Seasonal Variability and Source Diagnostics of Ambient PAHs in Agra, India Using CBPF and Health Risk Evaluation

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Supplementary Material

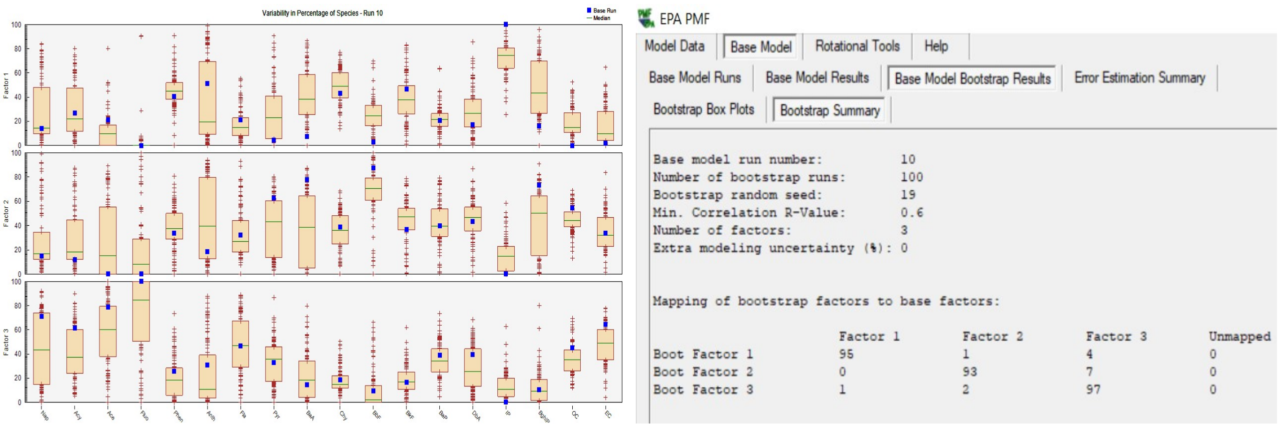

Figure S1. Bootstrap uncertainty analysis of PMF factor profiles.

