Electronic Supplementary Material (ESI) for Environmental Science: Atmospheres.

† Electronic Supplementary Information for "Comprehensive organic emission profiles, secondary organic aerosol production potential, and OH reactivity of domestic fuel combustion in Delhi, India"

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ESI1 – Schematic of burning chamber

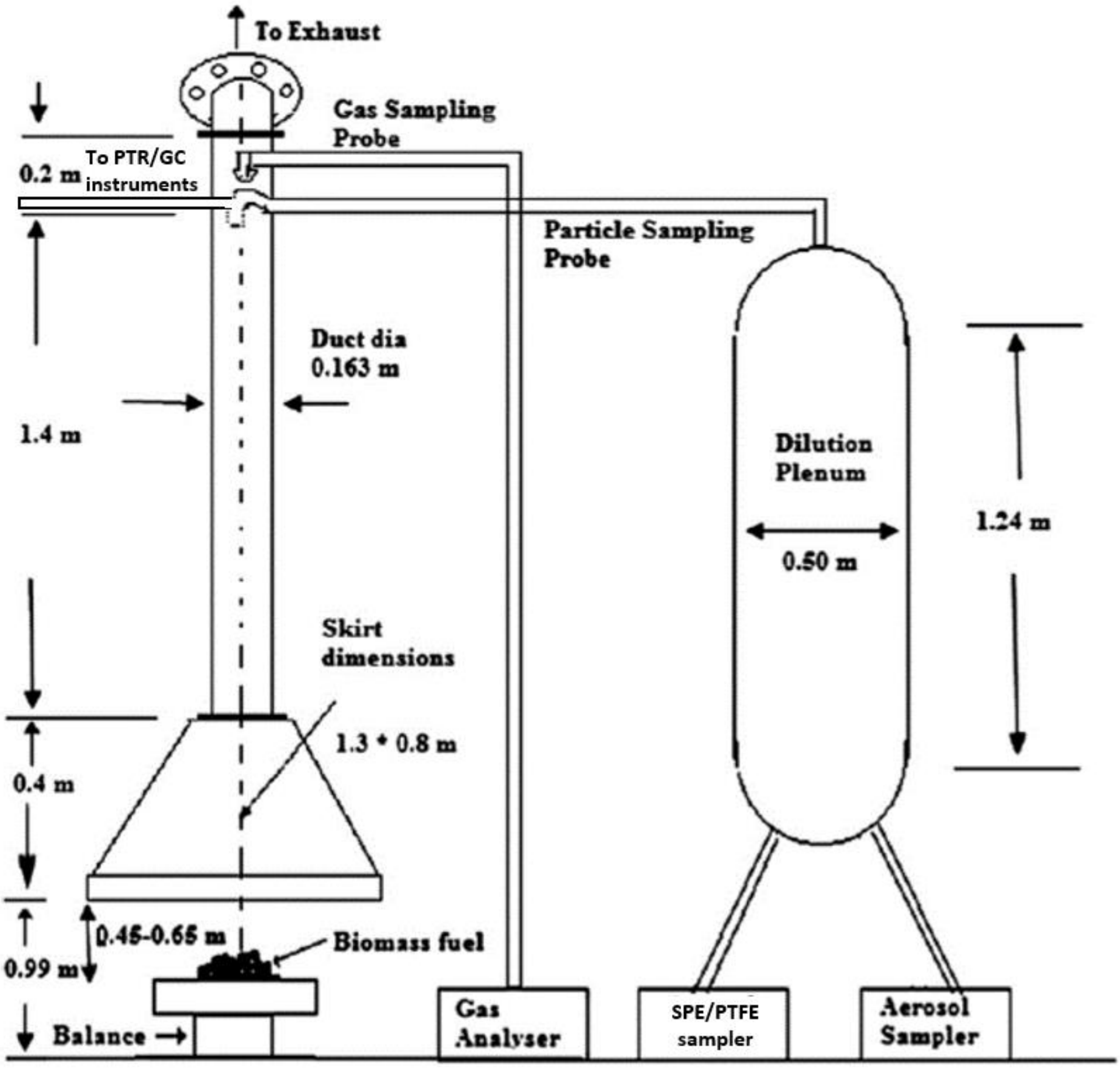

Figure S1. Schematic of combustion-dilution chamber with sampling locations for PTR-ToF-MS, DC-GC-FID and GC×GC-FID instruments and SPE/PTFE sample collection points.

