

GSMA Reims : UV – IR Spectroscopy of ozone

Genève, march 2010, 23-25

Ozone databank: S&MPO (GSMA Reims – IAO Tomsk)

<http://ozone.iao.ru> (S&MPO)

russian english

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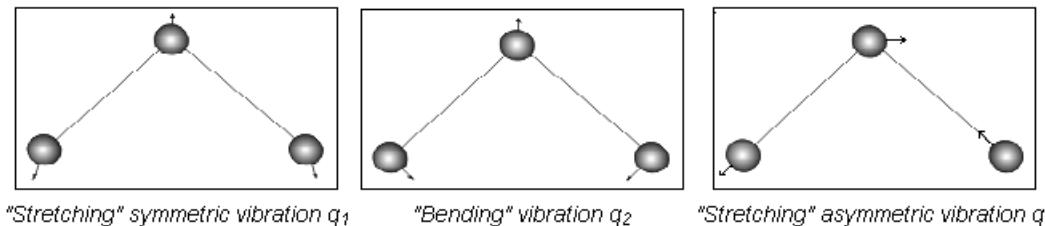
Spectroscopy & Molecular Properties of Ozone

EGS Structure and Spectroscopic Constants

Open configuration in the electronic ground state (EGS)

Equilibrium: tree oxygen atoms forming the isosceles triangle (apex angle $q_e=116.7542^\circ$, two equal bonds $r_e=1.27173 \text{ \AA}$)

Normal mode vibrations



Spectroscopic constants

Isotopic species				Calculated		Rot.parameters of Vib.ground state, cm ⁻¹				Fundamental vibration wavenumbers, cm ⁻¹			
formula	code	mass, a.u.	Q(296K)	(*)	abundance, %	A	B	C	(*)	v1	v2	v3	(*)
¹⁶ O ¹⁶ O ¹⁶ O	666	47.984745	3473.0		99.2901000000000	3.55366659	0.44528320	0.39475182		1103.137	700.931	1042.084	
¹⁶ O ¹⁶ O ¹⁸ O	668	49.988991	7385.0		0.398194000000	3.48818517	0.42000833	0.37400895		1090.354	684.613	1028.112	
¹⁶ O ¹⁸ O ¹⁶ O	686	49.988991	3599.0		0.199097000000	3.29049897	0.44539922	0.39132965		1074.308	693.306	1008.453	
¹⁶ O ¹⁶ O ¹⁷ O	667	48.988960	7159.0		0.074047500000	3.51880145	0.43201005	0.38386595		1095.693	692.435	1035.359	
¹⁶ O ¹⁷ O ¹⁶ O	676	48.988960	3543.0		0.037023700000	3.41407204	0.44534406	0.39299485		1087.829	697.079	1024.396	
¹⁶ O ¹⁸ O ¹⁸ O	688	51.993237	7747.0		0.000838457600	3.22506213	0.42006895	0.37077963		1060.708	677.504	993.925	
¹⁸ O ¹⁶ O ¹⁸ O	868	51.993237	4050.0		0.000419228800	3.42167473	0.39579007	0.35397425		1072.217	668.085	1019.349	
¹⁷ O ¹⁶ O ¹⁸ O	768	50.993206	7745.0	*	0.000155421400	3.45278049	0.40729198	0.36349812		1080.080	675.979	1024.026	*
¹⁶ O ¹⁸ O ¹⁷ O	687	50.993206	7565.0	*	0.000155421400	3.25564313	0.43210784	0.38055432		1066.365	685.153	1001.511	*
¹⁶ O ¹⁷ O ¹⁸ O	678	50.993206	7649.0	*	0.000155421400	3.34860682	0.42004153	0.37235370		1074.586	681.048	1010.129	*
¹⁶ O ¹⁷ O ¹⁷ O	677	49.993179	7353.9		0.000028809800	3.37920213	0.43206039	0.38217676		1080.153	688.758	1017.534	#
¹⁷ O ¹⁶ O ¹⁷ O	767	49.993179	7489.0	*	0.000014404900	3.48365021	0.41902918	0.37317932		1086.715	683.867	1030.037	*

Survey of Available Cross-Sections

Representation of WN/WL: Wavelength, nm ▼

select	$\lambda_{\min}, \text{nm}$	$\lambda_{\max}, \text{nm}$	$\lambda_{\text{step}}, \text{nm}$	T, K	P, torr	broad
<input type="checkbox"/>	194.5000	650.0100	0.010	218.00	n/a	air
<input type="checkbox"/>	194.5000	520.0100	0.010	228.00	n/a	air
<input type="checkbox"/>	194.5000	519.0100	0.010	243.00	n/a	air
<input type="checkbox"/>	299.5000	520.0100	0.010	273.00	n/a	air
<input type="checkbox"/>	195.0000	830.0000	0.010	295.00	n/a	air

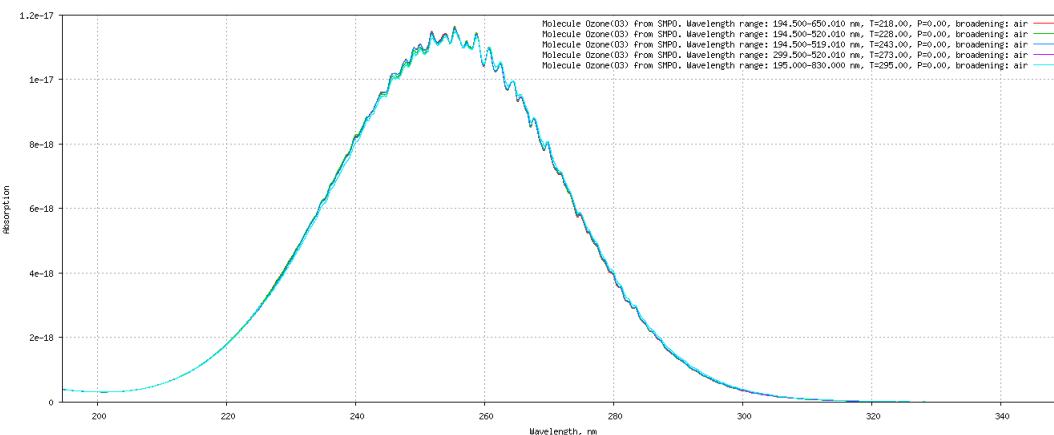
Show

Visible and ultraviolet spectra of the Hartley, Huggins, and Chappuis bands have been recorded in GSMA by J. Malicet, J. Brion, and D. Daumont. Fourier transform spectrometer Bomem DA3 was used for spectra registration. For more details see Refs. [36, 55, 67, 69, 84, 85, 103, 123] of the "Electronic structure" section in the references.