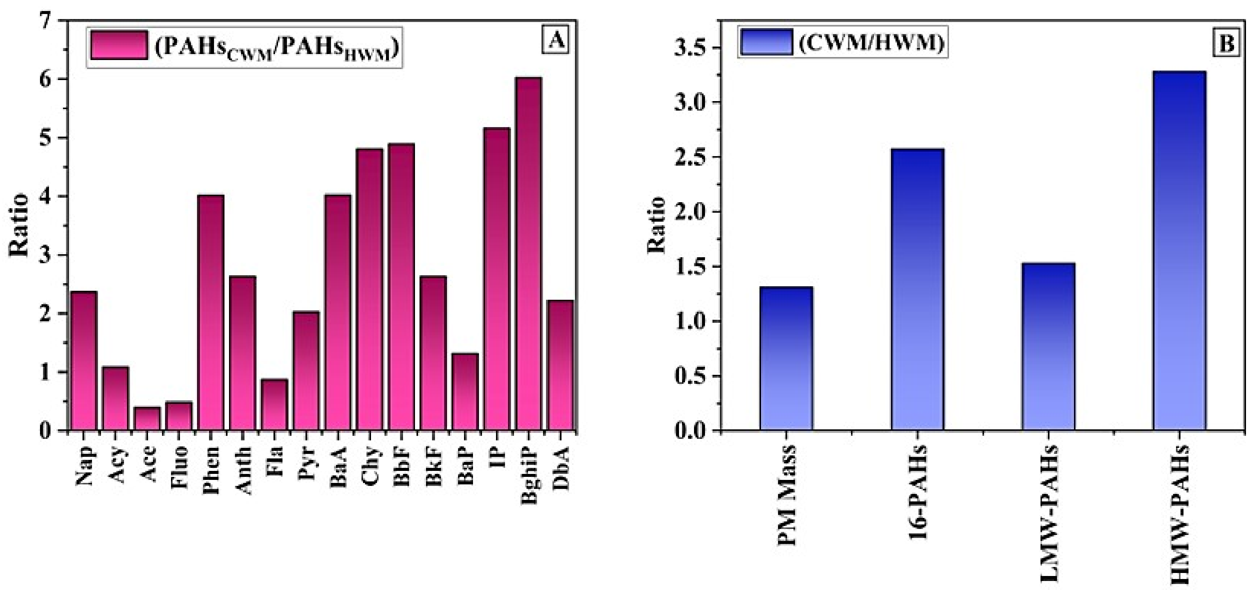

Figure S2. (a). Individual PAHs Ratios, (b). PM Mass, 16-PAHs, LMW-PAHs, and HMW-PAHs during the cold weather months and hot weather months.

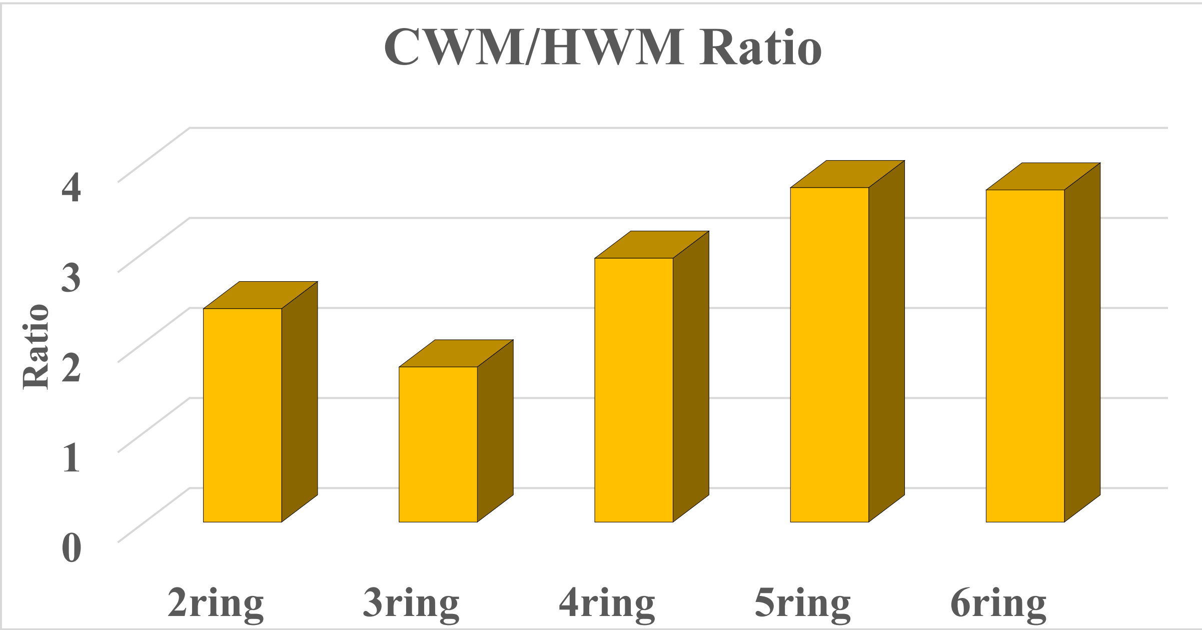

Figure S3. Cold weather months/Hot weather months ratio of 2, 3, 4, 5, and 6 ring PAHs average concentrations.

