



Supplement of

Overview of VOC emissions and chemistry from PTR-TOF-MS measurements during the SusKat-ABC campaign: high acetaldehyde, isoprene and isocyanic acid in wintertime air of the Kathmandu Valley

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Table S1. Most likely identity of VOCs (having average mixing ratios > 0.2 ppb) detected at specific protonated m/z ratios, molecular formula, likely mass assignment, reference of previous mass assignment, sensitivity, limit of detection (LOD), average ambient mixing ratios ($\pm 1 \sigma$)

Protonated m/z or ion	Formula	Most Likely Identity	References of some previously reported studies	Sensitivity (ncps/ppb)	LOD (ppb)	Average (sdev) mixing ratio (ppb)
28.007	HCN	Hydrogen Cyanide	Stockwell et al., 2015; Karl et al., 2003	18.48	0.241	1.56 (0.24)
31.018	HCHO	Formaldehyde	Inomata et al., 2010; Stockwell et al., 2015	18.88	0.103	1.78 (0.50)
33.034	CH ₃ OH	Methanol	Seco et al., 2011; de Gouw et al., 2003	19.16	0.090	7.42 (1.28)
41.039	C ₃ H ₄	Propyne	Akagi et al., 2011; Stockwell et al., 2015	7.167	0.080	7.67 (1.80)
42.034	CH ₃ CN	Acetonitrile*	Seco et al., 2011; de Gouw et al., 2003	20.91	0.043	1.08 (0.38)
43.055	C ₃ H ₆	Propene	Stockwell et al., 2015; Park et al., 2013	7.45	0.048	3.98 (1.21)
44.014	NHCO	Isocyanic acid	Warneke et al., 2011	20.64	0.067	0.90 (0.08)
45.033	C ₂ H ₄ O	Acetaldehyde*	De Gouw et al., 2003; Seco et al., 2011	20.04	0.262	8.81 (4.58)
45.990	NO ₂ ⁺	Nitronium ion from fragmentation of C1-C5 alkyl nitrates	Aoki et al., 2007	20.91	0.094	1.08 (0.24)
46.029	CH ₃ NO	Formamide		20.91	0.093	0.76 (0.16)
47.013	CH ₂ O ₂	Formic acid	Jordan et al., 2009; Williams et al., 2001	21.04	0.041	4.96 (1.02)
47.049	C ₂ H ₆ O	Ethanol	Park et al., 2013; Seco et al., 2011	21.05	0.361	1.59 (0.85)
51.044	C ₄ H ₂	1,3-Butadiyne ^{\$}	Yokelson et al., 2013	8.56	0.013	0.67 (0.14)
56.060	C ₃ H ₅ N	Propanenitrile ^{\$}	Yokelson et al., 2013	22.27	0.022	0.21 (0.05)
57.034	C ₃ H ₄ O	Acrolein* + Methylketene	Stockwell et al., 2015; Jordan et al., 2009	22.26	0.034	0.80 (0.26)
59.049	C ₃ H ₆ O	Acetone* + Propanal	de Gouw et al., 2003; Seco et al., 2011	23.47	0.074	4.21 (0.65)
60.051	C ₂ H ₅ NO	Acetamide		22.80	0.069	0.39 (0.05)
61.027	C ₂ H ₄ O ₂	Acetic acid (sum of parent ion contributions at m/z 61.027 and fragment ion contributions at m/z 43.018)	de Gouw et al., 2007; Stockwell et al., 2015; Seco et al., 2011	22.94	0.440	7.46 (2.93)
62.026	CH ₃ NO ₂	Nitromethane [@]	Inomata et al., 2014; Akagi et al., 2013	23.07	0.020	0.24 (0.08)
63.026	C ₂ H ₆ S	Dimethyl Sulfide	Akagi et al., 2011; Park et al., 2013	23.21	0.049	0.26 (0.03)
67.054	C ₅ H ₆	1,3-Cyclopentadiene	Stockwell et al., 2015	10.78	0.008	0.23 (0.06)
69.033	C ₄ H ₄ O	Furan	Stockwell et al., 2015; Jordan et al., 2009	24.02	0.009	0.46 (0.17)
69.070	C ₅ H ₈	Isoprene*	Stockwell et al., 2015; de Gouw et al., 2003; Seco et al., 2011	10.02	0.013	1.11 (0.24)
71.049	C ₄ H ₆ O	Methyl vinyl ketone; Methacrolein; Crotonaldehyde*	Seco et al., 2011; Stockwell et al., 2015; de Gouw et al., 2007	27.17	0.017	0.35 (0.10)