ESI2 - Temperatures above combustion experiments

Table S1. Mean maximum temperatures above different combustion experiments by fuel type.

Fuel	**Mean maximum flame temp ± σ / ºC**
Fuel wood	545 ± 122
Cow dung cake	303 ± 137
Charcoal	251 ± 57
Crop residue	432 ± 143
Sawdust	314 ± 163
LPG	721 ± 18
MSW	249 ± 161

ESI3– DC-GC-FID method

A 500 ml sample (1.5 L pre-purge of 100 ml min^{-1} for 15 minutes, sample at 17 mL min^{-1} for 30 minutes) was collected (Markes International CIA Advantage), passed through a glass finger at -30 ^{o}C to remove water and adsorbed onto a dual-bed sorbent trap (Markes International ozone precursors trap) at -20 ^{o}C (Markes International Unity 2). The sample was thermally desorbed (250 ^{o}C for 3 minutes) then split 50:50 and injected into two separate columns for analysis of NMHCs (50 m × 0.53 mm Al_2O_3 PLOT) and oxygenated NMVOCs (10 m × 0.53 mm LOWOX with 50 μm restrictor to balance flow). The oven was held at 40 ^{o}C for 5 minutes, then heated at 13 ^{o}C min^{-1} to 110 ^{o}C, then finally at 8 ^{o}C min^{-1} to 200 ^{o}C with a 30-minute hold. The instrument was calibrated using a 4 ppbv gas standard containing a range of alkanes, alkenes, alkynes and aromatics purchased from the British National Physical Laboratory.

ESI4 - GC×GC-FID method

The GC×GC-FID sampled 3 L samples (100 ml min^{-1} for 30 minutes) using an adsorption-thermal desorption system (Markes International Unity 2). NMVOCs were trapped onto a sorbent (Markes International U-T15ATA-2S) at -20 ^{o}C with water removed in a glass cold finger at -30 ^{o}C, removed and heated to ~ 100 ^{o}C after each sample to prevent carryover of unanalysed, polar interfering compounds. The sample was thermally desorbed (250 ^{o}C for 5 minutes) and injected splitless down a transfer line. Analytes were refocussed for 60 s using liquid CO_2 at the head of a non-polar BPX5 held at 50 psi (SGE Analytical 15m × 0.15 μm × 0.25 mm), which was connected to a polar BPX50 at 30 psi (SGE Analytical 2 m × 0.25 μm × 0.25 mm) *via*. a modulator held at 180 ^{o}C (5 s modulation, Analytical Flow Products ELDV2-MT). The oven was held for 2 minutes at 35 ^{o}C, then ramped at 2.5 ^{o}C min^{-1} to 130 ^{o}C and held for 1 minute with a final ramp of 10 ^{o}C min^{-1} to 180 ^{o}C and hold of 8 minutes. The instrument was calibrated using a 4 ppbv gas standard containing a range of alkanes and aromatics purchased from the British National Physical Laboratory. Blank measurements were made at the beginning, middle and end of the day, with mean values subtracted from measured emission factors for both GC instruments.

ESI5 – PTR-ToF-MS method

Additional details of the PTR-ToF-MS system used in this study are given in previous papers. [1, 2] The sample air was diluted into zero air, generated by passing ambient air (1 L min^{-1}) through a heated platinum filament at 550 ^{o}C, before entering the instrument with an inlet flow of 250 ml min^{-1}. Samples were diluted by either 5 or 6.25 times (50 ml min^{-1} in 200 ml min^{-1} zero air or 40 ml min^{-1} in 210 ml min^{-1} zero air). The instrument was operated with an electric field strength (E/N, where N is the buffer gas density and E is the electric field strength) of 120 Td. The drift tube temperature was 60 °C with a pressure of 2.3 mbar and 560 V applied across it.