Hartley band

Chosen Cross-Sections

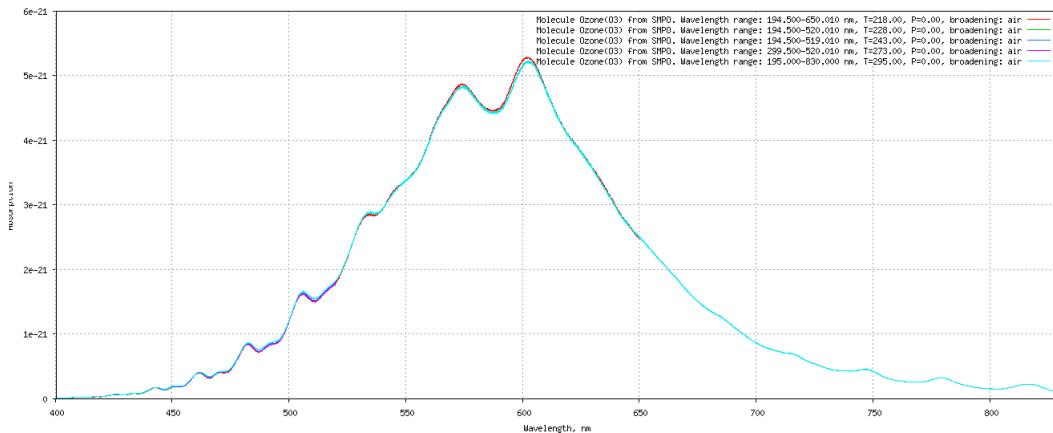
Representation of WN/WL: Wavelength, nm ▼



