Supplementary Information of

Source apportionment of VOCs in the Kathmandu Valley during the SusKat-ABC international field campaign using positive matrix factorization

Chinmoy Sarkar et al.

Correspondence to: Vinayak Sinha (vsinha@iisermohali.ac.in)

Table S1. Statistical parameters for the measured species used as PMF input

VOC Species	Category	S/N	Min	25th	Median	75th	Max	N[1]	Nbdl[2]
Hydrogen Cyanide	Weak	3.10	0.29	0.62	0.90	1.79	12.43	969	0
Formaldehyde	Strong	3.93	0.60	1.43	1.80	2.34	5.39	969	0
Methanol	Strong	4.00	3.31	6.69	8.51	10.32	21.79	969	0
Propyne	Strong	4.00	3.37	8.27	10.95	13.73	37.58	969	0
Acetonitrile	Strong	3.95	0.50	1.00	1.47	2.04	5.60	969	0
Propene	Strong	4.00	1.37	3.99	6.03	7.78	18.34	969	0
Isocyanic acid	Strong	3.91	0.94	1.22	1.36	1.61	2.39	969	0
Acetaldehyde	Strong	3.97	3.46	8.83	11.52	15.46	61.96	969	0
Nitronium ion	Strong	3.86	0.81	1.37	1.65	1.97	5.42	969	0
Formamide	Strong	3.71	0.55	0.93	1.20	1.51	2.67	969	0
Formic acid	Strong	4.00	2.42	6.85	7.92	9.61	17.74	969	0
Ethanol	Strong	2.78	bdl	1.16	2.21	3.49	18.63	969	51
1,3-Butadiyne	Strong	3.99	0.13	0.89	1.20	1.51	3.43	969	0
Propanenitrile	Strong	3.77	0.09	0.32	0.40	0.50	0.98	969	0
Acrolein + Methylketene	Strong	3.95	0.40	1.14	1.51	2.06	4.09	969	0
Acetone + Propanal	Strong	3.99	3.55	6.99	8.71	10.38	23.48	969	0
Acetamide	Strong	3.53	0.51	0.69	0.82	0.97	1.53	969	0
Acetic acid	Strong	3.88	4.69	9.31	11.99	15.56	35.04	969	0
Nitromethane	Strong	3.83	0.16	0.37	0.50	0.69	1.85	969	0
Dimethyl Sulfide	Strong	3.46	0.19	0.50	0.56	0.63	2.35	969	0
1,3-Cyclopentadiene	Strong	3.97	0.14	0.36	0.50	0.70	4.42	969	0
Furan	Strong	3.98	0.19	0.66	1.14	1.52	3.38	969	0
Isoprene	Strong	4.00	0.28	1.76	2.39	3.43	11.25	969	0
Methyl vinyl Ketone + Methacrolein	Strong	3.94	0.18	0.61	0.81	1.11	3.08	969	0
Methylglyoxal	Strong	3.89	0.18	0.56	0.76	1.01	2.27	969	0
Methyl ethyl ketone	Strong	3.93	0.37	1.30	1.73	2.18	4.93	969	0
Hydroxyacetone	Strong	3.74	0.27	1.17	1.54	2.15	4.47	969	0
Benzene	Strong	4.00	0.95	3.98	6.79	10.11	37.35	969	0
Assorted Hydrocarbons	Strong	3.99	0.10	0.78	1.10	1.66	6.88	969	0
2,3-Butanedione	Strong	3.86	0.16	0.80	1.04	1.36	3.35	969	0
Toluene	Strong	4.00	0.51	3.09	4.51	6.54	30.71	969	0
2-Furaldehyde (furfural)	Strong	3.96	0.18	0.61	0.83	1.15	2.23	969	0
Assorted Hydrocarbons	Strong	3.97	0.08	0.48	0.70	1.03	3.03	969	0
Styrene	Strong	3.98	0.09	0.41	0.67	1.06	3.32	969	0
Xylenes	Strong	4.00	0.31	2.12	3.19	4.79	24.73	969	0
Trimethylbenzenes	Strong	3.99	0.17	0.94	1.39	2.14	10.44	969	0
Naphthalene	Strong	3.97	0.28	0.92	1.44	2.00	6.94	969	0

