

Ozone Spectroscopy Evaluation Update

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This report supplements a previous O₃ evaluation performed in July 2020:

https://mark4sun.jpl.nasa.gov/report/O3_Spectroscopy_Evaluation_20200727.pdf

Main Changes since July 2020:

1) New window added centered at 832 cm⁻¹ and 57 cm⁻¹ wide. Although O₃ lines here are relatively weak, they can nevertheless easily be seen in KP lab spectra and MkIV balloon occultation spectra and so should be evaluated.

2) Three linelists are added to the evaluation:

Tenn_20: 449,569 lines covering 0 - 6697 cm⁻¹, obtained from the file:

72830178 Oct 27 O3_HITRAN2016-modified-by-UCL-intensities.par

SMPO_20: 505,868 lines covering 0 - 6997 cm⁻¹ from the file:

81961123 Nov 12 SMPO-hitraned-for-Geoff-v2.par

Birk_20: 99,186 lines covering 600 -1220 cm⁻¹ (gap 850-980 cm⁻¹ filled with HIT16) from the following files:

- 5932686 Oct 8 O3_nu2_export_full_HITRAN_with_Sscaled_gamma(J=KA)_updates_140920_V2.hit
- 4246622 Oct 8 O3_nu1_export_full_HITRAN_with_sigma_s_gamma(J=KA)_updates_140920_V3.hit
- 7639286 Oct 8 O3_nu3_export_full_HITRAN16_with_sigma_s_gammaeff_delta_updates_240720.hit

Lines above 1180 cm⁻¹ are not included in the evaluation (Manfred said that they weren't his).

Properties of the 37 windows used in fitting (Kitt Peak lab spectra)

#	Center	Width	MIT	A	I	F	Parameters to fit				Gases to fit				Iso_bar	S_max	S_tot	S_bar	W_bar	E''_bar
1	648.65	36.12	15	2	1	0	ncbf=15	fs	xo	cf	: o3	h2o	co2	hcooh	1.01	5.12E-22	8.25E-20	2.15E-22	0.0757	484.0
2	684.45	33.02	15	2	1	0	ncbf=11	fs	xo	cf	: o3	h2o	co2		1.01	1.22E-21	1.68E-19	4.54E-22	0.0765	287.0
3	752.40	102.82	15	2	1	0	ncbf=16	fs	xo	xf	: o3	h2o	co2		1.01	1.66E-21	3.45E-19	5.00E-22	0.0754	351.7
4	832.15	56.70	15	2	1	0	ncbf=18	fs	xo	xf	: o3	h2o	co2		1.00	1.13E-22	6.80E-21	4.49E-23	0.0729	958.7
5	1003.40	81.02	15	2	1	0	ncbf=14	fs	xo	cf	: o3	h2o			1.02	3.94E-20	8.27E-18	1.67E-20	0.0769	376.3
6	1060.00	32.52	15	2	1	0	ncbf=8	fs	xo	cf	: o3	h2o			1.00	4.06E-20	6.41E-18	2.12E-20	0.0761	308.3
7	1092.86	33.36	15	2	1	0	ncbf=11	fs	xo	cf	: o3	h2o	hcooh		1.02	5.74E-22	1.10E-19	2.60E-22	0.0739	416.8
8	1119.75	20.40	15	2	1	0	ncbf=10	fs	xo	cf	: o3	h2o	hcooh		1.01	2.02E-21	8.23E-20	1.00E-21	0.0731	305.7
9	1161.90	48.60	15	2	1	0	ncbf=11	fs	xo	cf	: o3	h2o			1.00	7.68E-22	8.56E-20	2.30E-22	0.0735	565.4
10	1199.25	22.20	15	2	1	0	ncbf=9	fs	xo	cf	: o3	h2o			1.00	9.40E-23	8.53E-21	4.50E-23	0.0721	878.2
11	1716.40	112.05	15	2	1	0	ncbf=12	fs	zo	cf	: o3	h2o			1.00	1.65E-22	5.97E-20	6.59E-23	0.0767	366.0
12	1775.44	44.93	15	2	1	0	ncbf=10	fs	xo	cf	: o3	h2o	hcooh		1.00	4.04E-23	7.45E-21	1.33E-23	0.0760	362.4
13	1812.50	24.50	15	2	1	0	ncbf=8	fs	xo	cf	: o3	h2o			1.00	1.05E-22	7.21E-21	4.40E-23	0.0740	306.0
14	1837.50	24.50	15	2	1	0	ncbf=8	fs	xo	cf	: o3	h2o			1.00	4.20E-23	4.28E-21	1.96E-23	0.0748	400.9
15	1865.00	29.40	15	2	1	0	ncbf=8	fs	xo	cf	: o3	h2o			1.00	2.63E-23	2.61E-21	1.42E-23	0.0742	476.0
16	1914.62	54.90	15	2	1	0	ncbf=8	fs	xo	cf	: o3	h2o			1.01	8.47E-24	1.55E-21	2.18E-24	0.0747	1139.7
17	1957.12	28.25	15	2	1	0	ncbf=9	fs	xo	cf	: o3	h2o			1.03	9.00E-24	1.46E-21	1.91E-24	0.0747	1200.5
18	1994.00	39.00	15	2	1	0	ncbf=8	fs	xo	cf	: o3	h2o			1.06	3.27E-23	7.99E-21	1.02E-23	0.0731	961.3
19	2028.22	27.05	15	2	1	0	ncbf=7	fs	xo	cf	: o3	h2o			1.09	5.43E-23	2.21E-20	2.04E-23	0.0750	903.3
20	2062.00	34.02	15	2	1	0	ncbf=8	fs	xo	cf	: o3	h2o	co		1.03	1.53E-21	1.64E-19	4.00E-22	0.0723	706.1
21	2095.15	32.40	15	2	1	0	ncbf=7	fs	xo	cf	: o3	h2o	co		1.01	3.52E-21	6.19E-19	1.66E-21	0.0779	280.4
22	2128.57	34.45	15	2	1	0	ncbf=7	fs	xo	cf	: o3	h2o	co		1.00	3.60E-21	5.61E-19	1.85E-21	0.0763	299.3
23	2188.00	64.40	15	2	1	0	ncbf=7	fs	xo	cf	: o3	h2o	co	n2o	1.01	1.61E-22	1.78E-20	4.59E-23	0.0729	426.9
24	2253.60	62.80	15	2	1	0	ncbf=7	fs	xo	cf	: o3	h2o	co	co2 n2o	1.00	4.78E-23	6.22E-21	1.12E-23	0.0730	637.7
25	2754.00	63.02	15	2	1	0	ncbf=11	fs	xo	cf	: o3	hdo			1.01	7.63E-23	1.79E-20	2.93E-23	0.0767	379.3
26	2797.50	21.02	15	2	1	0	ncbf=5	fs	xo	cf	: o3	hdo			1.00	7.49E-23	1.12E-20	3.87E-23	0.0765	288.1
27	2860.00	40.02	15	2	1	0	ncbf=10	fs	xo	cf	: o3	h2o	hdo	ch4	1.00	3.89E-24	3.55E-22	1.29E-24	0.0716	620.0
28	2916.00	72.02	15	2	1	0	ncbf=13	fs	xo	xf	: o3	h2o	hdo	ch4	1.00	8.83E-24	2.65E-21	2.72E-24	0.0747	1263.1
29	3011.00	114.02	15	2	1	0	ncbf=17	fs	xo	xf	: o3	h2o			1.00	4.28E-22	1.52E-19	1.94E-22	0.0766	331.2
30	3105.00	70.02	15	2	1	0	ncbf=11	fs	xo	xf	: o3	h2o			1.00	5.74E-23	6.20E-21	1.74E-23	0.0725	426.9
31	3164.50	45.02	15	2	1	0	ncbf=10	fs	xo	xf	: o3	h2o			1.00	2.16E-23	4.61E-21	9.79E-24	0.0769	331.6
32	3197.00	20.02	15	2	1	0	ncbf=7	fs	xo	xf	: o3	h2o			1.00	2.23E-23	3.48E-21	1.18E-23	0.0765	292.0
33	3985.88	69.76	15	2	1	0	ncbf=7	fs	xo	xf	: o3	h2o			1.00	3.84E-23	8.24E-21	1.56E-23	0.0767	335.7
34	4029.75	17.98	15	2	1	0	ncbf=7	fs	xo	xf	: o3	h2o			1.00	4.16E-23	5.93E-21	2.17E-23	0.0764	259.8
35	4640.00	70.02	15	2	1	0	ncbf=11	fs	xo	xf	: o3	h2o			1.00	2.87E-24	9.92E-22	1.25E-24	0.0767	279.2
36	4888.85	66.70	15	2	1	0	ncbf=8	fs	xo	xf	: o3	h2o			1.00	1.83E-24	6.56E-22	6.06E-25	0.0772	272.8
37	4927.35	10.35	15	2	1	0	ncbf=6	fs	xo	xf	: o3	h2o			1.00	2.13E-24	2.25E-22	1.17E-24	0.0765	214.6