Chappuis band

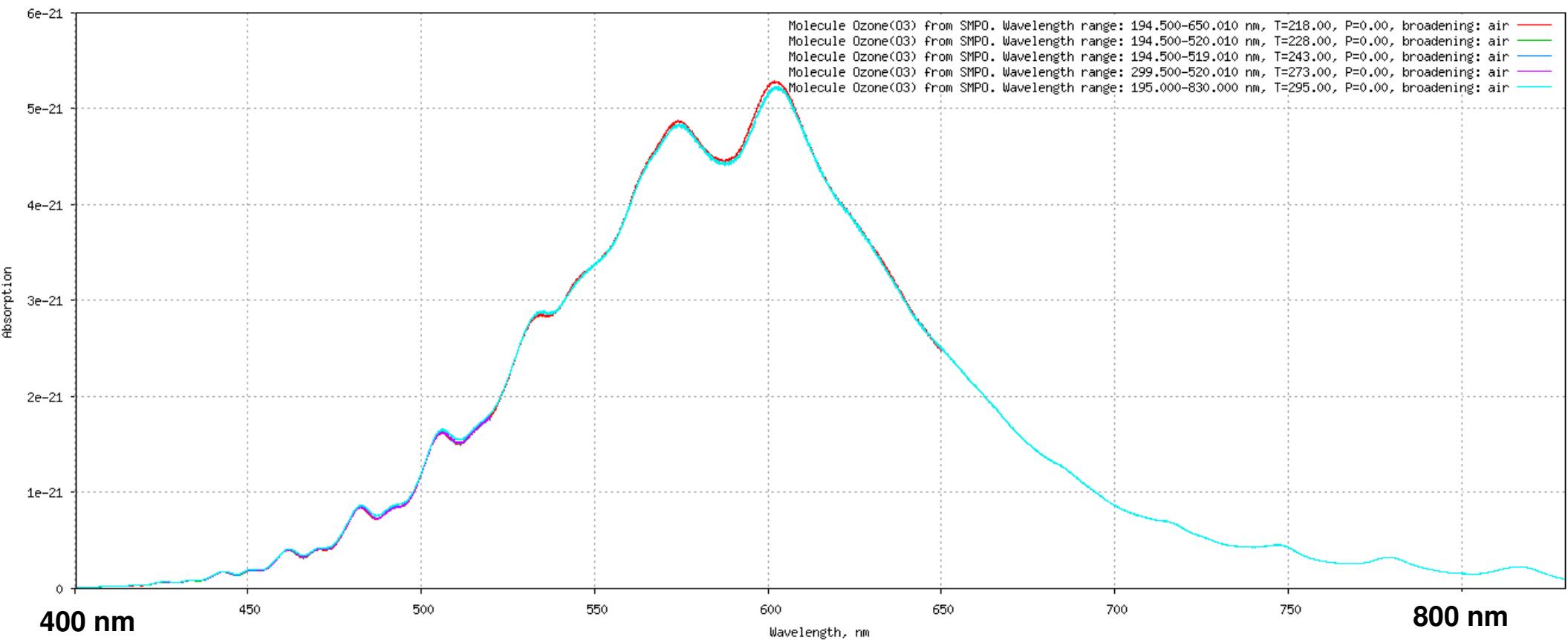
Chosen Cross-Sections

Representation of WN/WL: Wavelength, nm ▼