Calibrations were performed twice a week using a gas calibration unit (Ionicon Analytik, Innsbruck). The calibration gas (Apel-Riemer Enironmental Inc., Miami) contained 18 compounds: methanol, acetonitrile, acetaldehyde, acetone, dimethyl sulphide, isoprene, methacrolein, methyl vinyl ketone, 2-butanol, benzene, toluene, 2-hexanone, *m*-xylene, heptanal, α-pinene, 3-octanone and 3-octanol at 1000 ppbv (± 5%) and β-caryophyllene at 500 ppbv (± 5%). This standard was dynamically diluted into zero air to provide a 6-point calibration. The normalised sensitivity (ncps/ppbv) was then determined for each mass using a transmission curve. [3] The maximum error in this calibration approach has been shown to be 21%. Peak assignment was assisted with results reported by previous burning studies. [4-6]

Mass calibration and peak fitting of PTR-ToF-MS data were performed using PTRwid software. [7] Count rates (cps) of each mass spectral peak were normalised to the primary ion (H_3O^+) and water cluster $(H_3O.H_2O)^+$ peaks, and mixing ratios were then determined for each mass using the normalised sensitivity. Where compounds known to fragment in the PTR-ToF-MS were identified, the mixing ratio of these species was calculated by summing parent ion and fragment ion mixing ratios.

ESI6 – SPE/PTFE-GC×GC-ToF-MS analysis

Full details on GC×GC-ToF-MS sample collection, quality control and analyses are given elsewhere. [8] SPE disks and PTFE filters were spiked with an internal standard (50 μL at 20 μg mL^{-1}) containing 6 deuterated PAHs (1,4-Dichlorobenzene-d_4, naphthalene-d_8, acenaphthene-d_{10}, phenanthrene-d_{10}, chrysene-d_{12}, perylene-d_{12}; EPA 8270 Semivolatile Internal Standard Mix, 2000 μg mL^{-1} in DCM). SPE disks and PTFE filters were cut and extracted into ethyl acetate (EtOAc) using accelerated solvent extraction (ASE 350, Dionex, ThermoFisher Scientific) following the methodology of Farren et al. (2015). [9]

PTFE samples were analysed with a method that allowed well-resolved separation of hydrocarbons across a two-dimensional space from *n*-nonane to *n*-tetracontane (C_9-C_{40}) using GC×GC-ToF-MS (Leco Pegasus BT 4D) with a splitless injection (1 μL injection, 4mm taper focus liner, SHG 560302). The primary dimension column was a RXI-5SilMS (Restek, 30 m × 0.25 μm × 0.25 mm) connected to a second column of RXI-17SilMS (Restek, 0.25 μm × 0.25 mm, 0.17 m primary GC oven, 0.1 m modulator, 1.42 m secondary oven, 0.31 m transfer line) with a He flow of 1.4 mL min^{-1}. The primary oven was held at 40 ^{o}C for 1 minute, then ramped at 3 ^{o}C min^{-1} to 322 ^{o}C where it was held for 3 minutes. The secondary oven was held at 62 ^{o}C for 1 minute then ramped at 3.2 ^{o}C min^{-1} to 190 ^{o}C after which it was ramped at 3.6 ^{o}C min^{-1} to 325 ^{o}C and held for 19.5 minutes. The inlet was held at 280 ^{o}C and the transfer line at 340 ^{o}C. A 5 s cryogenic modulation was used with a 1.5 s hot pulse and 1 s cool time between stages. SPE samples were injected split (10:1) and analysed with a shorter analysis time with the primary oven held at 40 ^{o}C for 1 minute then ramped at 3 ^{o}C min^{-1} to 202 ^{o}C where it was held for 4 seconds. The secondary oven was held at 62 ^{o}C for 1 minute then ramped at 3.2 ^{o}C min^{-1} to 235 ^{o}C. All peaks, including those without mass spectral database matches, have been included in the analysis. Blank measurements were made by passing air from the chamber (6 L min^{-1} for 30 minutes) through the filter holder containing PTFE filters and SPE disks. Mean blank values from before and after relevant burning experiments were subtracted from samples.

ESI7 - Hierarchy of instruments used

Table S2 shows a summary of the instruments used to produce the volatility-basis dataset used in this study. Emission data was taken from [8, 10].

Table S2. Summary of instruments used for calculation of total emission factor.