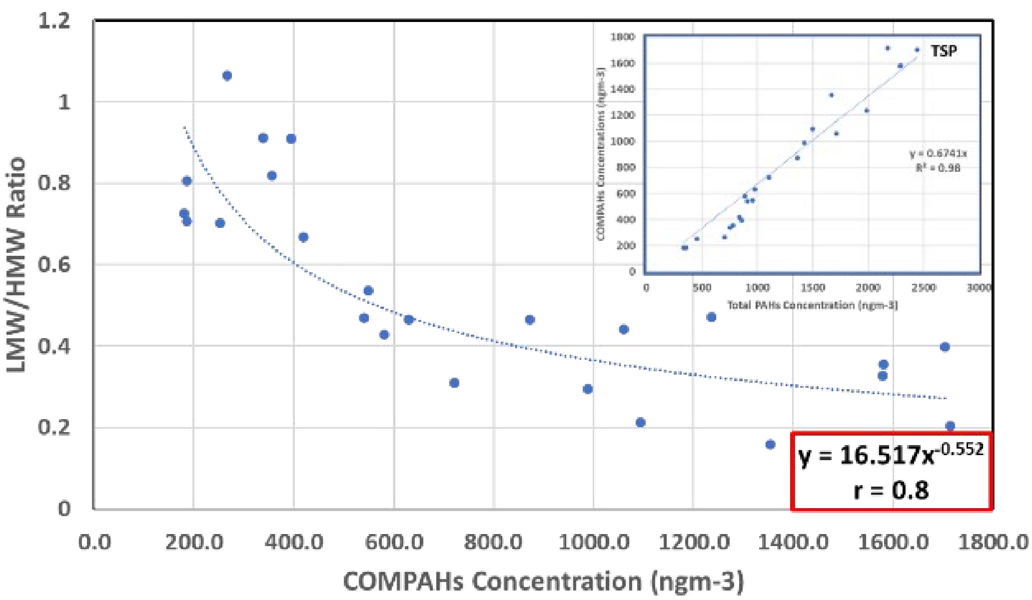

Figure S4. Relationship between COMPAHs concentration and LMW/HMW ratio; the relationship between COMPAHs and total PAHs concentrations in TSP.