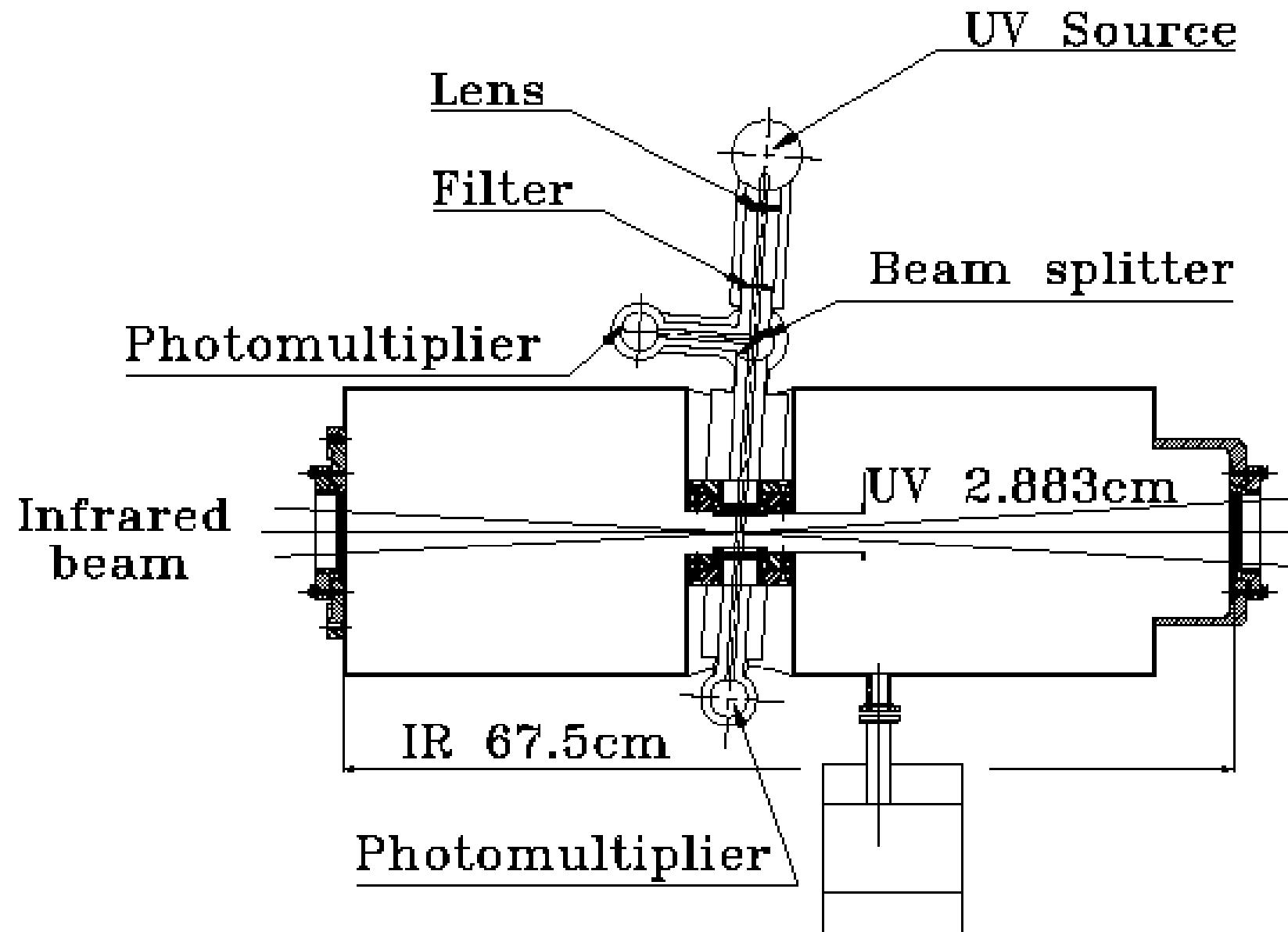


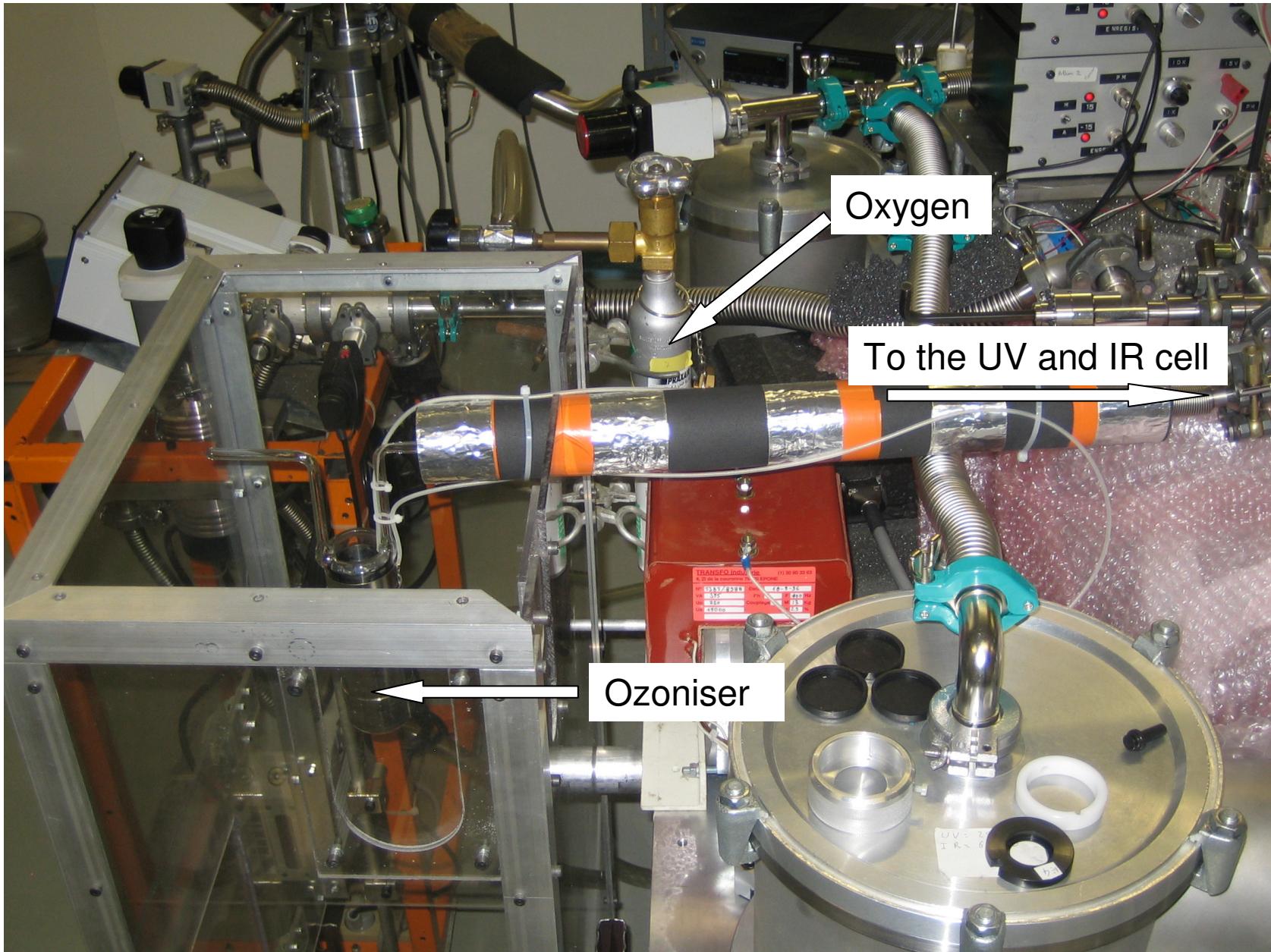
Chosen Cross-Sections

Representation of WN/WL: ▾