73.027	C ₃ H ₄ O ₂	Methylglyoxal	Stockwell et al., 2015; Muller et al., 2012	24.56	0.021	0.31 (0.10)
73.063	C ₄ H ₈ O	Methyl ethyl ketone*	de Gouw et al., 2003; Stockwell et al., 2015; Park et al., 2013	21.91	0.036	0.69 (0.12)
75.042	C ₃ H ₆ O ₂	Hydroxyacetone	Christian et al., 2003; Heigenmoser et al., 2013; Stockwell et al., 2015	24.83	0.066	0.63 (0.18)
79.054	C ₆ H ₆	Benzene*	Jordan et al., 2009; de Gouw et al., 2003	13.43	0.013	2.71 (1.17)
83.085	C ₆ H ₁₀	Assorted Hydrocarbons	Stockwell et al., 2015	13.01	0.008	0.45 (0.09)
87.042	C ₄ H ₆ O ₂	2,3-Butanedione	Stockwell et al., 2015; Karl et al., 2007	26.45	0.028	0.35 (0.08)
93.070	C ₇ H ₈	Toluene*	Seco et al., 2011; Jordan et al., 2009	15.78	0.006	1.53 (0.38)
97.031	C ₅ H ₄ O ₂	2-Furaldehyde (furfural)	Ruuskanen et al., 2011; Liu et al., 2012; Li et al., 2013	27.80	0.010	0.26 (0.07)
97.102	C ₇ H ₁₂	Assorted Hydrocarbons	Stockwell et al., 2015	14.96	0.006	0.23 (0.05)
105.070	C ₈ H ₈	Styrene	Jordan et al., 2009; Stockwell et al., 2015	16.07	0.004	0.21 (0.08)
107.086	C ₈ H ₁₀	Xylenes*	Jordan et al., 2009; Stockwell et al., 2015	15.36	0.004	0.97 (0.27)
121.101	C ₉ H ₁₂	Trimethylbenzenes	Muller et al., 2012; Jordan et al., 2009	18.30	0.004	0.38 (0.10)
129.070	C ₁₀ H ₈	Naphthalene	Jordan et al., 2009; Stockwell et al., 2015	19.40	0.009	0.33 (0.09)

* VOC sensitivities determined using VOC gas standards in calibration experiments

§ Observed mass accuracy for 1,3-Butadiyne and Propanenitrile were 21 mDa and 10 mDa, respectively

@ Corrected for the ¹³C isotopologues of acetic acid

Table S2. Top fifteen contributing VOCs to the total reactive carbon during SusKat-ABC campaign

VOCs	Campaign average reactive carbon (ppbC)	Percentage contribution to total reactive carbon
Propyne	23.01	13.1%
Acetaldehyde	17.62	10.0%
Benzene	16.26	9.2%
Acetic acid	14.92	8.5%
Acetone	12.63	7.2%
Propene	11.94	6.8%
Toluene	10.71	6.1%
Xylenes	7.76	4.4%
Methanol	7.42	4.2%
Isoprene	5.55	3.2%
Formic acid	4.96	2.8%
Trimethylbenzenes	3.42	1.9%
Naphthalene	3.30	1.9%
Ethanol	3.18	1.8%
MEK	2.76	1.6%