1. Number of valid hourly VOC samples; 2. Number of samples below detection limit

Table S2: Percentage contribution of PMF derived factors obtained from constrained runs with 5-, 6-, 7-, 8- and 9-Factors

PMF solutions	RB + WD	BK	BK2	MCS	TR	MI	UI	BG	MD	SE
5-Factor	19.2	23.7	-	23.9	-	-	-	13.4	19.8	-
6-Factor	15.6	18.4	-	-	20.1	21.5	-	11.7	12.7	-
7-Factor	12.3	14.7	-	-	17	19.5	-	8.2	13.8	14.7
8-Factor	10.9	10.4	-	-	16.8	14	17.9	10	9.2	10.8
9-Factor	10.5	12.2	7.7	-	15.6	9.5	15.5	7	9.8	12.2

RB + WD = Residential biofuel use and waste disposal; BK = Biomass co-fired brick kilns; BK2 = Second brick kiln factor; MCS = Mixed combustion sources; TR = Traffic; MI = Mixed industrial; UI = Unresolved industrial; BG = Biogenic; MD = Mixed daytime; SE = Solvent evaporation

Table S3. Correlation coefficient (r) between the PMF resolved factors and other independent meteorological parameters (solar radiation, ambient temperature, change in solar radiation, change in ambient temperature, wind speed, wind direction, relative humidity and absolute humidity) for a) daytime period (06:00 – 17:00 LT) and b) nighttime period (17:00 – 06:00 LT)

a)	**SE**	**MD**	**BG**	**RB+WD**	**BK**	**MI**	**UI**	**TR**	**SR**	**AT**	**ΔSR**	**ΔAT**	**WS**	**RH**	**AH**
SE	1.00	-													
MD	-0.22	1.00	-												
BG	-0.01	-0.01	1.00	-											
RB+WD	-0.01	-0.35	0.10	1.00	-										
BK	0.23	-0.55	-0.31	0.18	1.00	-									
MI	0.07	-0.68	-0.28	**0.51**	**0.54**	1.00	-								
UI	**0.55**	-0.49	-0.17	-0.24	0.37	0.06	1.00	-							
TR	0.05	-0.33	0.27	0.21	-0.19	0.17	-0.02	1.00	-						
SR	0.23	**0.58**	**0.57**	-0.35	-0.51	-0.65	-0.16	-0.10	1.00	-					
AT	-0.11	**0.74**	0.31	-0.41	-0.74	-0.79	-0.23	-0.07	**0.71**	1.00	-				
ΔSR	**0.62**	-0.47	0.15	0.14	0.38	0.29	0.46	-0.08	0.11	-0.46	1.00	-			
ΔAT	**0.64**	-0.06	0.33	-0.06	0.03	-0.07	0.28	-0.04	**0.50**	0.02	**0.67**	1.00	-		
WS	-0.35	**0.57**	-0.05	-0.23	-0.50	-0.48	-0.39	0.00	0.13	**0.63**	-0.71	-0.45	1.00	-	
RH	0.10	-0.82	-0.31	0.42	**0.65**	**0.74**	0.37	0.10	-0.75	-0.91	0.45	-0.05	-0.62	1.00	-
AH	0.21	-0.27	0.08	0.02	-0.17	-0.11	0.49	0.11	-0.02	0.13	0.20	0.16	-0.11	0.25	1.00