Species	**Instrument**
Aromatics	
Benzene-C_3 substituted monoaromatics	GCxGC-FID
C_4-C_5 substituted monoaromatics	PTR-ToF-MS
Phenolics	
All species	PTR-ToF-MS
Oxygenated aromatics	
All species	PTR-ToF-MS
Oxygenated aliphatics	
All species	PTR-ToF-MS
NVOCs	
All species	PTR-ToF-MS
Furanics	
All species	PTR-ToF-MS
Monoterpenes	
All species	PTR-ToF-MS [a]
PAHs	
All species	PTR-ToF-MS [a]
Alkenes	
All DC-GC-FID alkenes to C_5	DC-GC-FID
Remaining alkenes [b]	PTR-ToF-MS
Alkanes [c]	
C_2-C_6 alkanes	DC-GC-FID
C_7-C_{12} alkanes	GCxGC-FID
C_{13}-C_{20} alkanes	SPE-GCxGC-ToF-MS
Unidentified gas-phase I/SVOCs	
All peaks excluding those already identified by GCxGC-FID and PTR-ToF-MS.	SPE-GCxGC-ToF-MS [d]
Unidentified particle-phase I/SVOCs	
All peaks	PTFE-GCxGC-ToF-MS [d]

[a] PTR-ToF-MS signal used as may include isomers not measured by GCxGC-FID.

[b] Only alkenes not measured by DC-GC-FID.

[c] No peaks for > C_6 alkanes in PTR-ToF-MS spectra.

[d] Used to estimate the remaining unidentified organic mass in these regions, unidentified peaks from PTR-ToF-MS have not been included to avoid double counting in this region.

ESI8 - SOA yields

Table S3. SOA yields used for determining SOA from biomass burning NMVOC emissions

Compound	High NO_x yield	High NO_x ref	Notes	Low NO_x yield	Low NO_x ref	Notes
Dodecane	0.08	11		0.05	12	
Tridecane	0.21	11		0.21 [b]	11	Assumed same as low NO_x [13]
Tetradecane	0.28	11		0.28 [b]	11	Assumed same as low NO_x [13]
Pentadecane	0.34	11		0.34 [b]	11	Assumed same as low NO_x [13]
Hexadecane	0.38	11		0.38 [b]	11	Assumed same as low NO_x [13]
Heptadecane	0.42	11		0.42 [b]	11	Assumed same as low NO_x [13]
Octadecane	0.42	11		0.42 [b]	11	Assumed same as low NO_x [13]
Nonadecane	0.42	11		0.42 [b]	11	Assumed same as low NO_x [13]
Eicosane	0.42	11		0.42 [b]	11	Assumed same as low NO_x [13]
Naphthalene	0.21	11		0.66	14	Assumed same as low NO_x [13]
C1-Napthalene	0.27	11		0.57	14	Average of 1-MN and 2-MN
C2-Napthalene	0.31	11		0.57	14	Assumed same as C_1 napthalenes
Benzene	0.14	15		0.34	15	
Toluene	0.083	15		0.33	15	
C_2-Benzenes	0.047	15		0.27	15	
C_3-Benzenes	0.047	15	Assumed same as C_2 benzenes	0.27	15	

C_4-Benzenes	0.04	[11]		0.27	[15]	Assumed same as C_2 benzenes
C_5-Benzenes	0.08	[11]		0.27	[15]	Assumed same as C_2 benzenes
Salicylaldehyde	0.18	[a]	Average	0.31	[a]	Average
Phenol	0.54	[16]	Assumed same as phenol	0.40	[16]	
Cresol/anisole	0.54	[16]	Assumed same as phenol	0.40	[16]	Assumed same as phenol
Ethyl phenol	0.54	[16]	Assumed same as phenol	0.40	[16]	Assumed same as phenol
Guaiacol	0.46	[16]		0.45	[16]	
Vinyl guaiacol	0.46	[16]	Assumed same as guaiacol	0.45	[16]	Assumed same as guaiacol
Methyl guaiacol	0.46	[16]	Assumed same as guaiacol	0.45	[16]	Assumed same as guaiacol
Eugenol, isoeugenol	0.3	[16]	Assumed same as syringol	0.32	[16]	Assumed same as syringol
Syringol	0.3	[16]		0.32	[16]	
Vanillin	0.3	[16]	Assumed same as syringol	0.32	[16]	Assumed same as syringol
3-Methylcatechol	0.3	[16]	Assumed same as syringol	0.32	[16]	Assumed same as syringol
MVK, methacrolyn, crotonaldehyde	0.05	[17, 18]	Assumption of Hatch et al. (2015) applied to other oxygenated aliphatics > C_6	0.05	[17, 18]	Assumption of Hatch et al. (2015) applied to other oxygenated aliphatics > C_6.
Monoterpenes	0.15	[17, 19]		0.15	[17, 19]	Same as high NOx
Furan	0.05	[20]		0.05	[20]	
Methyl furans	0.09	[21]	Based on 3-methylfuran	0.12	[21]	Lower NO_x final, based on 3-methylfuran
Furfural	0.083	[15, 22]	Based on same SOAP as toluene Gilman et al. (2015)	0.33	[15, 22]	Based on same SOAP as toluene Gilman et al. (2015)