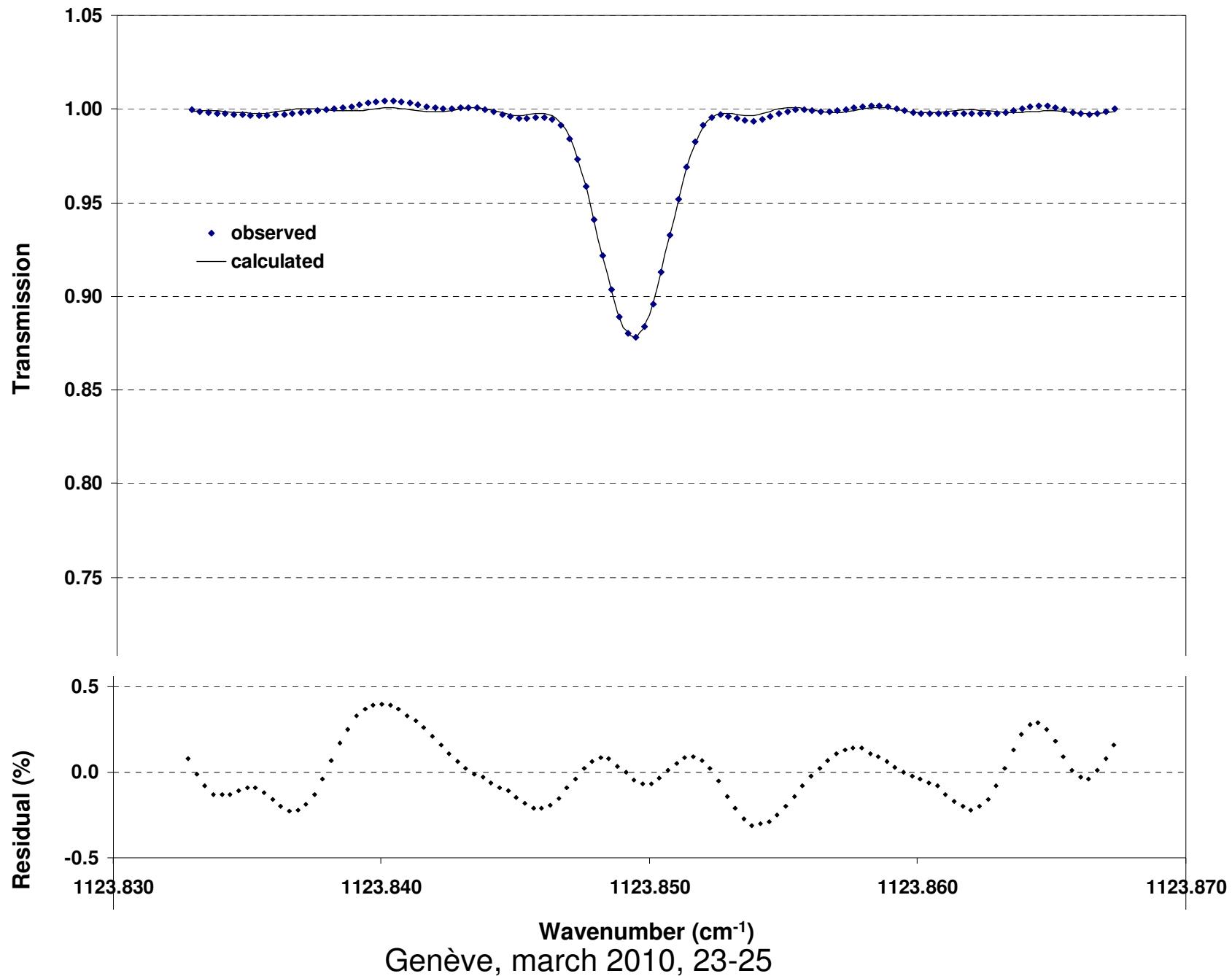


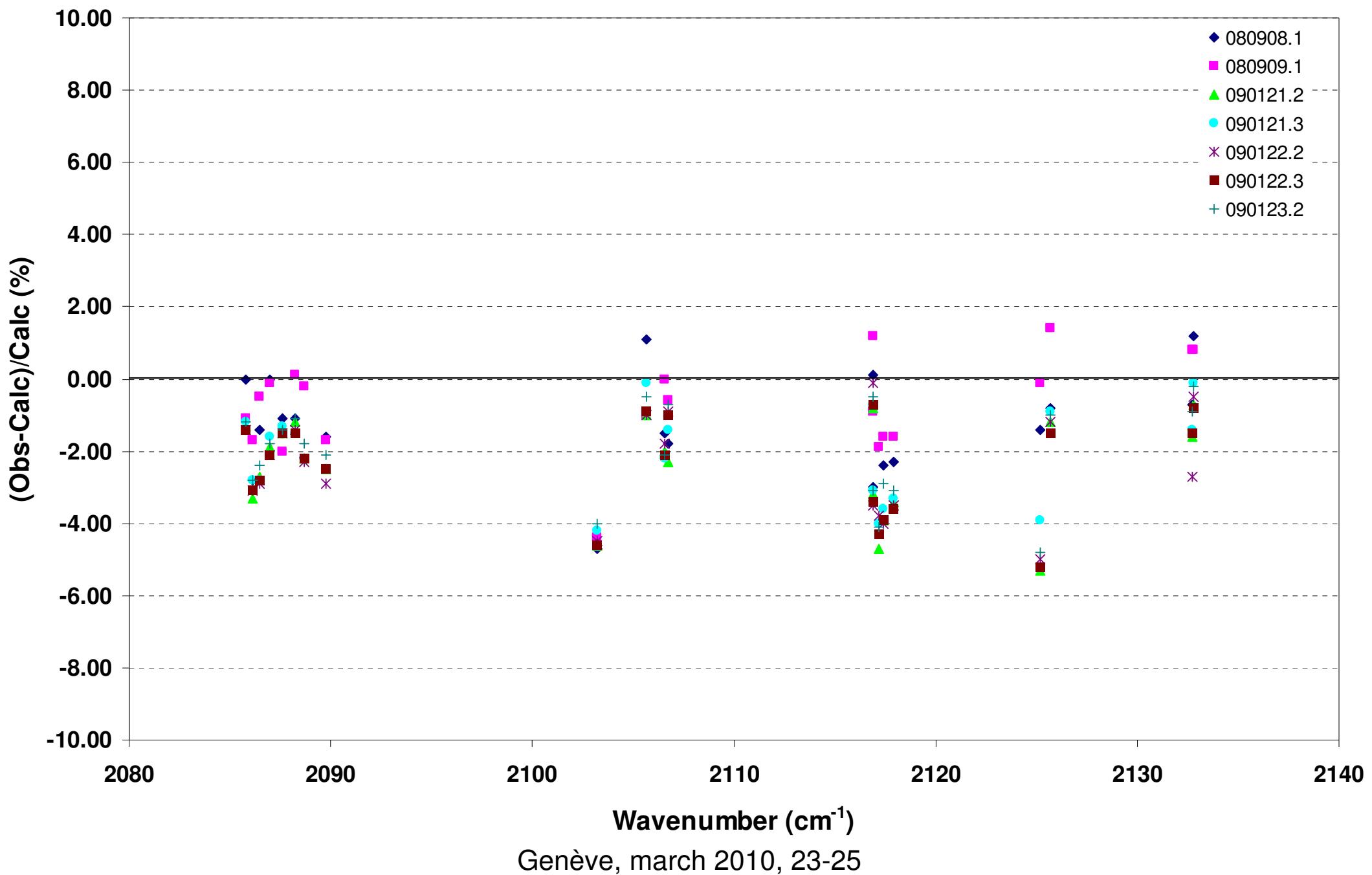
Recent studies (2009) concerning absolute intensities in the IR range.