b)	**SE**	**MD**	**BG**	**RB+WD**	**BK**	**MI**	**UI**	**TR**	**SR**	**AT**	**ΔSR**	**ΔAT**	**WS**	**RH**	**AH**
SE	1.00	-													
MD	0.14	1.00	-												
BG	-0.25	-0.18	1.00	-											
RB+WD	0.34	-0.10	**0.58**	1.00	-										
BK	-0.20	-0.38	-0.07	-0.33	1.00	-									
MI	-0.25	-0.60	0.08	0.04	0.32	1.00	-								
UI	0.29	-0.29	-0.58	-0.47	0.38	-0.03	1.00	-							
TR	0.17	-0.36	0.36	0.46	-0.24	0.14	-0.24	1.00	-						
SR	0.10	0.11	0.05	-0.04	-0.17	-0.28	-0.01	0.32	1.00	-					
AT	0.47	0.36	0.15	0.48	-0.59	-0.58	-0.18	0.37	0.44	1.00	-				
ΔSR	-0.17	-0.22	-0.03	-0.02	0.25	0.38	0.04	-0.34	-0.83	-0.59	1.00	-			
ΔAT	-0.12	0.00	-0.06	-0.21	0.09	0.08	0.08	-0.11	-0.09	-0.14	0.21	1.00	-		
WS	0.30	0.43	-0.02	0.07	-0.35	-0.53	-0.09	0.15	**0.55**	**0.70**	-0.78	-0.15	1.00	-	
RH	-0.59	-0.49	-0.07	-0.44	0.40	0.48	0.25	-0.26	-0.44	-0.80	**0.59**	0.16	-0.66	1.00	-
AH	0.04	-0.06	0.18	0.26	-0.43	-0.33	0.03	0.21	0.05	0.55	-0.08	-0.05	0.21	0.04	1.00

SE = Solvent evaporation; MD = Mixed daytime; BG = Biogenic; RB+WD = Residential biofuel use and waste disposal; BK = Biomass co-fired brick kilns; MI = Mixed industrial emissions; UI = Unresolved industrial emissions; TR = Traffic; SR = Solar radiation; AT = Ambient temperature; ΔSR = Rate of change in solar radiation (dSR/dt); ΔAT = Rate of change in ambient temperature (dT/dt); WS = Wind speed; RH = Relative humidity; AH = Absolute humidity