2-Methanol furanone	0.083	[15, 22]	Based on same SOAP as toluene Gilman et al. (2015)	0.33	[15, 22]	Based on same SOAP as toluene Gilman et al. (2015)
2-(3H)-furanone	0.083	[15, 22]	Based on same SOAP as toluene Gilman et al. (2015)	0.33	[15, 22]	Based on same SOAP as toluene Gilman et al. (2015)
5-hydroxymethyl-2[3H]-furanone	0.083	[15, 22]	Based on same SOAP as toluene Gilman et al. (2015)	0.33	Based on same SOAP as toluene Gilman et al. (2015)	Based on same SOAP as toluene Gilman et al. (2015)
C$_2$-furans	0.09	[21]	Based on 3-methylfuran	0.12	[21]	Lower NO$_x$ final, based on 3-methylfuran
C$_6$-diketone isomers, C$_6$-esters	0.05	[17, 18]	Assumption of Hatch et al. (2015) applied to other oxygenated aliphatics > C$_6$	0.05	[17, 18]	Assumption of Hatch et al. (2015) applied to other oxygenated aliphatics > C$_6$
Methyl furfurals	0.083	[15, 22]	Based on same SOAP as toluene Gilman et al. (2015)	0.33	[15, 22]	Based on same SOAP as toluene Gilman et al. (2015)
C$_2$-pyroles	0.083	[15, 22]	Based on same SOAP as toluene Gilman et al. (2015)	0.33	[15, 22]	Based on same SOAP as toluene Gilman et al. (2015)
Structurally assigned ≥ C$_6$ compounds [a]	0.18	[a]		0.31	[a]	
structurally unassigned ≥ C$_6$ compounds [a]	0.18	[a]		0.31	[a]	

[a] Average of applied yields from NMVOCs in the table with at least 6 carbon atoms per molecule.

[b] Low NO$_x$ alkane yields are poorly studied beyond *n*-dodecane, and alkane emission factors in this study are small. For *n*-dodecane the low NO$_x$ yield is comparable to high NO$_x$ yield of dodecane and high NO$_x$ yields have been used for heavier alkanes.

ESI9 – Rate constants for OH reactivity

C_4 substituted monoaromatics have been taken from the PTR-ToF-MS, as opposed to the speciated measurement with the GCxGC-FID, as these species have low emission factors and little influence on overall OH reactivity. Rate constants for reaction with the OH radical have largely been taken from those compiled in the Supplementary Information of Koss et al. (2018), [6] with additional species found from relevant literature.

Table S4. Rate constant used for calculation of OH reactivity.

No	VOC	Formula	Rate constant (10^{-12} cm^3 molecule^{-1} s^{-1})	Reference
1	Ethane	C_2H_6	0.248	[23]
2	Ethene	C_2H_4	8.52	[23]
3	Propane	C_3H_8	1.09	[23]
4	Propene	C_3H_6H	30	NIST database
5	Isobutane	C_4H_{10}	2.12	[23]
6	*n*-Butane	C_4H_{10}	2.36	[23]
7	Acetylene	C_2H_2	0.7	NIST database
8	*Trans*-2-butene	C_4H_8	64	[23]
9	1-Butene	C_4H_8	31.4	[23]
10	Isobutene	C_4H_8	51.4	[23]
11	*Cis*-2-butene	C_4H_8	56.4	[23]
12	Cyclopentane	C_5H_{10}	4.97	[23]
13	*i*-Pentane	C_5H_{12}	3.6	[23]
14	*n*-Pentane	C_5H_{12}	3.8	[23]
15	1,3-Butadiene	C_4H_6	66.6	[23]
16	*Trans*-2-pentene	C_5H_{10}	67	[23]
17	*Cis*-2-pentene	C_5H_{10}	65	[23]
18	Pent-1-ene	C_5H_{10}	31.4	[23]
19	*n*-Heptane	C_7H_{16}	6.76	[23]