Table S3. Top ten contributing VOCs to the total OH reactivity during SusKat-ABC campaign

VOCs	Campaign average speciated OH reactivity (s^{-1})	Percentage contribution to total average OH reactivity
Acetaldehyde	2.95	24.0%
Isoprene	2.47	20.2%
Propene	2.29	18.7%
Propyne	0.49	4.0%
1,3-Cyclopentadiene	0.43	3.5%
Furan	0.40	3.2%
Acrolein	0.34	2.8%
Formaldehyde	0.33	2.7%
Xylenes	0.29	2.4%
Trimethylbenzenes	0.25	2.0%

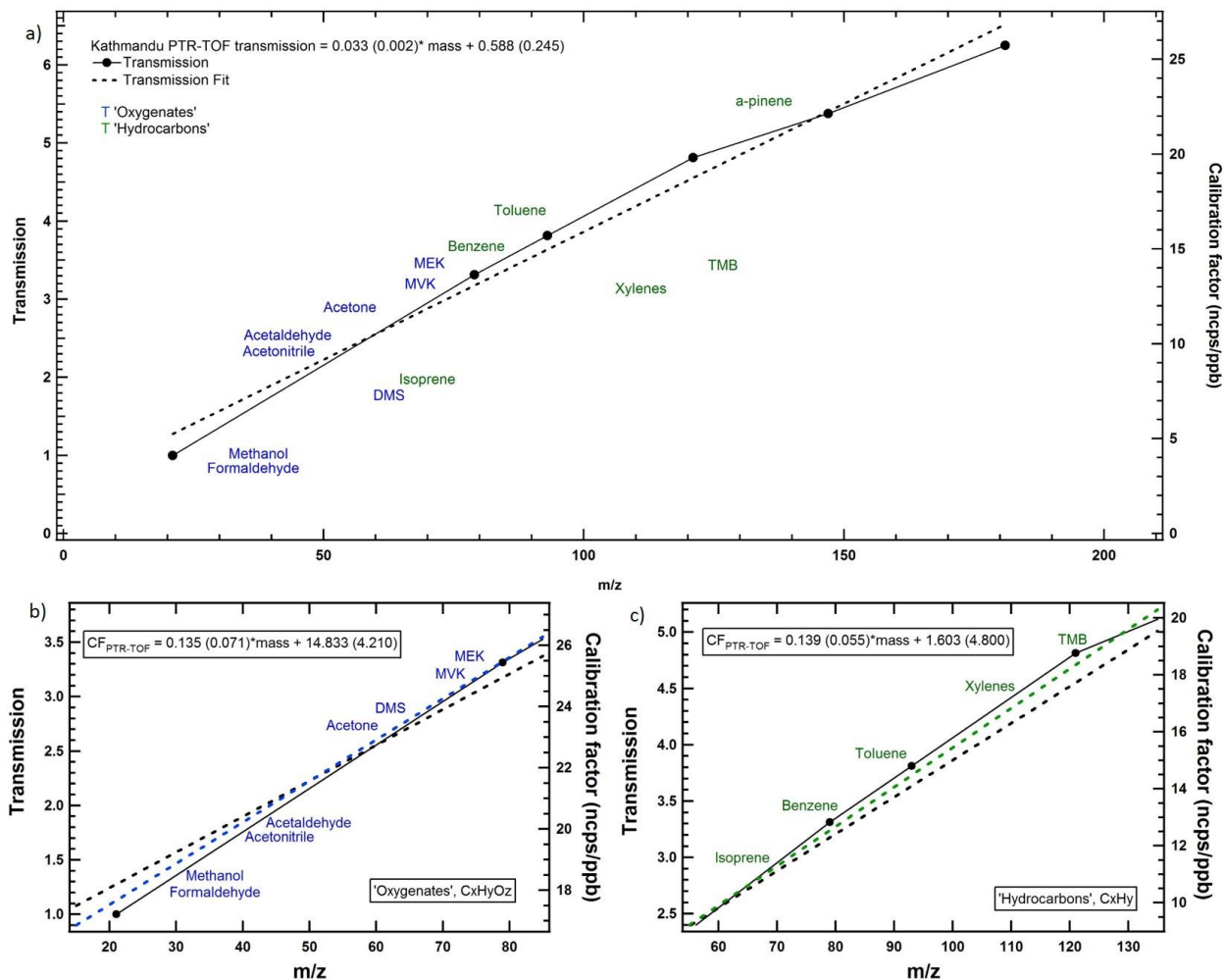