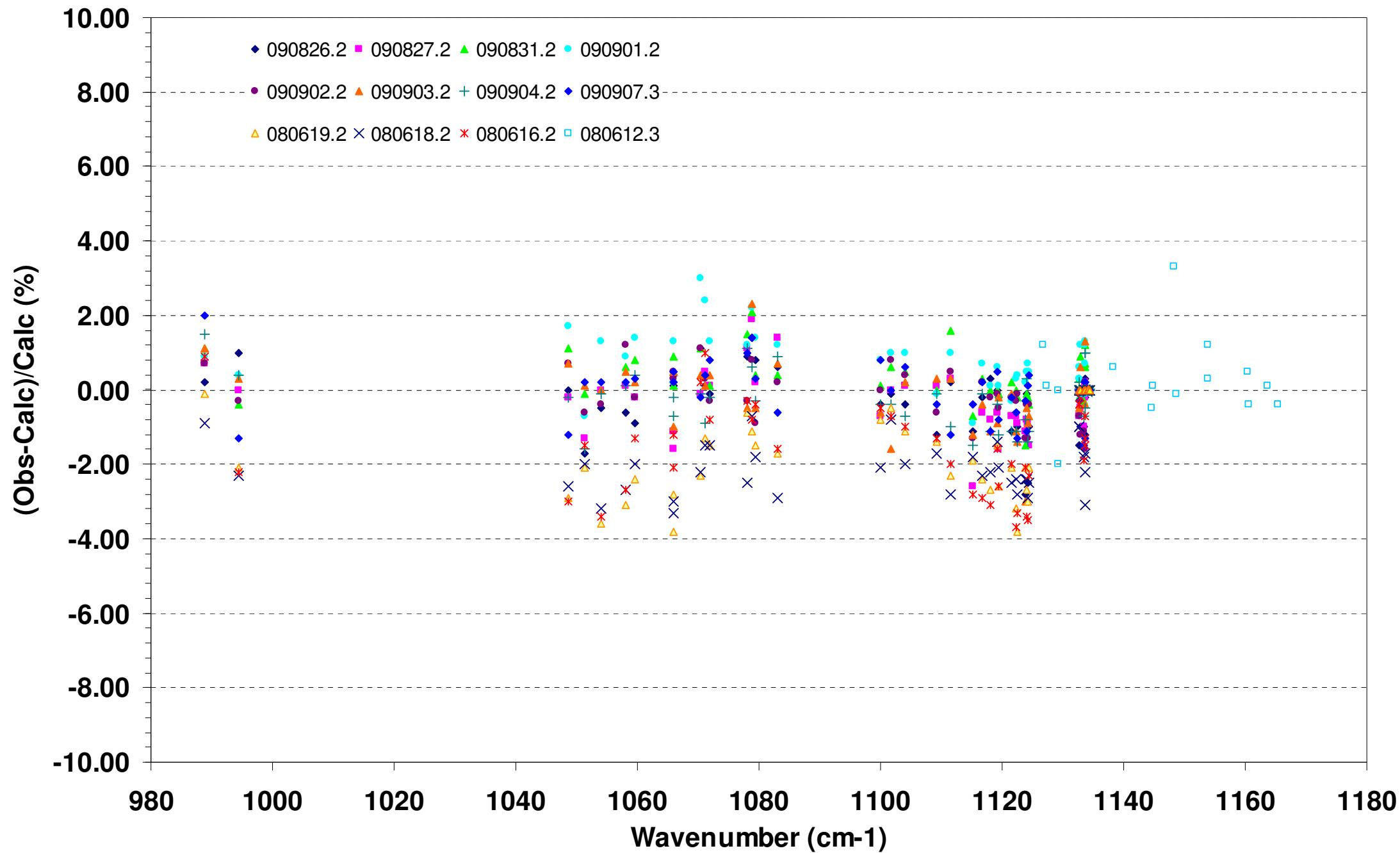




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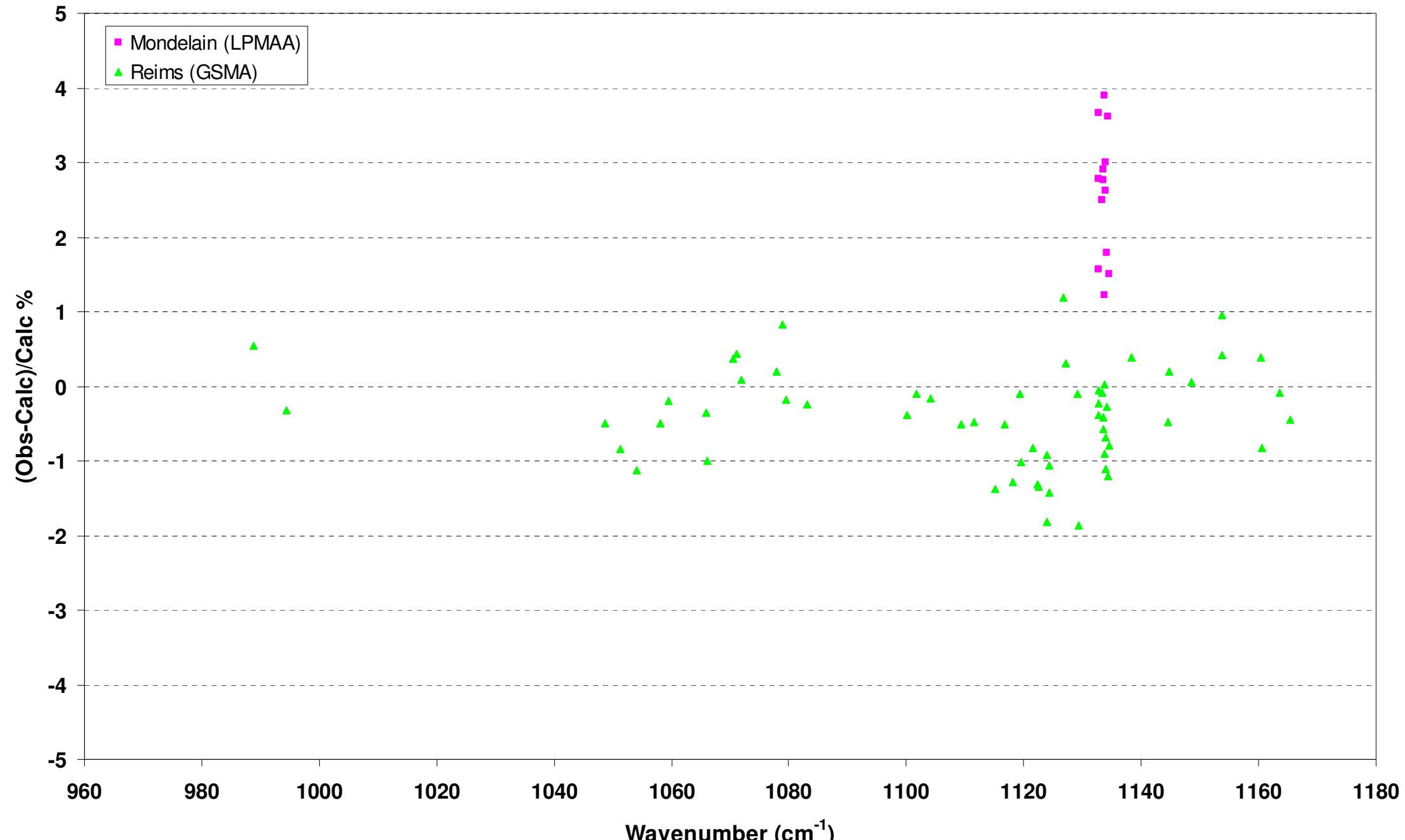