RMS Fitting residuals to Kitt Peak lab spectra

iwin	fcen	HWid	Nrow	Npp	hit12	atm16	hit16	hit16d	ten18b	hit20a	birk19	tenn20	smpo20	birk20
1	648.65	18.06	105 / 190		0.5065	0.5064	0.5064	0.5060	0.5069	0.5064	0.5064	0.5061	0.5081	0.5064
2	684.45	16.51	105 / 190		0.7019	0.7019	0.7019	0.7019	0.7034	0.7019	0.7020	0.7022	0.7037	0.7019
3	752.40	51.41	105 / 190		1.1137	1.1136	1.1136	1.1136	1.1137	1.1136	1.1137	1.1136	1.1151	1.1136
4	832.15	28.35	159 / 190		0.5975	0.5975	0.5975	0.5975	0.5974	0.5975	0.5973	0.5974	0.5974	0.5973
5	1003.40	40.51	162 / 190		0.3895	0.3880	0.3880	0.3868	0.3909	0.3880	0.3846	0.3889	0.3930	0.3846
6	1060.00	16.26	162 / 190		0.3525	0.3524	0.3523	0.3504	0.3664	0.3523	0.3512	0.3633	0.3550	0.3496
7	1092.86	16.68	162 / 190		0.2514	0.2514	0.2514	0.2507	0.2675	0.2514	0.2513	0.2698	0.2514	0.2514
8	1119.75	10.20	162 / 190		0.1903	0.1903	0.1903	0.1898	0.2040	0.1903	0.1903	0.2073	0.1905	0.1903
9	1161.90	24.30	162 / 190		0.2639	0.2666	0.2666	0.2633	0.2704	0.2666	0.2635	0.2727	0.2642	0.2634
10	1199.25	11.10	162 / 190		0.1572	0.1581	0.1581	0.1571	0.1575	0.1581		0.1578	0.1570	
11	1716.40	56.03	60 / 190		0.6139	0.6067	0.6139	0.6066	0.6087	0.6139		0.6057	0.6020	
12	1775.44	22.47	60 / 190		0.5893	0.5863	0.5893	0.5829	0.5886	0.5893		0.5883	0.5795	
13	1812.50	12.25	60 / 190		0.2494	0.2475	0.2494	0.2460	0.2498	0.2494		0.2494	0.2465	
14	1837.50	12.25	60 / 190		0.3003	0.2919	0.3003	0.2887	0.2996	0.3003		0.3002	0.2851	
15	1865.00	14.70	60 / 190		0.2268	0.2223	0.2268	0.2219	0.2268	0.2268		0.2267	0.2178	
16	1914.62	27.45	60 / 190		0.1456	0.1456	0.1456	0.1446	0.1454	0.1456		0.1456	0.1449	
17	1957.12	14.12	60 / 190		0.1510	0.1512	0.1512	0.1502	0.1498	0.1512		0.1503	0.1504	
18	1994.00	19.50	60 / 190		0.1769	0.1773	0.1774	0.1754	0.1754	0.1774		0.1756	0.1748	
19	2028.22	13.52	60 / 190		0.1652	0.1700	0.1704	0.1639	0.1702	0.1704		0.1671	0.1612	
20	2062.00	17.01	60 / 190		0.2976	0.2575	0.2620	0.2536	0.2775	0.2620		0.2432	0.2493	
21	2095.15	16.20	60 / 190		0.5064	0.4052	0.4079	0.4010	0.4194	0.4079		0.3985	0.4012	
22	2128.57	17.23	60 / 190		0.4947	0.3775	0.3855	0.3729	0.4247	0.3855		0.3880	0.3764	
23	2188.00	32.20	60 / 190		0.1568	0.1546	0.1546	0.1542	0.1563	0.1546		0.1545	0.1538	
24	2253.60	31.40	60 / 190		0.1519	0.1515	0.1515	0.1512	0.1525	0.1515		0.1512	0.1513	
25	2754.00	31.51	64 / 190		0.3112	0.3064	0.3106	0.3013	0.3096	0.3106		0.3068	0.3086	
26	2797.50	10.51	64 / 190		0.5582	0.5383	0.5641	0.5314	0.5422	0.5641		0.5247	0.5492	
27	2860.00	20.01	11 / 190		0.0529	0.0529	0.0529	0.0529	0.0529	0.0528		0.0528	0.0528	
28	2916.00	36.01	11 / 190		0.0910	0.0891	0.0890	0.0883	0.0878	0.0863		0.0881	0.0860	
29	3011.00	57.01	11 / 190		0.2293	0.2157	0.2234	0.2055	0.2109	0.2233		0.1946	0.2203	
30	3105.00	35.01	11 / 190		0.0788	0.0787	0.0787	0.0778	0.0770	0.0787		0.0769	0.0788	
31	3164.50	22.51	11 / 190		0.0732	0.0732	0.0732	0.0730	0.0735	0.0732		0.0728	0.0735	
32	3197.00	10.01	11 / 190		0.0815	0.0815	0.0815	0.0812	0.0774	0.0815		0.0765	0.0818	
33	3985.88	34.88	5 / 190		0.2806	0.2620	0.2641	0.2506		0.2261		0.2317	0.2198	
34	4029.75	8.99	5 / 190		0.4949	0.4542	0.4429	0.4183		0.3149		0.3903	0.3058	
35	4640.00	35.01	5 / 190		0.2697	0.2689	0.2705	0.2688		0.2705		0.2678	0.2662	
36	4888.85	33.35	6 / 190		0.3990	0.3995	0.3962	0.3642		0.3962		0.3996	0.3543	
37	4927.35	5.18	6 / 190		0.4353	0.4271	0.4199	0.3837		0.4199		0.4208	0.3951	
Mean RMS over windows:					0.3271	0.3167	0.3183	0.3115		0.3137		0.3142	0.3086	

The three right-most columns are the new, post-July 2020 linelists.

Blue values denote the lowest RMS in that row; red the highest.

Overall, smpo_20 is best, hit16d is second, and HIT12 the worst.