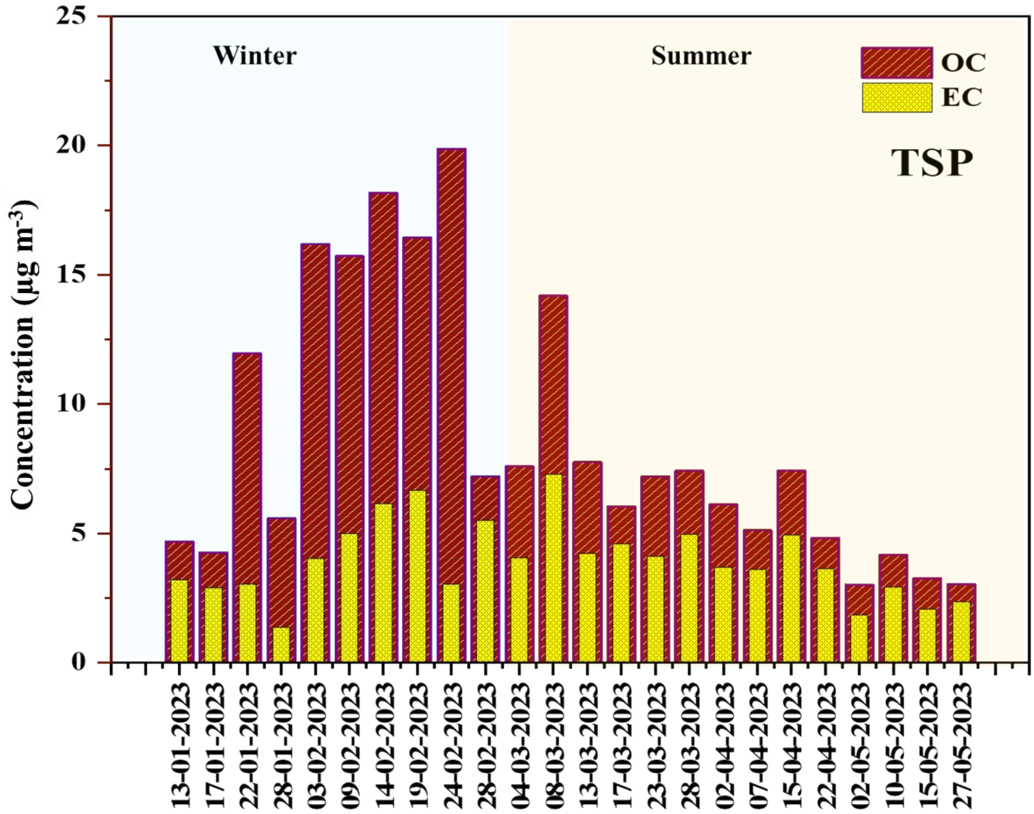

Figure S5. Temporal distribution of OC and EC in TSP

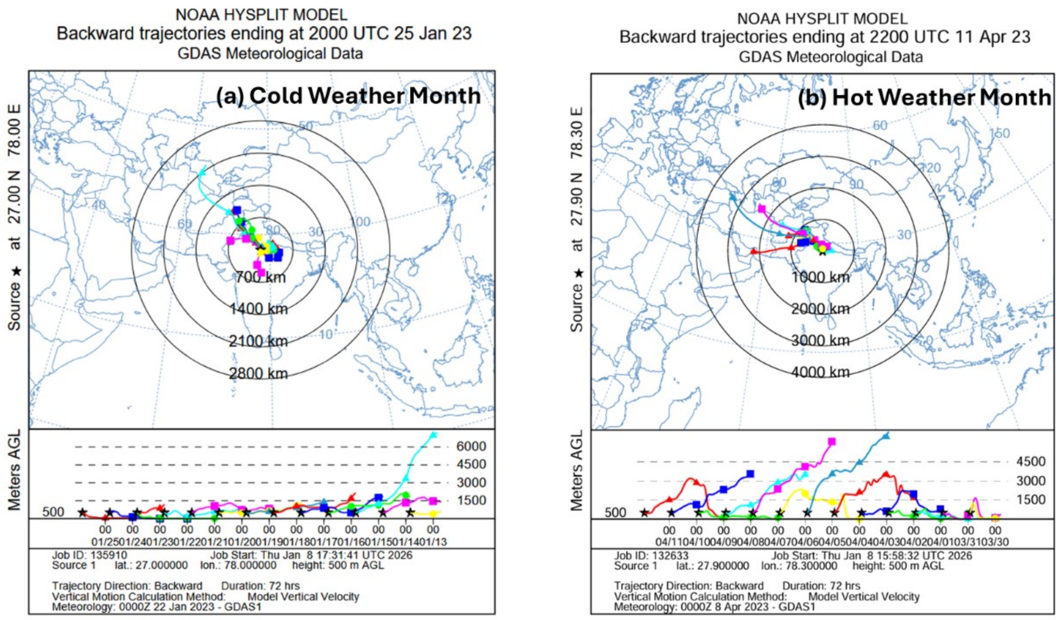

Figure S6. NOAA HYSPLIT 72-hour backward trajectories during (a) cold weather month (January) and (b) hot weather month (April) at the study site.