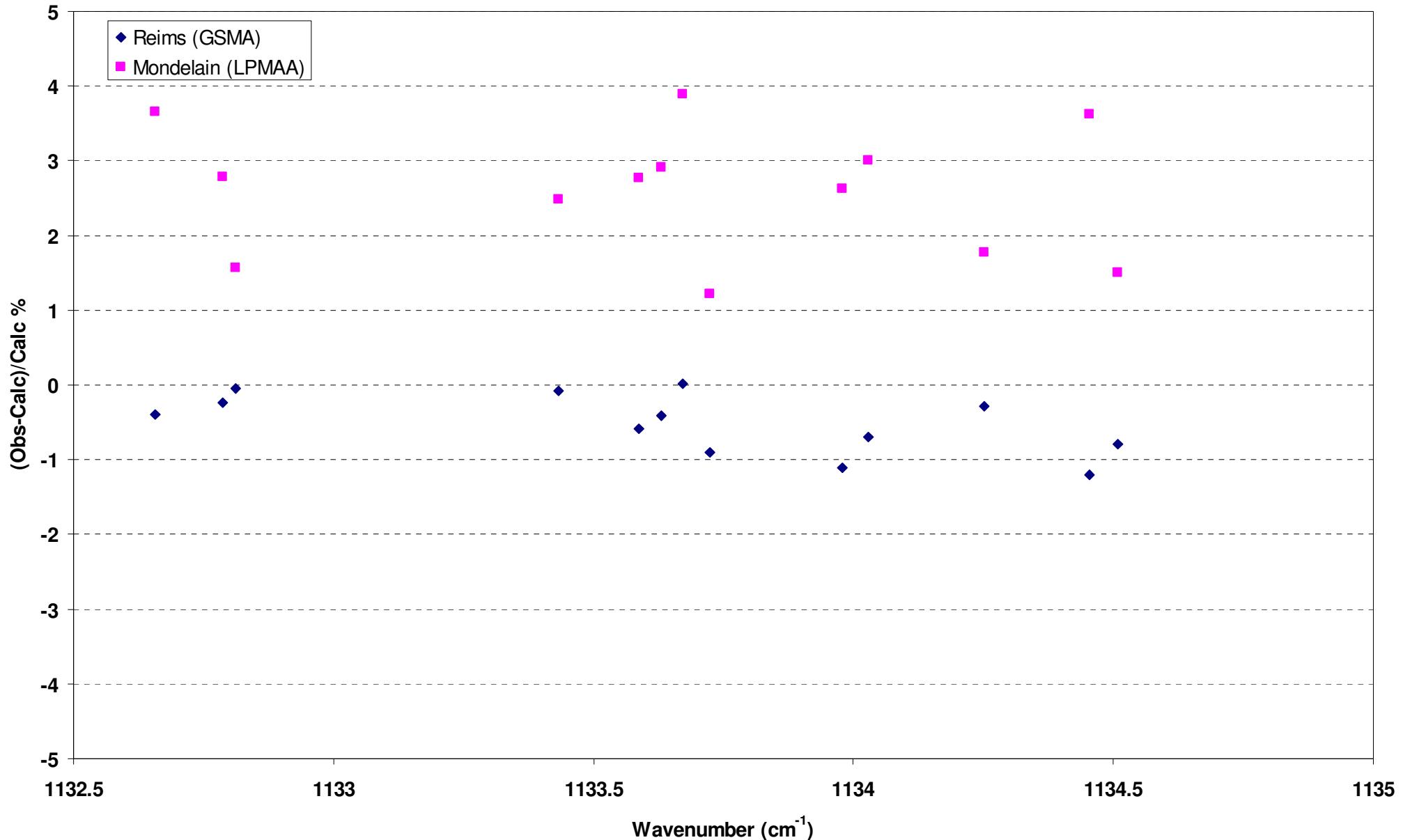
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Comparison (%) with the HITRAN 2004 database



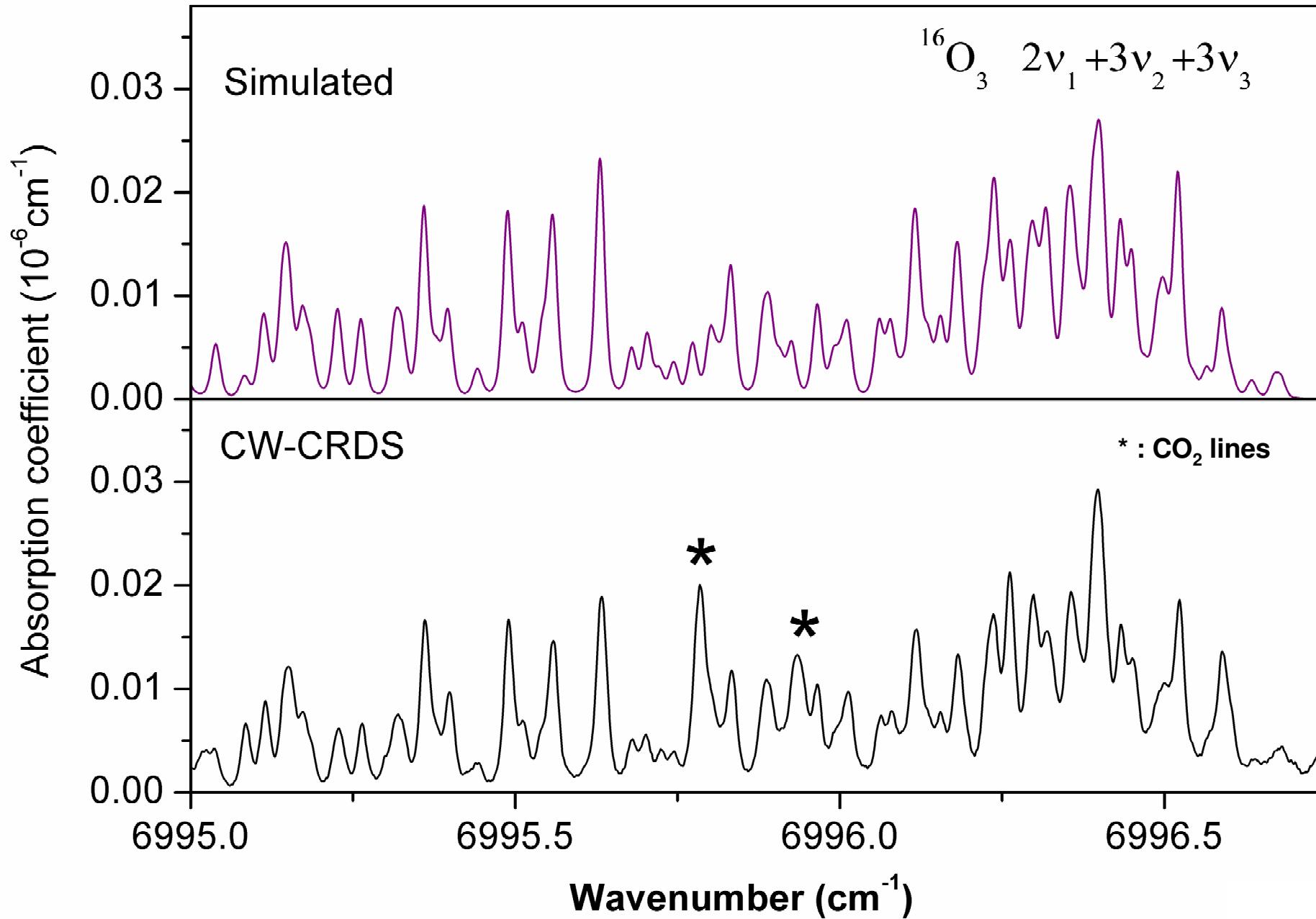
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Zoom in the SWIFT Instrument spectral : Comparison with the HITRAN 2004 database