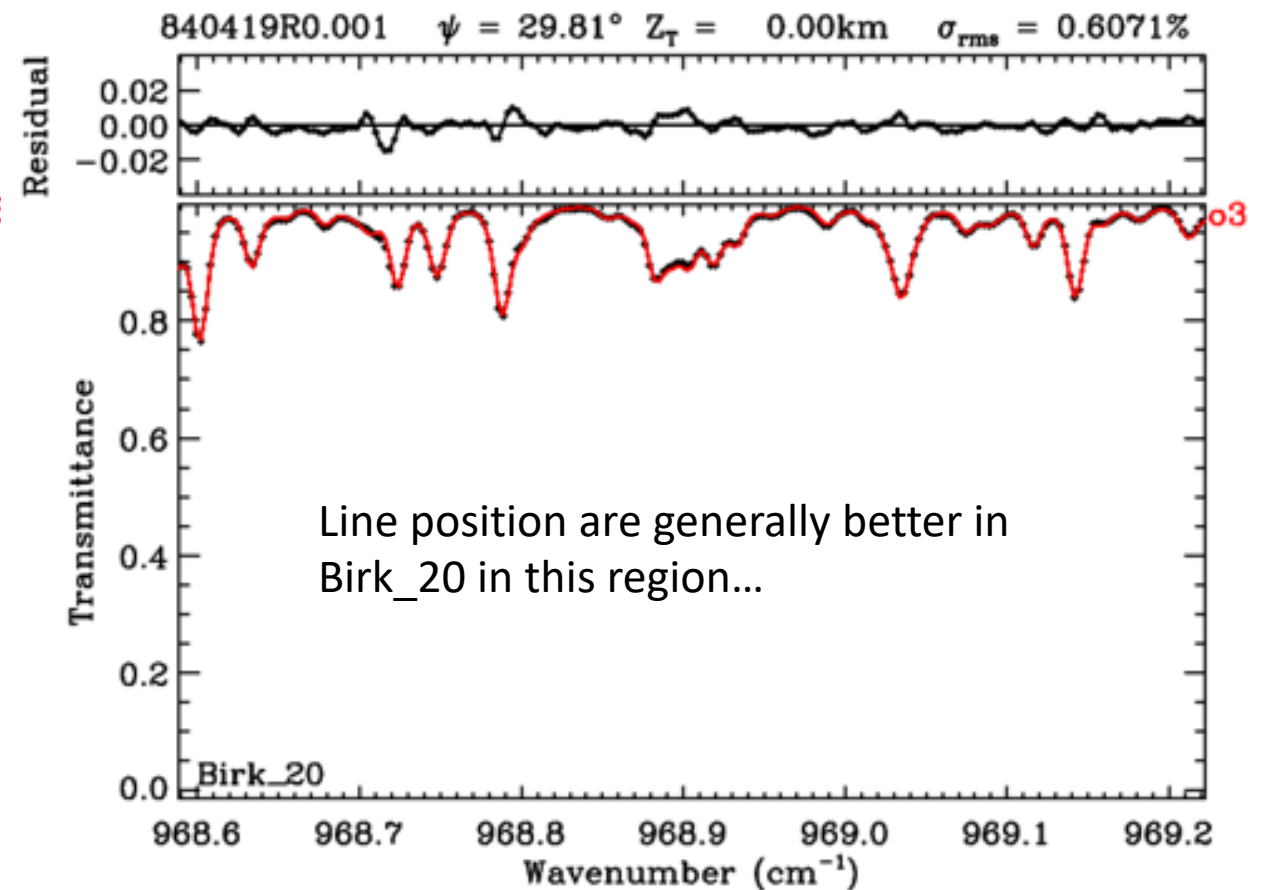
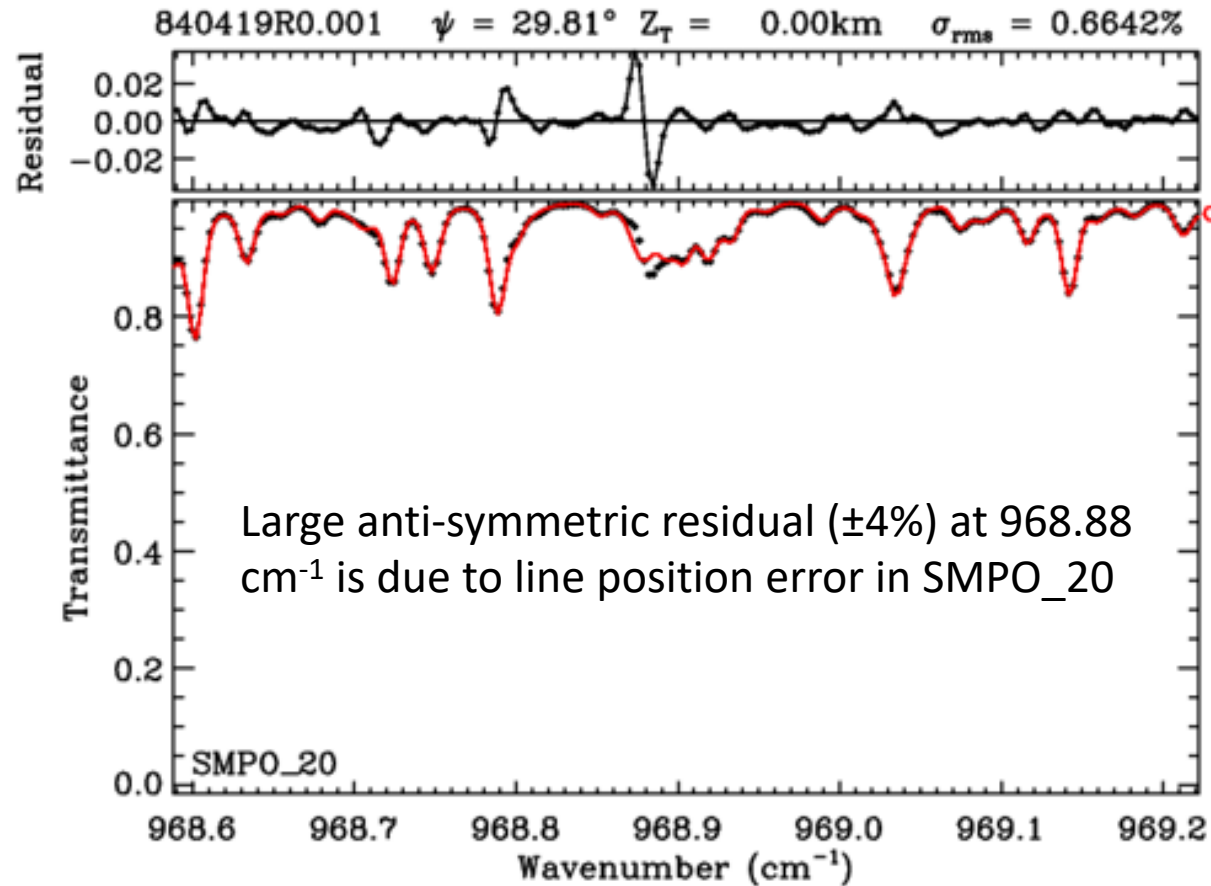
VMR Scale Factors (VSF) from fits to Kitt Peak lab spectra

iwin	fcen	HWid	Nrow	Npp	hit12	atm16	hit16	hit16d	ten18b	hit20a	birk19	tenn20	smpo20	birk20
1	648.65	18.06	105	190	0.9872	0.9873	0.9873	0.9872	0.9254	0.9873	0.9739	0.9336	0.9596	0.9740
2	684.45	16.51	105	190	0.9923	0.9923	0.9923	0.9919	0.9197	0.9923	0.9790	0.9274	0.9472	0.9790
3	752.40	51.41	105	190	1.0080	1.0080	1.0080	1.0080	0.9379	1.0080	0.9974	0.9425	0.9624	0.9946
4	832.15	28.35	159	190	0.9935	0.9935	0.9935	0.9935	0.9310	0.9935	0.9773	0.9342	1.0062	0.9774
5	1003.40	40.51	162	190	0.9995	0.9994	0.9994	0.9994	1.0045	0.9994	0.9778	0.9682	0.9710	0.9778
6	1060.00	16.26	162	190	0.9993	0.9993	0.9993	0.9993	1.0032	0.9993	0.9774	0.9660	0.9703	0.9774
7	1092.86	16.68	162	190	0.9966	0.9966	0.9966	0.9965	1.0442	0.9966	0.9778	1.0097	0.9829	0.9779
8	1119.75	10.20	162	190	1.0007	1.0007	1.0007	1.0013	1.0530	1.0007	0.9809	1.0208	0.9792	0.9809
9	1161.90	24.30	162	190	1.0063	1.0072	1.0072	1.0063	1.0617	1.0072	0.9862	1.0344	0.9810	0.9862
10	1199.25	11.10	162	190	1.0141	1.0162	1.0162	1.0139	1.0664	1.0162		1.0433	0.9897	
11	1716.40	56.03	60	190	0.9733	0.9738	0.9733	0.9738	1.1164	0.9733		1.0580	0.9436	
12	1775.44	22.47	60	190	1.0143	1.0146	1.0143	1.0152	1.0143	1.0143		0.9985	1.0180	
13	1812.50	12.25	60	190	0.9572	0.9573	0.9572	0.9573	0.9990	0.9572		0.9791	0.9845	
14	1837.50	12.25	60	190	0.9512	0.9514	0.9512	0.9515	1.0158	0.9512		0.9981	0.9940	
15	1865.00	14.70	60	190	0.9059	0.9107	0.9059	0.9110	0.9884	0.9059		0.9709	0.9712	
16	1914.62	27.45	60	190	0.8750	0.8794	0.8795	0.9026	1.0072	0.8795		0.9760	0.9705	
17	1957.12	14.12	60	190	0.8724	0.9458	0.9458	0.9783	1.0209	0.9458		1.0220	0.9760	
18	1994.00	19.50	60	190	0.8995	1.0010	1.0008	1.0132	0.9804	1.0008		0.9896	0.9788	
19	2028.22	13.52	60	190	0.9249	1.0071	1.0070	1.0210	0.9757	1.0070		0.9865	0.9899	
20	2062.00	17.01	60	190	0.9936	1.0227	1.0228	1.0227	0.9873	1.0228		0.9738	0.9825	
21	2095.15	16.20	60	190	1.0084	1.0092	1.0091	1.0093	0.9812	1.0091		0.9595	0.9690	
22	2128.57	17.23	60	190	1.0267	1.0149	1.0147	1.0150	0.9874	1.0147		0.9638	0.9736	
23	2188.00	32.20	60	190	0.9425	1.0176	1.0176	1.0177	0.9734	1.0176		0.9682	0.9767	
24	2253.60	31.40	60	190	0.9463	1.0056	1.0056	1.0057	0.9919	1.0056		0.9737	0.9651	
25	2754.00	31.51	64	190	0.9377	0.9377	0.9377	0.9375	0.9882	0.9377		0.9378	0.9666	
26	2797.50	10.51	64	190	0.9654	0.9645	0.9664	0.9647	0.9863	0.9664		0.9384	0.9962	
27	2860.00	20.01	11	190	0.9505	0.9505	0.9510	0.9510	0.9546	0.9500		0.9580	0.9402	
28	2916.00	36.01	11	190	0.8956	0.9006	0.9009	0.9029	0.9926	0.9428		0.9626	0.9654	
29	3011.00	57.01	11	190	0.9098	0.9093	0.9095	0.9087	0.9835	0.9095		0.9440	0.9786	
30	3105.00	35.01	11	190	0.9052	0.9057	0.9057	0.9059	0.9765	0.9057		0.9367	0.9066	
31	3164.50	22.51	11	190	0.9401	0.9401	0.9401	0.9402	0.8957	0.9401		0.8829	0.9388	
32	3197.00	10.01	11	190	0.9298	0.9298	0.9298	0.9300	0.8884	0.9298		0.8819	0.9286	
33	3985.88	34.88	5	190	0.9656	0.9669	0.9672	0.9688		1.0976		0.8416	0.9468	
34	4029.75	8.99	5	190	0.9377	0.9388	0.9386	0.9398		1.0918		0.8380	0.9410	
35	4640.00	35.01	5	190	0.9910	0.9925	0.9892	0.9890		0.9892		0.7980	0.9904	
36	4888.85	33.35	6	190	1.0657	1.0642	1.0668	1.0805		1.0668		0.9113	0.8940	
37	4927.35	5.18	6	190	0.9198	0.9446	0.9485	0.9699		0.9485		0.8209	0.8659	
Average VSF (over windows)					0.9788	0.9939	0.9942	0.9946		0.9954		0.9784	0.9749	
RMS deviation from mean					0.0332	0.0292	0.0296	0.0296		0.0301		0.0360	0.0152	