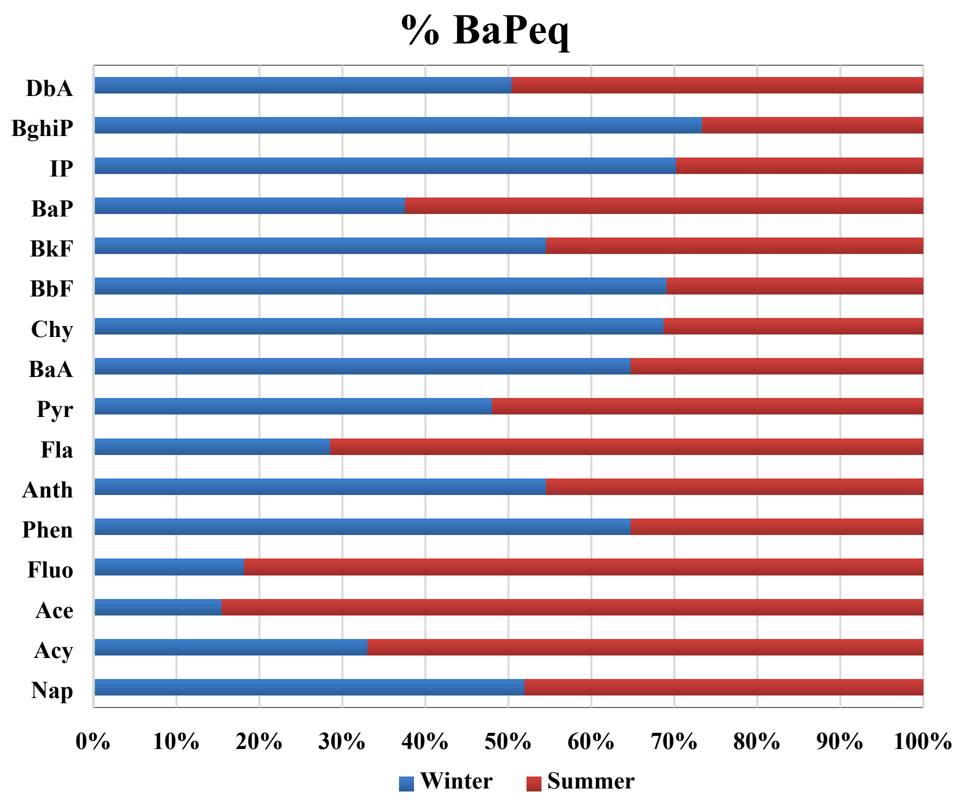

Figure S7. % BaP_{eq} contribution of individual PAH during the Cold weather months and the hot weather months in TSP.

Table S1. Meteorological conditions at the study site.

Parameter	Range / Value	Seasonal Variation
Temperature (°C)	11.1 – 36.1	Highest in May: 36.1 ± 3.2°C Lowest in January: 11.1 ± 10.1°C
Relative Humidity (%)	19.4 – 87.6	Highest in January: 87.6% Lowest in April: 19.4%
Wind Speed (km/h)	1 – 3	Generally low and stable
Wind Direction (degrees)	Winter: North/Northwest Summer: Southwest/East	Seasonal shift in prevailing wind directions
Solar Intensity (W/m^2)	14.8 – 88.9	Highest in May: 88.9 Wm-2 Lowest in January: 14.8 Wm-2

Table S2. Details of ions and ion ratios quantified per compound.

S.No	Compound	Quantifier Ion (m/z)	Qualifier Ion (m/z)	Ion Ratio Q2/Q1 : Q3/Q1	Retention Time (min)
1.	Naphthalene	128	127,102	0.85: 0.42	5.9
2.	Acenaphthylene	152	151, 153	0.90: 0.35	7.4
3.	Acenaphthene	154	152, 153	0.88: 0.47	8.4
4.	Fluorene	166	165, 167	0.83: 0.38	12.1
5.	Phenanthrene	178	176, 179	0.89: 0.41	14.3
6.	Anthracene	178	176, 179	0.93: 0.40	17.1
7.	Fluoranthene	202	101, 200	0.65: 0.38	20.5
8.	Pyrene	202	101, 200	0.68: 0.37	21.8
9.	Benz(a)anthracene	228	226, 229	0.78: 0.32	29.4
10.	Chrysene	228	226, 229	0.82: 0.36	29.6
11.	Benzo(b)Fluoranthene	252	250, 253	0.84: 0.33	35.3
12.	Benzo(k)fluoranthene	252	250, 253	0.79: 0.35	35.4
13.	Benzo(a)pyrene	252	250, 253	0.86: 0.39	36.8
14.	Indeno(1,2,3-cd)pyrene	276	138, 278	0.72: 0.30	41.8
15.	Dibenz(a,h)anthracene	278	139, 276	0.76: 0.34	41.9
16.	Benzo(g,h,i)perylene	276	138, 278	0.74: 0.31	42.9