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Example of agreement between observed (CRDS, Grenoble) and our calculations.



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CRDS spectra recorded in Grenoble and analysed in Reims : 33 bands published

References

- [1] De-Backer-Barily M-R, Barbe A, Tyuterev VL.G, Romanini D, Moeskop B, Campargue A, "Fourier transform and high sensitivity cw-cavity ringdown absorption spectroscopies of ozone in the 6030-6130 cm-1 region. First observation of the 3v1+3v3 and 2v2+ 5v3 bands". J. Mol. Structure (2006), 780-781, 225-233.
- [2] Barbe A., De Backer-Barily M.-R., Tyuterev VI. G., Campargue A., Romanini D., and Kassi S., "CW-Cavity Ring Down Spectroscopy of the ozone molecule in the 5980-6280 cm-1 region". J. Mol. Spectroscopy (2007), 242 (2), 156-175.
- [3] Barbe A., De Backer-Barily M.-R., Tyuterev VI. G., Campargue A., Romanini D., and Kassi S., "CW-Cavity Ring Down Spectroscopy of the ozone molecule in the 6220-6400 cm-1 region.". J. Mol. Spectroscopy (2007), 246(1), 22-38.
- [4] Campargue A., Kassi S., Romanini D., Barbe A., De Backer-Barily M.-R., Tyuterev VI. G., "CW-Cavity Ring Down Spectroscopy of the ozone molecule in the 6625-6830 cm-1 region". J. Mol. Spectroscopy (2006), vol. 240, 1-13.
- [5] Kassi S., Campargue A., De Backer-Barily M.-R. and. Barbe A., "The v1+3v2+3v3 and 4v1+v2+v3 bands of ozone by CW-Cavity Ring Down Spectroscopy between 5900 and 5960 cm-1". J. Mol. Spectroscopy (2007), 44(2), 122-129.
- [6] Campargue A., Barbe A., De Backer-Barily M.-R., Tyuterev VI.G., Kassi S., "The near infrared spectrum of ozone by CW-cavity ring down spectroscopy between 5850 and 7000 cm-1: New observations and exhaustive review". Physical Chemistry Chemical Physics, (2008), 10 (20), 2925-2946.
- [7] Campargue A., Liu A.W., Kassi S., De Backer-Barily M.-R., Barbe A., Starikova E. N., Tashkun S.A., Tyuterev VI.G., "CW-Cavity Ring Down spectroscopy of $^{18}\text{O}_3$ Part 1: Experiment and analysis of the 6200-6400 cm-1 spectral region", J. Mol. Spectroscopy, (2009), 255, 75-87.
- [8] Starikova E.N., De Backer-Barily M.-R., Barbe A., Tyuterev VI.G., Campargue A., Liu A. W., Kassi S., "CRDS Spectroscopy of $^{18}\text{O}_3$. Part 2: Analysis of six interacting bands between 5930 and 6080 cm-1", J. Mol. Spectroscopy, (2009), 255, 144-156.
- [9] Starikova E.N. , Barbe A De Backer-Barily M.-R.,, Tyuterev VI.G., Campargue A., Kassi S., "CW-Cavity Ring Down Spectroscopy of $^{18}\text{O}_3$. Part 3: Analysis of the 6490 - 6900 cm-1 and overview comparison with the $^{16}\text{O}_3$ main isotologue. Part 3", J. Mol. Spectroscopy, (2009), 257, 40-56.
- [10] Barbe A., Tyuterev VI. G., De-Backer M.-R., Bourgeois M.-T., Kassi S., Campargue A., Taskhun S. A., "CW-CRDS infrared spectra of $^{16}\text{O}_3$ in the 5850-7000 cm-1 region : Analyses. Comparisons of band centers and rotational constants with theoretical predictions", ASA prodeedings, (2008), available from <http://asa.univ-reims.fr>
- [23] Starikova E. N., De-Backer M.-R., Tyuterev VI. G., Barbe A., Campargue A., Liu A., Kassi S., Taskhun S. A., "CW-CRDS infrared spectra of $^{18}\text{O}_3$ in the 5900-7000 cm-1 region : Analyses, isotopic effects for band centers, wave functions and rotational constants.", ASA prodeedings, (2008), available from <http://asa.univ-reims.fr>.

Work in progress : analyses of spectra in the 7000-8000 cm⁻¹ spectral range.