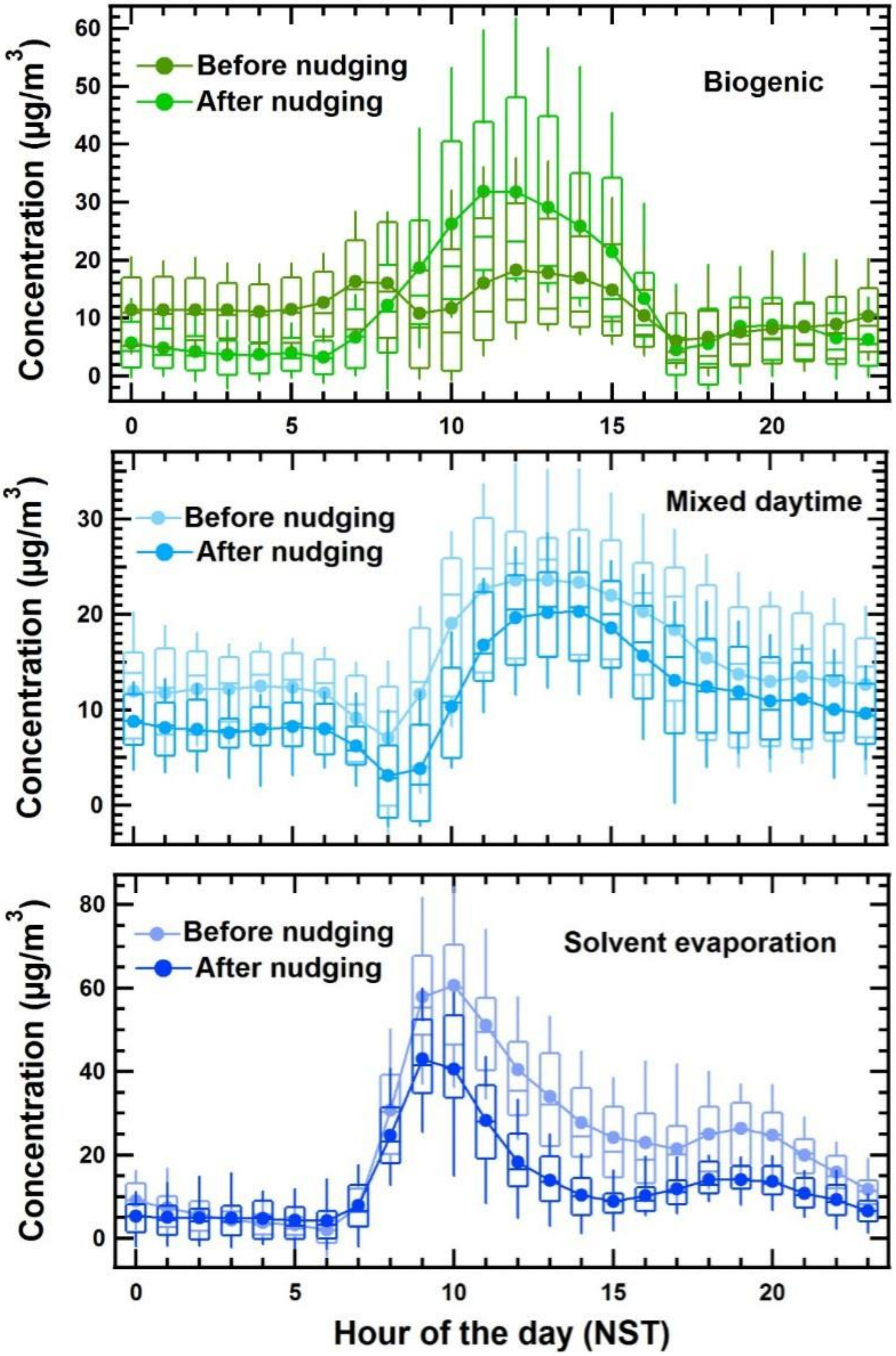

Figure S1. Comparison of the diel profiles of biogenic emissions, mixed daytime and solvent evaporation factors before and after nudging