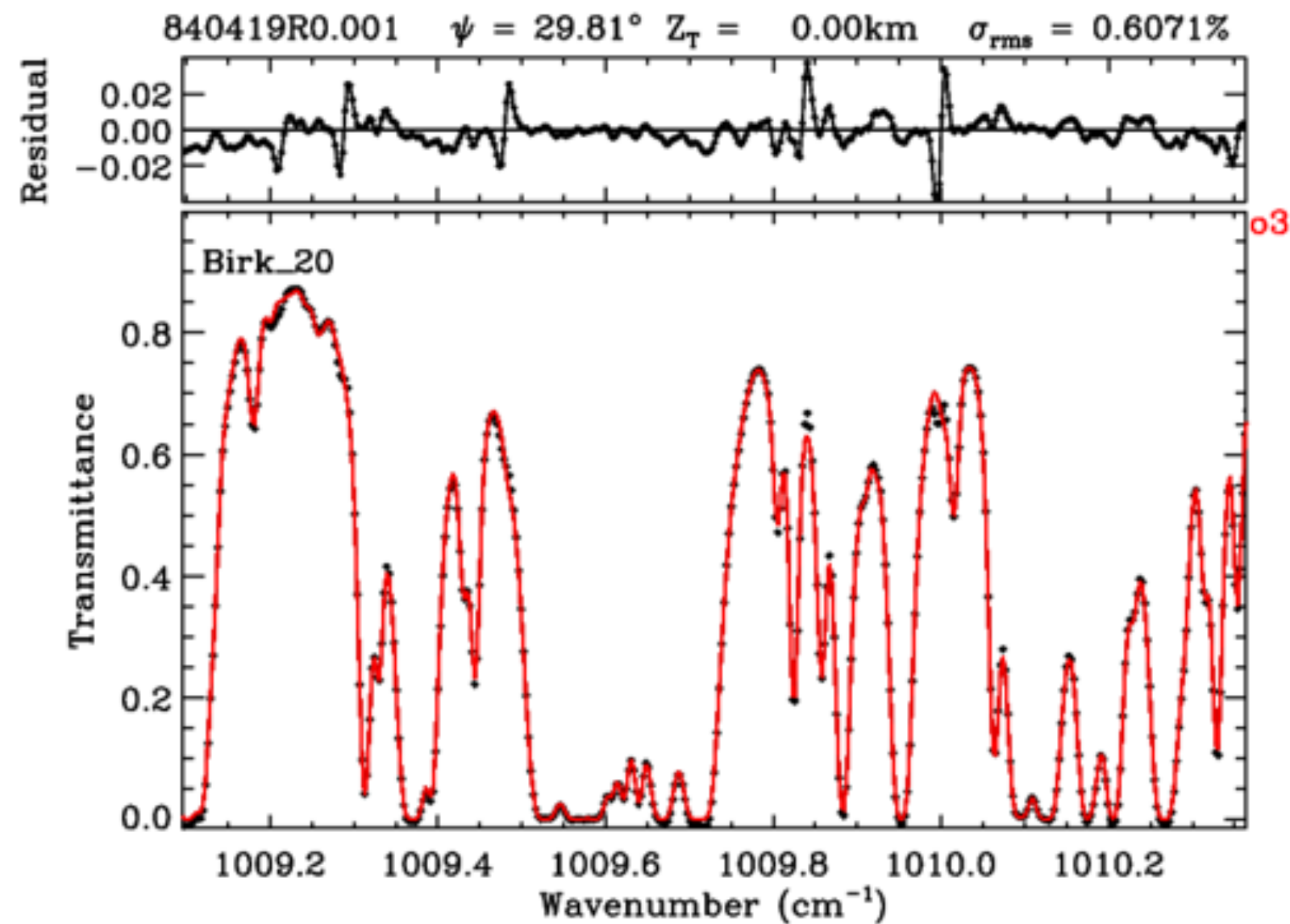
VSFs should all be 1.0

smpo_20 linelist gives the smallest window-to-window RMS deviation (1.5%), but retrievals are biased low by nearly 3%. In particular, retrievals in the 4888 and 4927 cm⁻¹ windows are biased low by more than 10%.

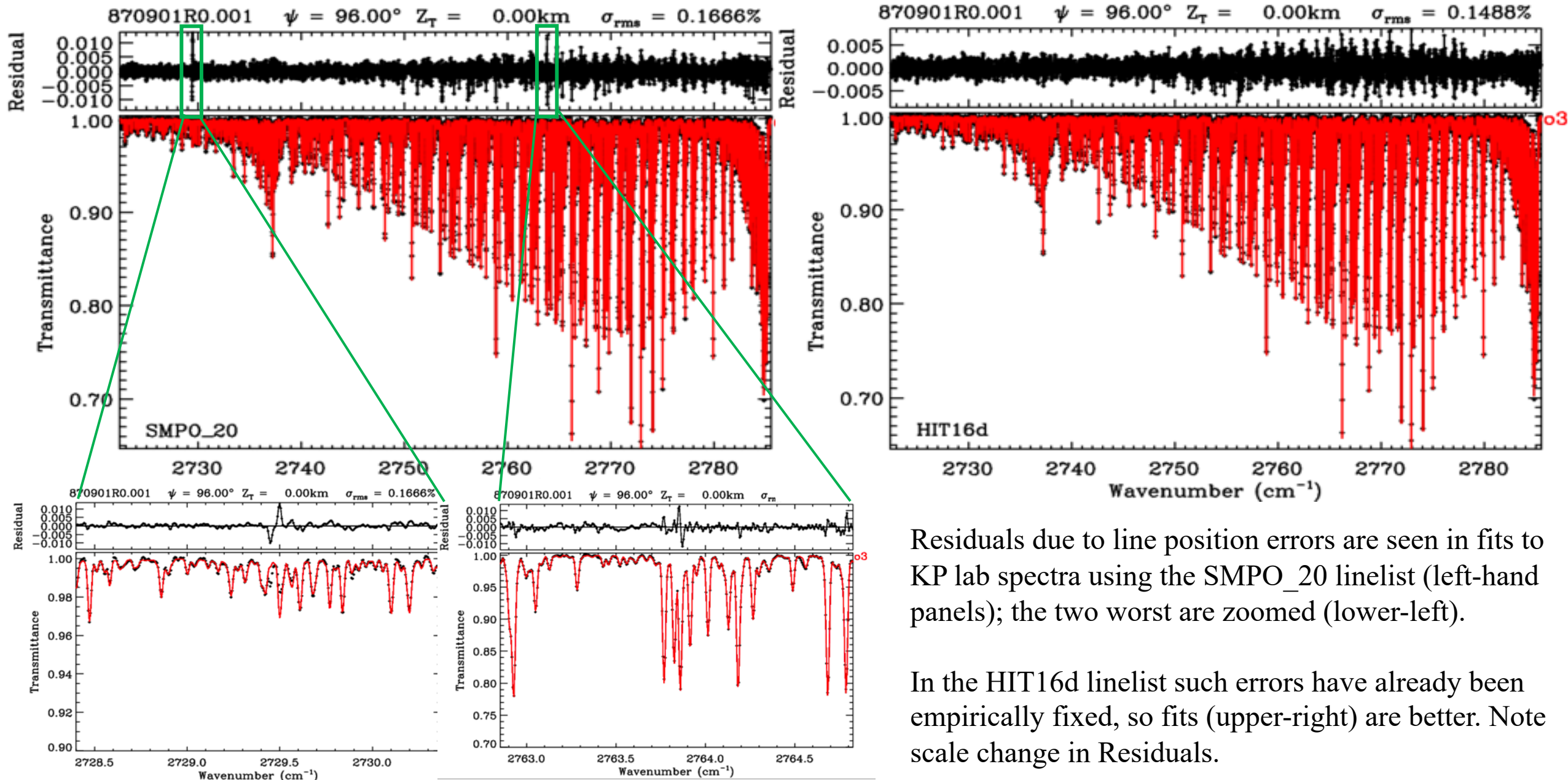
Example of fit to Kitt Peak lab spectrum -- 24 Torr of pure O₃ at 296K