Figure S1. a) Normalized response of calibration factors (“CF,” ncps/ppb) vs mass (calibrated species labeled by name) overlaid with linearly fitted mass-dependent transmission curve (black markers and dotted line). Approximate calibration factors for all observed masses where explicit calibrations were not available were determined using separate linear approximations namely b) oxygenated (blue) and c) hydrocarbon (green) species

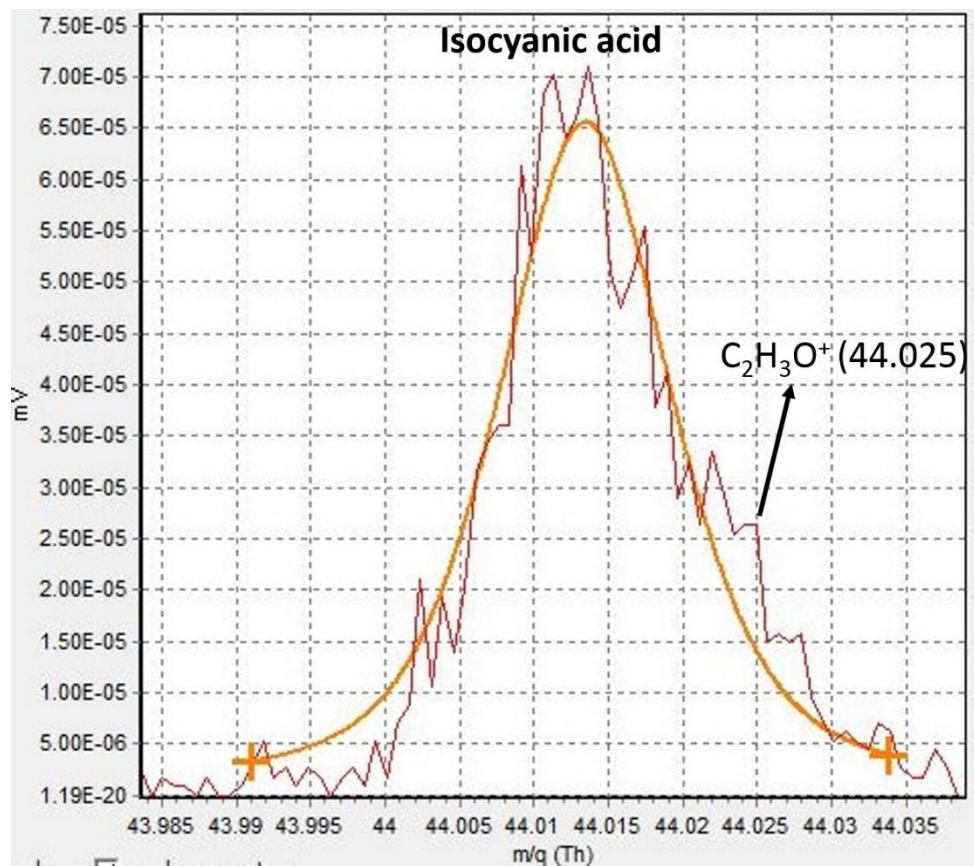


Figure S2. Illustrative mass spectra (30 second average) of isocyanic acid obtained at 09:24 LT on 13 January 2013