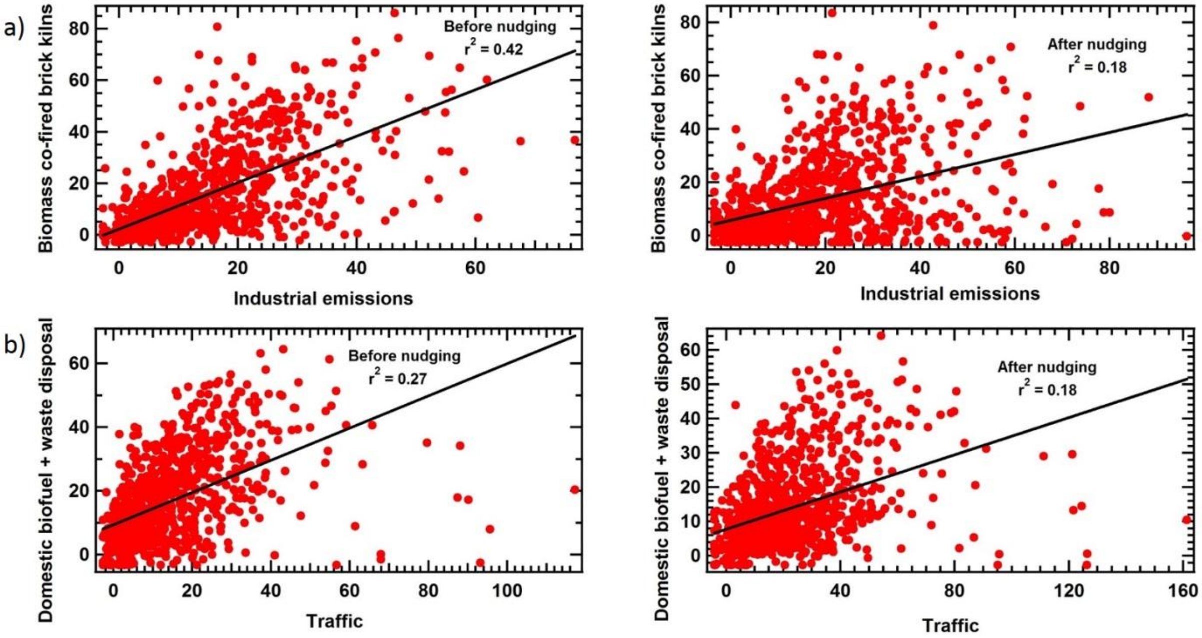

Figure S2. Comparison of the G-space plots between a) biomass co-fired brick kilns and mixed industrial emissions and b) residential biofuel use and waste disposal and traffic before and after nudging

Figure S3. Collection of garbage burning grab samples in the Kathmandu Valley (on left) and the instrumental setup for the analysis (on right)