20	*n*-Octane	C_8H_{18}	8.11	[23]
21	*n*-Nonane	C_9H_{20}	9.7	[23]
22	*n*-Decane	$C_{10}H_{22}$	11	[23]
23	*n*-Undecane	$C_{11}H_{24}$	12.3	[23]
24	*n*-Dodecane	$C_{12}H_{26}$	13.2	[23]
25	*n*-Tridecane	$C_{13}H_{28}$	15.1	[23]
26	*n*-Tetradecane	$C_{14}H_{30}$	17.9	[23] *312K
27	C_8 grouped aliphatics	C_8H_{18}	8.11	[23]
28	C_9 grouped aliphatics	C_9H_{20}	9.7	[23]
29	C_{10} grouped aliphatics	$C_{10}H_{22}$	11	[23]
30	C_{11} grouped aliphatics	$C_{11}H_{24}$	12.3	[23]
31	C_{12} grouped aliphatics	$C_{12}H_{26}$	13.2	[23]
32	C_{13} grouped aliphatics	$C_{13}H_{28}$	15.1	[23]
33	C_{14} grouped aliphatics	$C_{14}H_{30}$	17.9	[23] *312K
34	Benzene	C_6H_6	1.22	[23]
35	Toluene	C_7H_8	5.6	[23]
36	Ethylbenzene	C_8H_{10}	7	[23]
37	*m*-/*p*-Xylene	C_8H_{10}	18.7	[23] *mean *m*/*p*-xylene
38	*o*-Xylene	C_8H_{10}	13.6	[23]
39	*i*-Propylbenzene	C_9H_{12}	6.3	[23]
40	*n*-Propylbenzene	C_9H_{12}	5.8	[23]
41	3/4-Ethyltoluene	C_9H_{12}	15.2	[23] *mean 3/4-ethyl toluene
42	1,3,5-TMB	C_9H_{12}	56.7	[23]
43	2-Ethyltoluene	C_9H_{12}	11.9	[23]
44	1,2,4-TMB	C_9H_{12}	32.5	[23]
45	*t*-Butylbenzene	$C_{10}H_{14}$	4.5	[23]
46	1,2,3-TMB	C_9H_{12}	32.7	[23]
47	Indan	C_9H_{10}	23.01429	[23] *mean C_3 substituted monoaromatic

48	α-Pinene	$C_{10}H_{16}$	52.3	[23]
49	Camphene	$C_{10}H_{16}$	53	[23]
50	Sabinene	$C_{10}H_{16}$	117	[23]
51	β-Pinene	$C_{10}H_{16}$	74.3	[23]
52	Myrcene	$C_{10}H_{16}$	215	[23]
53	α-Phellandrene	$C_{10}H_{16}$	313	[23]
54	3-Carene	$C_{10}H_{16}$	88	[23]
55	α-Terpinene	$C_{10}H_{16}$	363	[23]
56	Limonene	$C_{10}H_{16}$	164	[23]
57	β-Ocimene	$C_{10}H_{16}$	252	[23]
58	γ-Terpinene	$C_{10}H_{16}$	177	[23]
59	Terpinolonene	$C_{10}H_{16}$	225	[23]
60	Ammonia [a]	NH_3	0.2	[22]
61	Acetylene	C_2H_2	0.7	NIST database
62	Hydrogen cyanide [a]	HCN	0.0	Cicerone 1983
63	Methanimine	CH_3N	0.2	*from ammonia
64	Formaldehyde	CH_2O	9.4	[23]
65	Methanol	CH_3OH	0.8	[23]
66	Acetonitrile	C_2H_3N	0.0	[22]
67	Isocyanic acid	HNCO	0.0	[22]
68	Acetaldehyde	C_2H_4O	15.0	[23]
69	Formamide	CH_3NO	1.5	NIST database: $CH_2=NOH$
70	Formic acid	CH_2O_2	0.4	NIST database
71	Ethanol	C_2H_5OH	3.2	[23]
72	Nitrous acid	HNO_2	6.0	[22]
73	Methane thiol	CH_4S	33.0	NIST database
74	Methanediol	CH_4O_2	7.0	NIST database
75	Propyne nitrile	C_3HN	4.0	* From acrylonitrile

