

Supplement material

Formaldehyde and Glyoxal Measurement Deploying a Selected Ion Flow Tube Mass Spectrometer (SIFT-MS)

Antonia G. Zogka, Manolis N. Romanias,* and Frederic Thevenet

¹ IMT Nord Europe, Institut Mines-Télécom, Univ. Lille, CERI EE, F-59000 Lille, France

*Corresponding author: emmanouil.romanias@imt-lille-douai.fr

Table S1. Detection limits (in ppb) of glyoxal as a function of relative humidity for standard operation conditions of the SIFT-MS.

I_{37}/I_{19}	RH (%)	m/z 59			m/z 88		
		DL (1 sec)	DL (10 sec)	DL (1 min)	DL (1 sec)	DL (10 sec)	DL (1 min)
0.001	0.008 (Dry)	0.810	0.420	0.280	50.9	28.2	14.4
0.06 ^a	7.1	1.60	0.840	0.550	47.4	26.2	13.4
0.09	10	1.80	0.950	0.620	43.5	24.0	12.3
0.27	30	4.80	2.50	1.60	41.8	23.1	11.8
0.41	50	7.70	4.00	2.60	40.2	22.2	11.3
0.54	70	10.7	5.60	3.70	46.7	25.8	13.2

^a: Determined in THALAMOS Chamber

Table S2. Detection limits (in ppb) of glyoxal as a function of relative humidity for custom operation conditions of the SIFT-MS)

I_{37}/I_{19}	RH (%)	m/z 59			m/z 88		
		DL (1 sec)	DL (10 sec)	DL (1 min)	DL (1 sec)	DL (10 sec)	DL (1 min)
0.005	0.008 (Dry)	0.360	0.190	0.124	6.50	3.60	1.80
0.28	10	1.80	0.930	0.610	6.10	3.40	1.70
0.56	30	5.10	2.70	1.80	5.70	3.10	1.60
0.79	50	8.40	4.40	2.90	4.80	2.70	1.40
1.00	70	14.0	7.30	4.80	4.70	2.60	1.30

Table S3. Data points extracted from the study of Stoner et al. and used to prepare Fig. 5 right panel. Data points were round to two decimal places.

I_{39}/I_{21}	sensitivity	Normalized sensitivity
0.02	0.80	1
0.035	0.79	0.99
0.055	0.68	0.84
0.10	0.52	0.65
0.16	0.40	0.50
0.21	0.29	0.36
0.24	0.26	0.32

Table S4. Data points extracted from the study of Lacko et al. and used to prepare Fig. 6 right panel. Data points were round to two decimal places.

H	Absolute signal of FM ⁺	Normalized signal of FM ⁺	H	Absolute signal of GL ⁺	Normalized signal of GL ⁺
0.04	0.07	1.00	0.04	0.84	1.00
0.05	0.08	1.24	0.06	0.79	0.94

0.07	0.10	1.50	0.06	0.77	0.92
0.09	0.12	1.75	0.07	0.74	0.89
0.10	0.13	1.93	0.09	0.71	0.85
0.12	0.15	2.28	0.10	0.68	0.81
0.14	0.18	2.68	0.12	0.64	0.77
0.15	0.19	2.78	0.14	0.60	0.71
0.20	0.24	3.59	0.15	0.59	0.70
0.22	0.26	3.84	0.21	0.51	0.61
0.25	0.28	4.15	0.22	0.49	0.59
0.30	0.33	4.93	0.25	0.46	0.56
0.36	0.38	5.65	0.30	0.41	0.49
0.36	0.38	5.65	0.36	0.36	0.43
0.42	0.43	6.43	0.42	0.33	0.39
0.51	0.48	7.11	0.51	0.30	0.35
0.57	0.51	7.65	0.57	0.26	0.31
0.69	0.53	7.95	0.69	0.26	0.31
0.78	0.59	8.83	0.78	0.22	0.26
0.87	0.60	8.95	0.88	0.21	0.25
0.99	0.62	9.22	0.99	0.19	0.22