...but there's still plenty of scope for improvement



In the 2700-2900 cm^{-1} region the HIT16d linelist provides the best fits



Residuals due to line position errors are seen in fits to KP lab spectra using the SMPO_20 linelist (left-hand panels); the two worst are zoomed (lower-left).

In the HIT16d linelist such errors have already been empirically fixed, so fits (upper-right) are better. Note scale change in Residuals.

RMS fitting residuals to MKIV balloon spectra

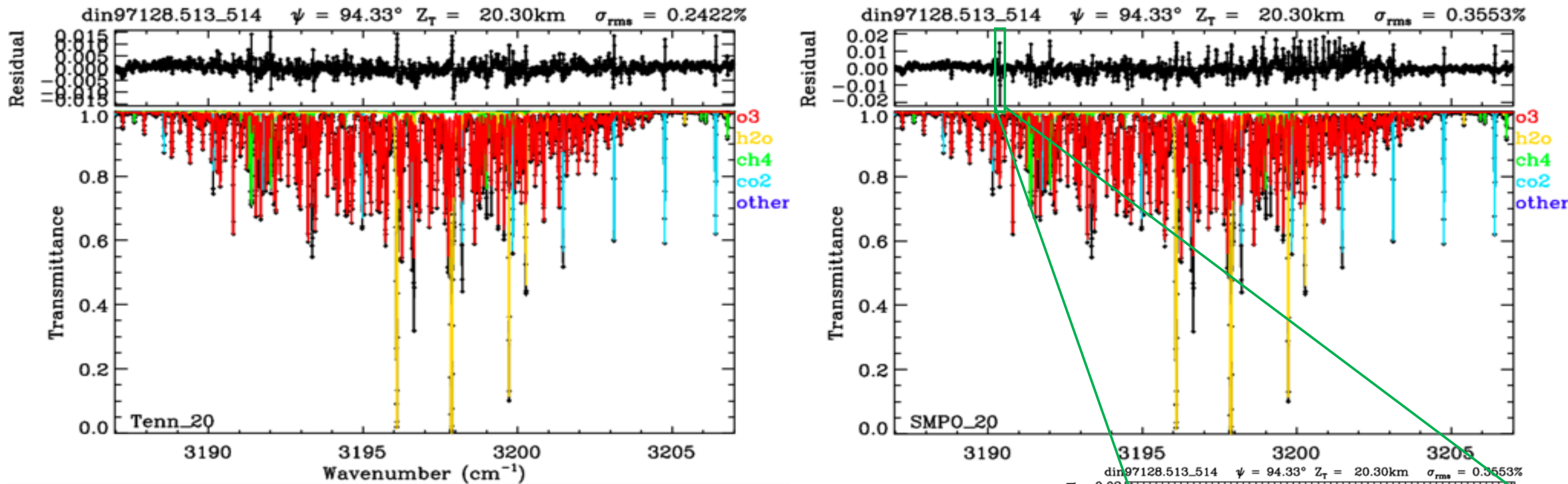
iwin	fcen	hwid	Nrow	Npp	hit12	atml6	hit16	hit16d	ten18b	hit20a	birk19	tenn20	smpo20	birk20
2	684.00	17.01	17	/ 17	0.9789	0.9779	0.9779	0.9788	0.9792	0.9779	0.9796	0.9789	0.9796	0.9790
3	752.40	51.41	17	/ 17	1.1136	1.1135	1.1135	1.1135	1.1150	1.1135	1.1134	1.1139	1.1109	1.1135
4	832.15	28.35	17	/ 17	0.5059	0.5059	0.5059	0.5059	0.5061	0.5059	0.5062	0.5060	0.5052	0.5062
5	1003.40	40.51	17	/ 17	0.5308	0.5213	0.5220	0.5209	0.5076	0.5220	0.5095	0.5020	0.5360	0.4901
6	1059.40	16.30	17	/ 17	0.3588	0.3586	0.3591	0.3429	0.4266	0.3591	0.3500	0.4536	0.3779	0.3385
7	1092.86	16.68	17	/ 17	0.3379	0.3379	0.3379	0.3375	0.6138	0.3379	0.3335	0.6673	0.3502	0.3328
8	1122.58	13.04	17	/ 17	0.3784	0.3787	0.3787	0.3778	0.6132	0.3787	0.3790	0.6765	0.3797	0.3788
9	1161.90	24.31	17	/ 17	0.3230	0.3569	0.3569	0.3201	0.4124	0.3569	0.3220	0.4445	0.3189	0.3220
10	1199.25	11.10	17	/ 17	0.2798	0.2828	0.2828	0.2785	0.2866	0.2828		0.2883	0.2766	
11	1706.90	46.53	17	/ 17	1.4252	1.4244	1.4252	1.4244	1.4243	1.4252		1.4230	1.4165	
12	1775.44	22.47	17	/ 17	0.8966	0.8963	0.8966	0.8963	0.8896	0.8966		0.8895	0.8904	
13	1812.50	12.25	17	/ 17	0.6642	0.6632	0.6642	0.6625	0.6650	0.6642		0.6628	0.6621	
14	1837.50	12.25	17	/ 17	0.8663	0.8550	0.8663	0.8548	0.8653	0.8663		0.8651	0.8641	
15	1865.00	14.70	17	/ 17	0.6707	0.6682	0.6707	0.6681	0.6702	0.6707		0.6699	0.6669	
16	1905.82	25.25	17	/ 17	0.6170	0.6169	0.6169	0.6166	0.6166	0.6169		0.6169	0.6169	
17	1953.12	18.12	17	/ 17	0.5485	0.5476	0.5476	0.5468	0.5472	0.5476		0.5472	0.5468	
18	1992.00	20.50	17	/ 17	0.5426	0.5326	0.5328	0.5303	0.5327	0.5328		0.5323	0.5091	
19	2027.22	14.52	17	/ 17	0.6281	0.6540	0.6568	0.6108	0.6047	0.6568		0.6125	0.5469	
20	2059.00	17.01	17	/ 17	0.6609	0.6202	0.6404	0.6137	0.5627	0.6404		0.5355	0.5670	
21	2095.15	16.20	17	/ 17	0.6628	0.5861	0.5922	0.5805	0.5403	0.5922		0.5274	0.5672	
22	2128.57	17.23	17	/ 17	0.9359	0.5678	0.5728	0.5673	0.6084	0.5728		0.5784	0.5748	
23	2183.00	37.20	17	/ 17	0.5109	0.5026	0.5027	0.5027	0.5066	0.5027		0.5019	0.5003	
24	2252.60	32.40	17	/ 17	0.5265	0.5253	0.5253	0.5252	0.5251	0.5253		0.5227	0.5251	
25	2754.00	31.51	17	/ 17	0.2707	0.2528	0.2734	0.2514	0.2786	0.2734		0.2701	0.2598	
26	2796.30	10.51	17	/ 17	0.3295	0.2872	0.3290	0.2864	0.3303	0.3290		0.3116	0.2999	
27	2860.00	20.01	17	/ 17	0.5246	0.5246	0.5246	0.5246	0.5251	0.5246		0.5247	0.5245	
28	2916.00	36.01	17	/ 17	0.8247	0.8235	0.8234	0.8233	0.8273	0.8258		0.8260	0.8257	
29	3011.00	59.01	17	/ 17	0.5833	0.5169	0.5475	0.4927	0.5540	0.5473		0.5407	0.5423	
30	3104.50	34.51	17	/ 17	0.4498	0.4495	0.4495	0.4494	0.4468	0.4495		0.4463	0.4502	
31	3164.50	22.51	17	/ 17	0.3178	0.3178	0.3178	0.3176	0.3178	0.3178		0.3159	0.3192	
32	3197.00	10.01	17	/ 17	0.2236	0.2236	0.2236	0.2227	0.1980	0.2236		0.1866	0.2290	
33	3985.88	34.88	17	/ 17	0.4084	0.3940	0.3979	0.3845		0.3593		0.3565	0.3555	
34	4029.75	8.99	17	/ 17	0.6047	0.5574	0.5557	0.5291		0.4255		0.4996	0.4194	
35	4640.00	35.01	17	/ 17	0.2731	0.2645	0.2658	0.2629		0.2658		0.2627	0.2580	
36	4888.85	33.35	17	/ 17	0.4407	0.4394	0.4389	0.4371		0.4389		0.4397	0.4380	
37	4927.35	5.18	17	/ 17	0.4055	0.3896	0.3857	0.3820		0.3857		0.3870	0.3808	
Mean RMS over windows:					0.5573	0.5388	0.5426	0.5335		0.5381		0.5536	0.5292	