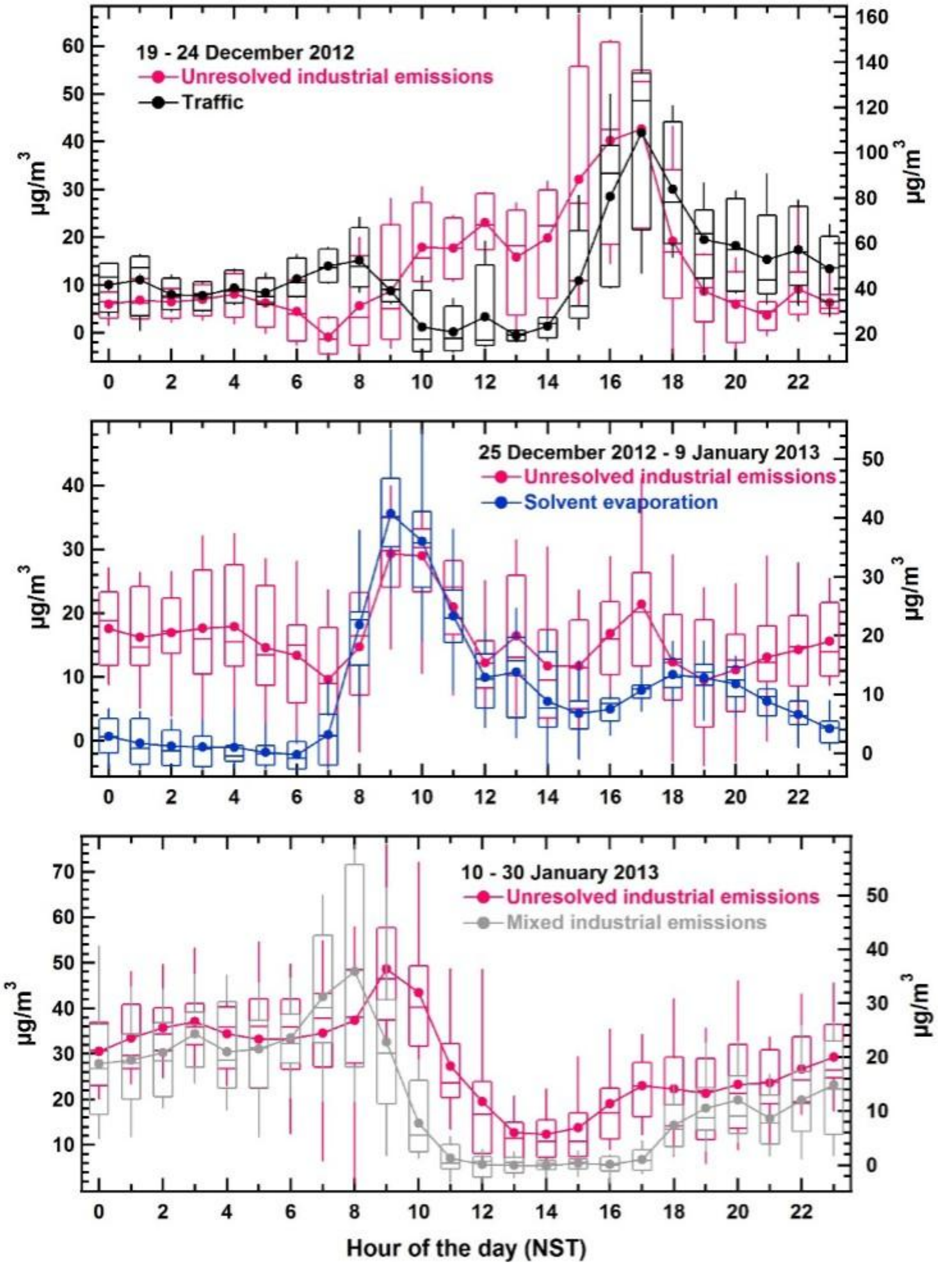

Figure S4. Comparison of the diel profile of the unresolved industrial emissions with that of traffic (19 – 24 December 2012), solvent evaporation (25 December 2012 – 9 January 2013) and mixed industrial emissions (10 – 30 January 2013)

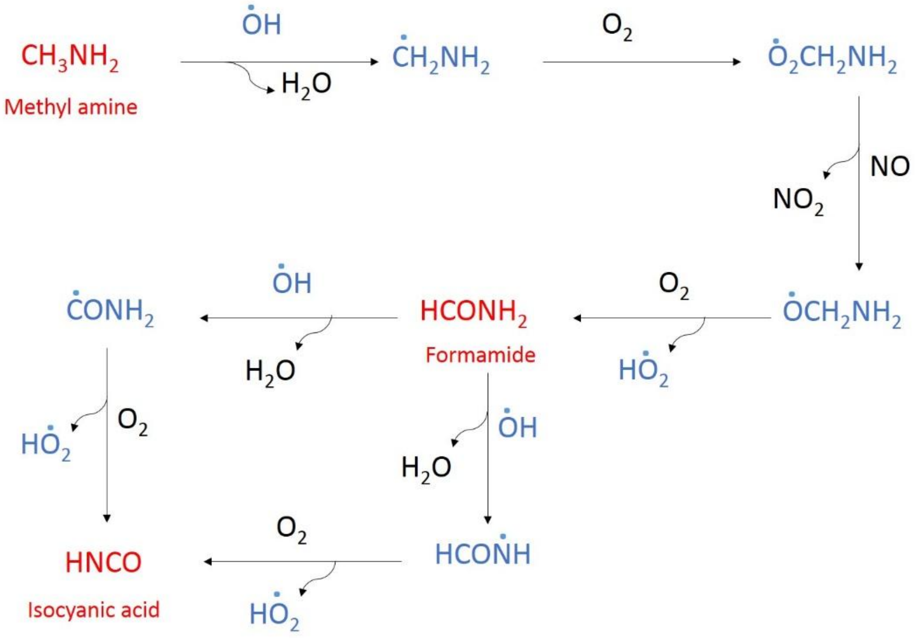

Figure S5. Reaction schematic for the formation of formamide and isocyanic acid (blue colored species represents radicals)

Figure S5 represents the reaction schematic of the proposed mechanism for the formation of formamide, acetamide and isocyanic acid based on the previous laboratory experiments which shows that photooxidation of alkyl amines leads to the formation of formamide and acetamide which undergoes further photooxidation to form isocyanic acid which can have severe health impact at concentration thresholds above 1 ppb (Roberts et al., 2011;Roberts et al., 2014). This study provides the first ambient evidence of the photochemical source of isocyanic acid by quantification of both the amides (the precursor) and isocyanic acid (the product) collectively and the source apportionment of these compounds in the Kathmandu Valley.

References

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