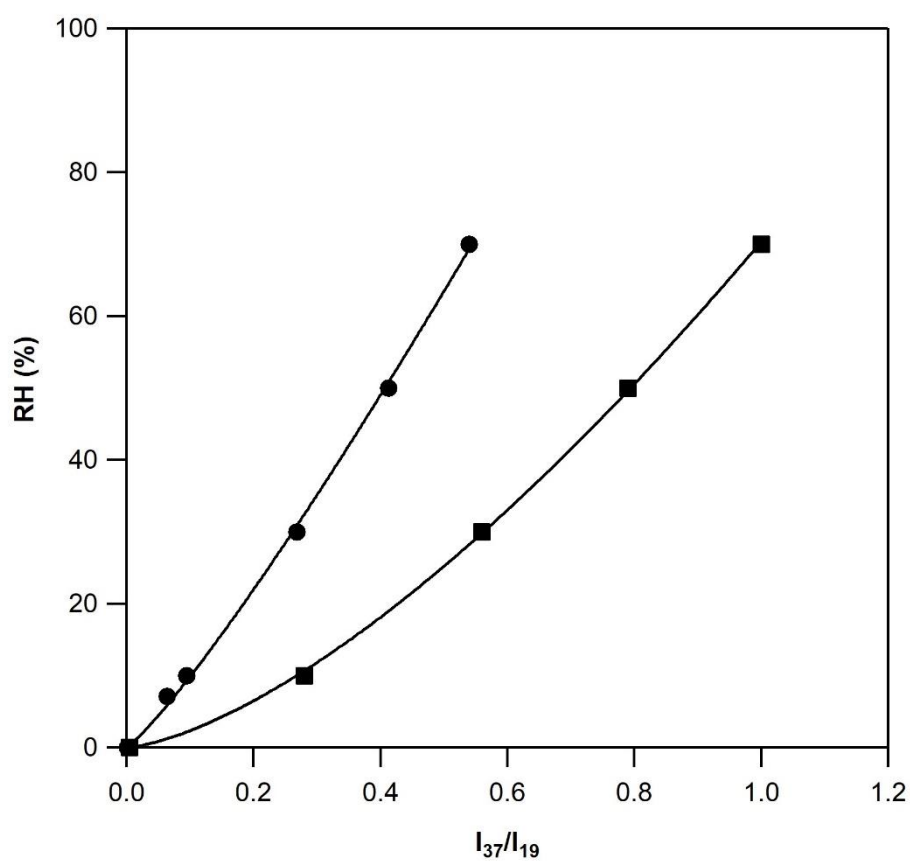


Figure S1. Relationship between the relative ratio of mass peaks 37 ($\text{H}_3\text{O}^+\cdot\text{H}_2\text{O}$ cluster) and 19 (H_3O^+) with the relative humidity (in %) under SC (circles) and CC (squares) operational conditions.

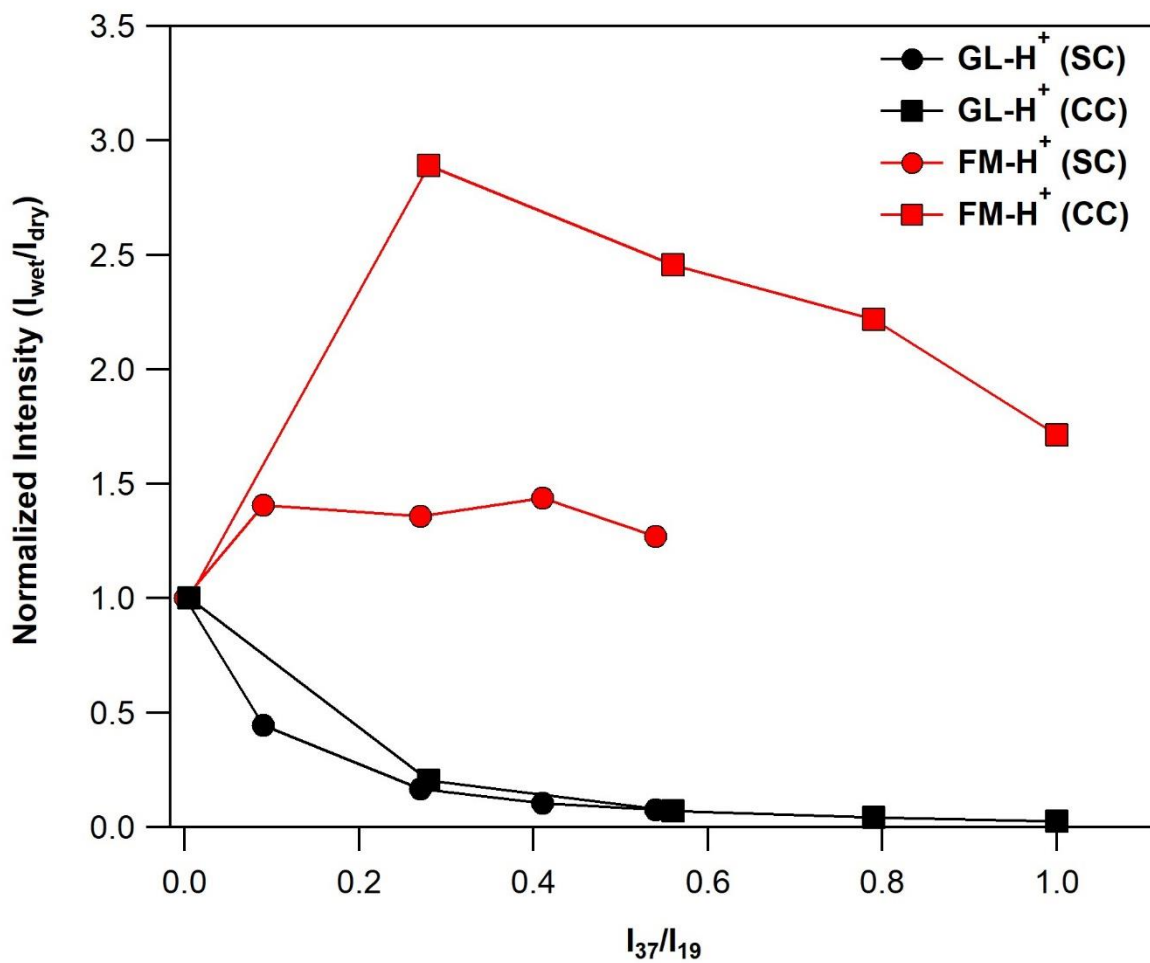


Figure S2. Normalized intensity of signals recorded for GL-H⁺ and FM-H⁺ under SC and OC conditions, versus the I_{37}/I_{19} . This Figure aims to evaluate the impact of water concentrations in the presence of GL-H⁺ and FM-H⁺ inside the SIFT-MS flow tube. Therefore, although the fragmentation of GL-H⁺ to FM-H⁺ is less under CC, the impact of water to FM-H⁺ formation is greater.