Blue denotes the lowest RMS in that row; Red denotes the highest.

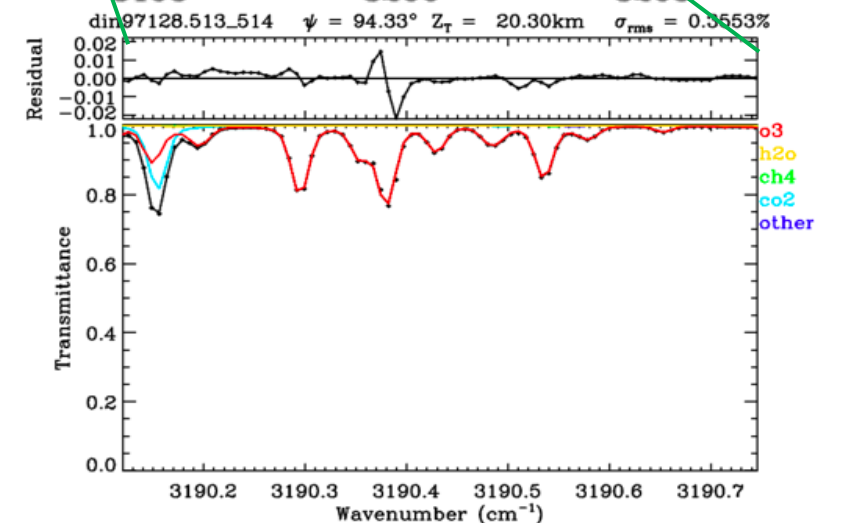
Overall, smpo20 best, followed by hit16d. HIT12 is the worst.

Window #1 is too blacked out in balloon spectra.

Fits to the 3197 cm⁻¹ window in MkIV balloon spectrum (20 km tangent altitude)



Tenn_20 linelist (left) produces much better fits than SMPO_20 (right). In left-hand panel, residuals are dominated by inconsistency between H₂O, CH₄, and CO₂ line positions. In right-hand panel, residuals are mainly due to O₃. Biggest residual is due to a line position error in line at 3190.38 cm⁻¹ in SMPO_20 (zoomed lower right).



VMR Scale Factors (VSF) from fits to MkIV balloon spectra

iwin	fcen	hwid	Nrow	Npp	hit12	atml6	hit16	hit16d	ten18b	hit20a	birk19	tenn20	smpo20	birk20
2	684.00	17.01	17 / 17		1.2013	1.2013	1.2013	1.2008	1.1138	1.2013	1.1862	1.1214	1.1428	1.1862
3	752.40	51.41	17 / 17		1.1078	1.1078	1.1078	1.1078	1.0299	1.1078	1.0931	1.0355	1.0695	1.0931
4	832.15	28.35	17 / 17		1.0404	1.0404	1.0404	1.0404	0.9746	1.0404	1.0288	0.9781	1.0587	1.0288
5	1003.40	40.51	17 / 17		1.0433	1.0416	1.0413	1.0420	1.0518	1.0413	1.0234	1.0199	1.0188	1.0283
6	1059.40	16.30	17 / 17		1.0462	1.0463	1.0461	1.0466	1.0665	1.0461	1.0263	1.0280	1.0237	1.0252
7	1092.86	16.68	17 / 17		1.0791	1.0791	1.0791	1.0794	1.1325	1.0791	1.0567	1.0979	1.0625	1.0571
8	1122.58	13.04	17 / 17		1.0925	1.0925	1.0925	1.0914	1.1755	1.0925	1.0676	1.1478	1.0681	1.0677
9	1161.90	24.31	17 / 17		1.0784	1.0825	1.0825	1.0788	1.1444	1.0825	1.0541	1.1176	1.0509	1.0542
10	1199.25	11.10	17 / 17		1.0555	1.0567	1.0567	1.0555	1.1118	1.0567		1.0879	1.0312	
11	1706.90	46.53	17 / 17		1.0307	1.0308	1.0307	1.0308	1.1666	1.0307		1.1055	0.9994	
12	1775.44	22.47	17 / 17		1.0305	1.0305	1.0305	1.0305	1.0295	1.0305		1.0138	1.0329	
13	1812.50	12.25	17 / 17		0.9906	0.9907	0.9906	0.9906	1.0316	0.9906		1.0132	1.0175	
14	1837.50	12.25	17 / 17		0.9611	0.9609	0.9611	0.9610	1.0252	0.9611		1.0079	1.0032	
15	1865.00	14.70	17 / 17		0.9139	0.9149	0.9139	0.9148	0.9960	0.9139		0.9788	0.9711	
16	1905.82	25.25	17 / 17		0.8911	0.8915	0.8915	0.8937	0.9922	0.8915		0.9737	0.9664	
17	1953.12	18.12	17 / 17		0.8371	0.9226	0.9225	0.9400	0.9512	0.9225		0.9740	0.9169	
18	1992.00	20.50	17 / 17		0.9152	1.0287	1.0286	1.0304	0.9861	1.0286		1.0057	0.9892	
19	2027.22	14.52	17 / 17		0.9527	1.0433	1.0428	1.0512	1.0030	1.0428		1.0142	1.0136	
20	2059.00	17.01	17 / 17		0.9826	1.0377	1.0376	1.0378	1.0125	1.0376		1.0062	1.0049	
21	2095.15	16.20	17 / 17		1.0536	1.0694	1.0701	1.0696	1.0469	1.0701		1.0272	1.0312	
22	2128.57	17.23	17 / 17		1.0531	1.0585	1.0582	1.0585	1.0309	1.0582		1.0065	1.0149	
23	2183.00	37.20	17 / 17		0.9588	1.0384	1.0384	1.0385	0.9944	1.0384		0.9896	0.9966	
24	2252.60	32.40	17 / 17		1.0041	1.0687	1.0687	1.0688	1.0510	1.0687		1.0313	1.0257	
25	2754.00	31.51	17 / 17		0.9653	0.9642	0.9655	0.9638	1.0158	0.9655		0.9643	0.9943	
26	2796.30	10.51	17 / 17		0.9992	0.9974	1.0002	0.9971	1.0211	1.0002		0.9703	1.0305	
27	2860.00	20.01	17 / 17		0.9376	0.9376	0.9376	0.9376	0.9422	0.9376		0.9461	0.9375	
28	2916.00	36.01	17 / 17		1.0010	1.0120	1.0119	1.0132	1.0536	1.0129		1.0189	1.0278	
29	3011.00	59.01	17 / 17		0.9479	0.9477	0.9477	0.9451	1.0230	0.9477		0.9807	1.0175	
30	3104.50	34.51	17 / 17		0.9486	0.9487	0.9487	0.9481	1.0113	0.9487		0.9690	0.9485	
31	3164.50	22.51	17 / 17		0.9813	0.9813	0.9813	0.9813	0.9289	0.9813		0.9164	0.9801	
32	3197.00	10.01	17 / 17		0.9682	0.9682	0.9682	0.9681	0.9210	0.9682		0.9125	0.9674	
33	3985.88	34.88	17 / 17		1.0345	1.0341	1.0347	1.0353		1.1681		0.8921	1.0081	
34	4029.75	8.99	17 / 17		1.0061	1.0056	1.0053	1.0064		1.1615		0.8963	1.0036	
35	4640.00	35.01	17 / 17		1.0286	1.0364	1.0363	1.0351		1.0363		0.8241	1.0439	
36	4888.85	33.35	17 / 17		1.0516	1.0607	1.0638	1.0788		1.0638		0.8807	0.8698	
37	4927.35	5.18	17 / 17		0.9583	0.9982	1.0044	1.0206		1.0044		0.8516	0.9148	
Average VSF (over windows)					1.0160	1.0206	1.0227	1.0211		1.0366		0.9878	1.0162	
RMS deviation from mean					0.0521	0.0486	0.0486	0.0484		0.0637		0.0716	0.0325	

