCO effort are absorption coefficients (available upon request from the ABSCO group) rather than spectral parameters, which are available in the publications. Moreover, these absorption coefficients are empirically scaled by the factors of 0.6% and 1.4% for the 1.6-μm and 2.06-μm bands respectively, due to lingering data and/or model biases (the use of partition function HITRAN 2012/TIPS is up to 0.3% of this factor). After these studies, an update of the multi spectrum fitting code with CDSD partition functions was done. Additional methods to adjust the intensity distribution closer to the UCL list by scaling experimental conditions within the uncertainties are under evaluation. The intensities of the band at 2.06 μm are already within 0.7% of Zak et al. [82], indicating that the additional 0.7% scaling of ABSCO cross-sections may be unrelated to intensities. These issues will be considered for future editions of the database.

For wavenumbers greater than 8000 cm^{-1}, two sources of the line intensities are used: CDSD-296 [92] and the newly-generated line list in the 9800–10,500 cm^{-1} and 11,600–12,400 cm^{-1} regions based on the new measurements [105–108]. The uncertainty codes of the CDSD-296 line intensities were transferred to HITRAN2016. Based on the uncertainties of the line intensity measurements in the 10,700–10,860 cm^{-1} region [106], we use uncertainty code 5 (5% – 10%) for the line intensities of the 3003i-00001 (i = 1,2,3,4) series of bands and based on the uncertainties of the line intensity measurements in the 10,000–10,300 cm^{-1} and 11,600–12,400 cm^{-1} [107] wavenumber regions we use uncertainty code 3 (> 20%) for the line intensities of the 4003i-00001 (i = 1,2,3,4,5) and of the 6001i-00001 (i = 1,2,3,4,5,6,7) series of bands.

The Voigt line-shape parameters throughout the entire database were calculated using the predictive routine of Gamache and Lamouroux explained in Refs. [114–116]. For the line mixing, we now provide a code from Lamouroux et al. [117] which has been updated to operate with HITRAN2016. We note that Lamouroux et al. [117] line mixing coupled with the HITRAN2012 data has worked really well and in fact produced residuals hardly exceeding 1% when applied to the TCCON data in Ref. [113], although slightly inferior to the ABSCO cross-sections in the 2.06-μm region.