Table S3. Method Detection Limits (MDLs) of PAHs

S.No	PAHs	LOD (ng m^{-3})
1.	Nap	0.71
2.	Acy	1.21
3.	Ace	0.04
4.	Flu	0.53
5.	Phen	0.73
6.	Anth	0.07
7.	Fla	0.03
8.	Pyr	0.03
9.	BaA	0.15
10.	Chy	0.02
11.	BbF	0.16
12.	BkF	0.15
13.	BaP	1.31
14.	IP	0.16
15.	DbA	0.11
16.	BghiP	0.07

Table S4. Summary of Displacement Analysis Results

Parameter	Result
DISP error code	0
Maximum ΔQ	0.000
Factor swaps	None
Rotational ambiguity	Low

Table S5. Parameters used in ILCR

Parameters	Unit	Infants	Children	Adult	Reference
Body Weight (BW)	Kg	5	30	70	2
Inhalation Rate (IR_{inh})	m^3day^{-1}	5.05	9.67	12.44	3
Ingestion Rate (IR_{ing})	$mgday^{-1}$	30	200	100	2
Exposed surface area of skin (SA)	cm^2	719	860	1530	1, 2, 4
Soil to skin adhere factor (AF)	mg cm^2	0.04	0.65	0.49	5
Dermal absorption factor (ABS)	Unitless	0.13	0.13	0.13	5
Exposure frequency (EF)	Days $year^{-1}$	180	180	180	2
Exposure Duration (ED)	Year	1	14	52	2, 6
Average Time (AT)	Days	25,550	25,550	25,550	6

These values were adopted from the United States EPA Risk Assessment Guidance and related publications as listed below (under References at bottom).

Table S6. Comparison of TSP and PAH concentrations reported in Agra with other urban and global locations.

Location (City)	Region	TSP (µg m⁻³)	PAHs (ng m⁻³)	Reference(s)
Agra	IGP	317.7 ± 96.2	1194.9 ± 351.2	Present Study
Agra	IGP			
Traffic Site		562.4 ± 104.7	2658 ± 2925	Verma et al., 2022
Rural Site		322.4 ± 64.5	269 ± 121	Rajput et al., 2012;
Delhi	IGP	162.9–262.8	122–625	Jahangir et al., 2022;
				Hazarika et al., 2015
		246–996		
Kanpur	IGP	141 ± 73	—	Ram and Sarin, 2010
Hisar	IGP	177 ± 64	—	Islam et al., 2020a, 2020b
Varanasi	IGP	220.4–536.6		Sen et al., 2014;
Agra		50.1–251.4		
Lucknow		220.4–536.6		
Kathmandu	Nepal	199 ± 124	—	Chen et al., 2015
Lumbini	Nepal	209.1 ± 113.4	91.6 ± 54.6	Chen et al., 2017
Harbin City	China	119–180	26.6–3240.97	Zhu et al., 2021; Yan et al., 2017
Bengbu	China	—	1.71–43.85	Wu et al., 2024
South Pars	Iran	173.4–413.5	8.77–21.8	Ghadrshenas et al., 2023
Erzurum	Turkey	108–211	—	Paloluoğlu et al., 2016
Istanbul	Turkey	49.8–101.2	109–212	Hanedar et al., 2014
Monterrey Metropolitan Area	Mexico	45–182	1.34–8.76	Longoria-Rodríguez et al., 2020; López-Ayala et al., 2019
Ulaanbaatar	Mongolia	—	1.4–773	Byambaa et al., 2019

Ulsan	South Korea	—	5.1–11.1	Nguyen et al., 2018

Table S7. Diagnostic ratios of PAH isomers.