Windows # 1 is too blacked out in balloon spectra of the atmosphere to derive a useful VSF value.

SMPO_20 linelist has the smallest/best window-to-window biases (3.25%), although Birk20 is also very good where it exists.

MkIV ground-based atmospheric spectra: RMS fitting residuals (%)

iwin	fcen	Hwid	Nrow	Npp	hit12	atm16	hit16	hit16d	ten18b	hit20a	birk19	tenn20	smpo20	birk20
3	752.40	51.41	78	/ 78	1.2593	1.2593	1.2593	1.2593	1.2597	1.2593	1.2593	1.2594	1.2610	1.2593
4	832.15	28.35	78	/ 78	0.5295	0.5295	0.5295	0.5295	0.5295	0.5295	0.5295	0.5295	0.5297	0.5295
5	1003.40	40.51	78	/ 78	0.4640	0.4611	0.4613	0.4611	0.4789	0.4613	0.4565	0.4668	0.4676	0.4534
6	1059.40	16.30	78	/ 78	0.4378	0.4377	0.4379	0.4377	0.5081	0.4379	0.4478	0.5114	0.4462	0.4406
7	1092.86	16.68	78	/ 78	0.3406	0.3406	0.3406	0.3405	0.4598	0.3406	0.3398	0.4833	0.3433	0.3401
8	1122.68	13.14	78	/ 78	0.3642	0.3642	0.3642	0.3638	0.4648	0.3642	0.3616	0.4733	0.3647	0.3616
9	1161.90	24.31	78	/ 78	0.4429	0.4428	0.4428	0.4426	0.4554	0.4428	0.4419	0.4576	0.4410	0.4419
10	1199.25	11.10	78	/ 78	0.7203	0.7203	0.7203	0.7203	0.7206	0.7203		0.7203	0.7198	
11	1706.90	46.53	78	/ 78	0.1197	0.1197	0.1197	0.1197	0.1197	0.1197		0.1197	0.1196	
12	1775.44	22.47	78	/ 78	0.2437	0.2437	0.2437	0.2437	0.2437	0.2437		0.2436	0.2441	
13	1812.50	12.25	62	/ 78	0.2328	0.2358	0.2328	0.2297	0.2456	0.2328		0.2483	0.2395	
14	1837.50	12.25	62	/ 78	0.1298	0.1293	0.1298	0.1283	0.1358	0.1298		0.1363	0.1334	
15	1865.00	14.70	78	/ 78	0.3926	0.3927	0.3926	0.3927	0.3837	0.3926		0.3823	0.3819	
16	1905.82	25.25	78	/ 78	0.3875	0.3875	0.3875	0.3875	0.3875	0.3875		0.3875	0.3875	
17	1953.12	18.12	78	/ 78	0.5074	0.5092	0.5092	0.5089	0.5074	0.5092		0.5074	0.5088	
18	1992.00	20.50	78	/ 78	0.5278	0.5277	0.5277	0.5277	0.5277	0.5277		0.5277	0.5274	
19	2027.22	14.52	78	/ 78	0.4969	0.4968	0.4969	0.4965	0.4970	0.4969		0.4968	0.4962	
20	2059.00	17.01	78	/ 78	0.5142	0.5141	0.5144	0.5137	0.5199	0.5144		0.5153	0.5145	
21	2095.15	16.20	78	/ 78	0.7528	0.7298	0.7305	0.7289	0.7462	0.7305		0.7322	0.7331	
22	2128.57	17.23	78	/ 78	0.8326	0.7968	0.7974	0.7962	0.8223	0.7974		0.7988	0.7978	
23	2183.00	37.20	78	/ 78	0.3248	0.3250	0.3250	0.3250	0.3251	0.3250		0.3251	0.3250	
24	2252.60	32.40	78	/ 78	0.1431	0.1431	0.1431	0.1431	0.1431	0.1431		0.1431	0.1431	
25	2754.00	31.51	78	/ 78	0.3624	0.3616	0.3632	0.3611	0.3632	0.3632		0.3629	0.3622	
26	2796.30	10.51	78	/ 78	0.4313	0.4298	0.4305	0.4295	0.4298	0.4305		0.4301	0.4302	
27	2860.00	20.01	78	/ 78	0.7140	0.7140	0.7140	0.7140	0.7140	0.7140		0.7140	0.7140	
28	2916.00	36.01	78	/ 78	1.2022	1.2022	1.2022	1.2022	1.2023	1.2022		1.2022	1.2023	
29	3011.00	59.01	78	/ 78	0.5752	0.5739	0.5746	0.5737	0.5763	0.5746		0.5747	0.5750	
30	3104.50	34.51	78	/ 78	0.4932	0.4932	0.4932	0.4932	0.4932	0.4932		0.4932	0.4933	
31	3164.50	22.51	78	/ 78	0.9611	0.9611	0.9611	0.9611	0.9611	0.9611		0.9610	0.9610	
32	3197.00	10.01	78	/ 78	0.5345	0.5345	0.5345	0.5345	0.5346	0.5345		0.5346	0.5346	
33	3985.88	34.88	78	/ 78	0.3602	0.3602	0.3601	0.3575		0.3580		0.3559	0.3592	
34	4029.75	8.99	78	/ 78	0.4840	0.4835	0.4836	0.4832		0.4822		0.4836	0.4821	
35	4640.00	35.01	78	/ 78	0.3165	0.3162	0.3162	0.3161		0.3162		0.3162	0.3159	
36	4888.85	33.35	78	/ 78	0.6191	0.6190	0.6190	0.6190		0.6190		0.6191	0.6190	
37	4927.35	5.18	78	/ 78	0.5203	0.5201	0.5199	0.5199		0.5201		0.5201	0.5201	
Mean RMS over windows:					0.4913	0.4896	0.4897	0.4892		0.4896		0.4993	0.4898	

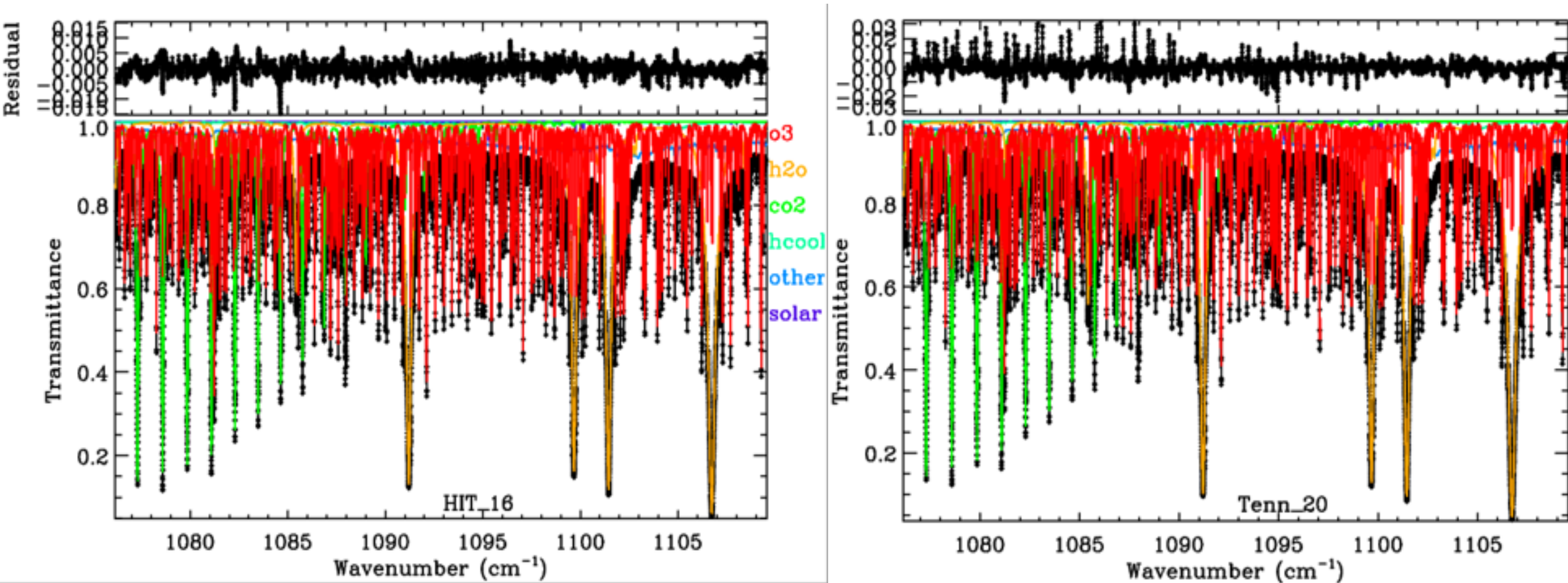
Blue values denote the lowest RMS in that row; red the highest. Overall hit16d is best, closely followed by smpo20.

Ground-based spectral fits are sensitive to line widths and pressure shifts.

VSF values retrieved from MKIV ground-based spectra

iwin	fcen	Hwid	Nrow	Npp	hit12	atml6	hit16	hit16d	ten18b	hit20a	birk19	tenn20	smpo20	birk20	
3	752.40	51.41	78 \	78	1.0154	1.0154	1.0154	1.0154	0.9477	1.0154	1.0017	0.9523	0.9858	1.0017	
4	832.15	28.35	78 \	78	1.0291	1.0291	1.0291	1.0291	0.9621	1.0291	1.0099	0.9659	1.0383	1.0099	
5	1003.40	40.51	78 \	78	1.0216	1.0213	1.0213	1.0213	1.0281	1.0213	0.9965	0.9921	0.9941	0.9984	
6	1059.40	16.30	78 \	78	1.0255	1.0255	1.0255	1.0257	1.0429	1.0255	1.0019	1.0063	0.9997	1.0024	
7	1092.86	16.68	78 \	78	1.0091	1.0091	1.0091	1.0091	1.0653	1.0091	0.9890	1.0315	0.9937	0.9890	
8	1122.68	13.14	78 \	78	1.0105	1.0105	1.0105	1.0102	1.0740	1.0105	0.9893	1.0460	0.9882	0.9893	
9	1161.90	24.31	78 \	78	1.0187	1.0189	1.0189	1.0187	1.0803	1.0189	0.9973	1.0534	0.9931	0.9973	
10	1199.25	11.10	78 \	78	1.0084	1.0087	1.0087	1.0083	1.0625	1.0087		1.0409	0.9852		
11	1706.90	46.53	78 \	78											
12	1775.44	22.47	78 \	78											
13	1812.50	12.25	62 \	78	0.9187	0.9177	0.9187	0.9177	0.9607	0.9187		0.9425	0.9473		Windows # 1, 2, 11, 12 are too blacked out in ground-based spectra to determine a worthwhile VSF value
14	1837.50	12.25	62 \	78	0.8071	0.8062	0.8071	0.8063	0.8614	0.8071		0.8452	0.8396		
15	1865.00	14.70	78 \	78	0.8478	0.8484	0.8478	0.8479	0.9250	0.8478		0.9087	0.9010		
16	1905.82	25.25	78 \	78											
17	1953.12	18.12	78 \	78											
18	1992.00	20.50	78 \	78	0.8835	0.9942	0.9942	0.9945	0.9450	0.9942		0.9677	0.9543		
19	2027.22	14.52	78 \	78	0.9423	1.0375	1.0375	1.0401	0.9809	1.0375		1.0004	1.0010		
20	2059.00	17.01	78 \	78	0.9744	1.0188	1.0189	1.0187	0.9788	1.0189		0.9726	0.9793		
21	2095.15	16.20	78 \	78	1.0102	1.0135	1.0134	1.0136	0.9852	1.0134		0.9637	0.9731		In windows #16, 17, 27, 28, 35, 36, and 37, O ₃ lines are too weak in ground-based spectra to ascertain a useful VSF value.
22	2128.57	17.23	78 \	78	1.0201	1.0111	1.0112	1.0111	0.9842	1.0112		0.9602	0.9706		
23	2183.00	37.20	78 \	78	0.9408	1.0179	1.0179	1.0178	0.9746	1.0179		0.9694	0.9768		
24	2252.60	32.40	78 \	78	0.9356	0.9992	0.9992	0.9992	0.9977	0.9992		0.9688	0.9590		
25	2754.00	31.51	78 \	78	0.9425	0.9429	0.9425	0.9431	0.9946	0.9425		0.9439	0.9720		
26	2796.30	10.51	78 \	78	0.9658	0.9662	0.9660	0.9665	0.9941	0.9660		0.9445	0.9970		
27	2860.00	20.01	78 \	78											
28	2916.00	36.01	78 \	78											
29	3011.00	59.01	78 \	78	0.9011	0.9013	0.9012	0.9013	0.9741	0.9012		0.9348	0.9686		
30	3104.50	34.51	78 \	78	1.0234	1.0236	1.0236	1.0242	1.0766	1.0236		1.0285	1.0179		SMPO_20 linelist has the smallest/best window-to-window biases (1.48%), although Birk20 is also very good where it exists.
31	3164.50	22.51	78 \	78	0.8923	0.8923	0.8923	0.8922	0.8488	0.8923		0.8367	0.8920		
32	3197.00	10.01	78 \	78	0.9740	0.9740	0.9740	0.9741	0.9195	0.9740		0.9096	0.9722		
33	3985.88	34.88	78 \	78	1.0064	1.0071	1.0073	1.0089		1.1544		0.8678	0.9946		
34	4029.75	8.99	78 \	78	0.9603	0.9603	0.9600	0.9615		1.1186		0.8502	0.9654		
35	4640.00	35.01	78 \	78											
36	4888.85	33.35	78 \	78											
37	4927.35	5.18	78 \	78											
Average VSF (over windows)					1.0002	1.0049	1.0050	1.0049		1.0056		0.9985	0.9892		
RMS deviation from mean					0.0322	0.0290	0.0290	0.0290		0.0300		0.0443	0.0148		

Example of Fits to MkIV ground-based spectra in 1092 cm⁻¹ window



HIT_16 (left) has peak residuals of 1.5% and a RMS of 0.34%. Tenn_20 (right) has peak residuals of 3% and a RMS of 0.48%. Note the factor 2 scale change between the two residuals panels. In Tenn_20 a subset of lines below 1090 cm⁻¹ seem inconsistent (too strong) compared with the other lines in the window. For example, the intensity of the following line in HIT16

31	1082.87766	2.895E-22	286.5665	.0698	.1010	.79	-.001	1	0	0	0	25	1	25	26	0	26	0065501412	4	2	2	1	51.0	53.0
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became 3.300E-22 in Tenn_20, which is 14% stronger, causing a large upward residual. Many other examples can be seen.

Conclusions

Based on the results of fitting KP lab spectra, plus MkIV balloon & ground-based atmospheric spectra, using 10 linelists:

- HIT_12 has the worst RMS fitting residuals, which are indicative of position errors and inconsistent intensities
- Birk_20 produces better RMS fits than Birk_19, especially in windows # 5 and 6.
- Birk_20 is the best linelist below 1135 cm^{-1} , in terms of RMS fitting residuals, and probably absolute intensities.
- SMPO_20 is the best linelist above 1135 cm^{-1} , except for $3070\text{-}3210\text{ cm}^{-1}$ where it is the worst.
- Tenn_20 is worse than Ten_18b in windows # 7, 8, 9, but is generally better elsewhere.
- There are still several windows (e.g. $2040\text{-}3070\text{ cm}^{-1}$) where the HIT16d O₃ linelist has the smallest fitting residuals. (HIT16d is an empirically modified version of the HIT16)
- Would be nice for HITRAN_2024 to have linelists for the doubly-substituted isotopologs (e.g. 688, 868) in order to better analyze ¹⁸O-enriched lab spectra in the ν_3 band.