S.No	Ratio	Sources	References	This study
1.	**Anth/Anth+Phen**	<0.1 Petrogenic (oil source) >0.1 Pyrogenic (High heat action)	Nadali et al., 2021	0.52 Pyrogenic
2.	**IP/IP+BghiP**	0.2-0.5 Fossil Fuel emissions >0.5 Biomass/Coal combustion >0.7 Gasoline emission	Wu et al., 2024; Cao et al., 2018	0.47 Fossil fuel emissions
3.	**BaA/BaA+Chy**	<0.2 Petroleum emission 0.2-0.35 Biomass/Coal combustion >0.35 Vehicular emission	Wu et al., 2024; Hu et al., 2012	0.51 Vehicular emission
4.	**BaP/BghiP**	>0.6 Petrogenic/traffic emission <0.6 Pyrogenic emission	Gbeddy et al., 2021; Naydenova et al., 2022	1.3 Coal combustion
5.	**Fla/Fla+Pyr**	0.4-0.5 Fossil fuel combustion/vehicular emission >0.5 Biomass/Coal combustion >0.35 Petroleum emission	Akyuz et al., 2010; Naydenova et al., 2022	0.41 Fossil fuel combustion /vehicular emission
6.	**Flu/Flu+Pyr**	<0.4 unburned petroleum (Oil source) 0.4-0.5 liquid fossil fuel >0.5 coal and wood combustion	Hu et al., 2012; Ontiveros-Cuadras et al., 2019	0.46 Liquid fossil fuel
7.	**COMB-PAHs/PAHs**	>1 Combustion Sources <1 Petrogenic Sources		

Table S8. Comparison of Diagnostic Ratios of PAH isomers with other national studies

	Anth/Anth +Phen	IP/IP+ BghiP	BaA/BaA+ Chy	Fla/Fla +Pyr	BaP/ BghiP	Flu/Flu+ Pyr	LMW/ HMW	Particle Size	References
Agra	0.52	0.47	0.51	0.41	1.30	0.46	0.54	TSP	Present Study
Delhi	-	0.51	0.45	0.65	0.59	0.27	-	PM10	Singh et al., 2011
Delhi JNU	-	0.62	-	-	0.85	-	-	PM2.5	Singh et al., 2021
Amritsar	0.46	0.68-0.8	0.53-0.55	0.47	0.15-5.9	-	1.03	PM10	Kaur et al., 2022; Kaur et al., 2013
Jamshedpur	0.63-0.72	0.40-0.52	0.60-0.64	0.24	-	0.50	-	PM2.5	Ambade et al., 2021; Kumar et al., 2020
Agra	-	0.35-0.72	0.46-0.50	0.5	0.53-1.38	-	0.018 - 4.67	TSP	Lakhani 2012; Rajput et al., 2010
Kolkata	0.12	0.44	0.32	-	-	-	-	TSP	Saha et al., 2017
Odisha	>0.1	0.5	<0.3	>0.5l				PM10	Ekka et al., 2021
Ranchi	0.43	-	0.46	-	0.6	0.50	-	PM2.5	Ambade et al., 2022
Bokaro	0.46	-	0.44	-	0.6	0.52	-		
Gamhari (One year)	0.44	-	0.41	-	0.6	0.52	-		

Table S9. Variation in the OC/EC ratio concerning the source of PM

S. No	PM Source	OC/EC Ratio	References
1.	Diesel vehicles	0.2 - 0.8	Park et al., 2018; Dallmann et al., 2016
2.	Vehicle Exhaust	2.5 - 5.0	Zhang et al., 2020; Chen and Liao, 2006
3.	Gasoline vehicles	1.0 - 2.0	Fraser et al., 2012; Chow et al., 2007
4.	Biomass burning	3.8 - 13.2	Elkins et al., 2020; Zhang et al., 2020
5.	Coal combustion	2.5 - 10.5	Wang et al., 2020; Zhang et al., 2020
6.	Secondary Organic Aerosols (SOA)	0.1 - 0.3	Ng et al., 2010; Kroll et al., 2011; Shrivastava et al., 2017

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