76	1-Buten-3-yne	C_4H_4	20.0	[22]
77	Acrylonitrile	C_3H_3N	4.0	[22]
78	2-Propynal	C_3H_2O	20.0	* From acrolein
79	Butadienes	C_4H_6	58.8	[23]
80	Propanenitrile	C_3H_5N	0.3	[22]
81	Acrolein	C_3H_4O	20	[22]
82	Butenes, other hydrocarbon	C_4H_8	31.8	[23]
83	Methyl isocyanate	C_2H_3NO	0.1	* From isocyanic acid, methanol [6]
84	Acetone	C_3H_6O	0.2	[23]
85	Acetamide	C_2H_5NO	8.6	NIST database
86	C_3 Amines	C_3H_9N	60.0	NIST database
87	Acetic acid	$C_2H_4O_2$	3.7	NIST database
88	Nitromethane	CH_3NO_2	0.0	[22]
89	Dimethylsulfide [a]	CH_3NO_2	0.02	[22]
90	1,3-Cyclopentadiene	C_5H_6	92.0	[22]
91	Butenenitrile isomers, pyrole	C_4H_5N	111.4	[22]
92	Carbon suboxide	C_3O_2	1.5	[22]
93	Furan	C_4H_4O	40.0	[22]
94	Isoprene	C_5H_8	100.0	[23]
95	Butane nitriles, dihydropyrole	C_4H_7N	7.7	SONGNEX PTRToF paper
96	Propiolic acid	$C_3H_2O_2$	26.0	* From acrylic acid
97	MVK, methacrolyn, crotonaldehyde	C_4H_6O	24.8	[23], NIST database
98	Methoxyacetonitrile or acrylamide	C_3H_5NO	0.02	From acetonitrile [22]

99	Butene amines, tetrahydropyrole	C_4H_9N	25.0	* From butenes, ammonia see [6]
100	Methylglyoxal, acrylic acid	$C_3H_4O_2$	21.0962	Methylglyoxal [23], Acrylic acid [22]
101	MEK	C_4H_8OH	5.46	[23] weighted average
102	Formamide N,N-dimethyl- or propanamide 2, ethyl or acetamide, N-methyl	C_3H_7NO	1.41	NIST Database
103	Hydroxyacetone, methyl acetate, ethyl formate	$C_3H_6O_2$	2.19763	NIST Database hydroxyacetone
104	Benzene	C_6H_6	1.22	[23]
105	Pyridine, C_5 nitriles	C_5H_5N	5.64607	NIST Database pyridine; *from pentane nitriles, pentyne nitrile
106	2,4-Cyclopentadiene-1-one, other hydrocarbon	C_5H_4O	19.9929	2-Methylfuran [22]
107	Methyl cyclopentadiene	C_6H_8	91.0	Estimated as cyclopentadiene [22]
108	Methylpyrole, pentanenitriles	C_5H_7N	62.6792	[22]
109	Methylfurans, other hydrocarbon	C_5H_6O	37.0887	Cyclopentenone [22]
110	Hexenol fragment or cyclohexene or hexenes or 1,3-hexadiene	C_6H_{10}	67.4	NIST database for cyclohexene
111	Pentane nitriles	C_5H_9N	0.5	* From butane nitriles
112	2-(3H)-Furanone	$C_4H_4O_2$	44.5	[22]
113	3-Methyl-3-butene-2-one, cyclopentanone, other hydrocarbon	C_5H_8O	11.5	[23], NIST Database

114	1-Hexene, C_6-alkenes	C_6H_{12}	37.0	[23]
115	2,3-Butnaedione, methyl butanals, pentanones	$C_4H_6O_2$	0.8	[22], NIST Database
116	Propanamide 2-methyl- or butanamide or acetamide N-ethyl-	C_4H_9NO	1.78	Estimated as propanamide, NIST database.
117	Pyruvic acid	$C_3H_4O_3$	0.1	[22]
118	Methyl propanoate	$C_4H_8O_2$	0.9	NIST Database
119	Methyl pyridines	C_6H_7N	2.6	NIST Database methylpyridines average
120	Phenol	C_6H_5OH	28.0	[22]
121	Pyrydinamine, methyl diazina	$C_5H_6N_2$	10	Average of 3 isomers, [22]
122	C_2 substituted pyrroles	C_5H_7N	145	* From pyyrole [6]
123	Furfurals, other hydrocarbons	$C_5H_4O_2$	35.6	[22]
124	C_2 substituted furans	C_6H_8O	132.0	2,5-Dimethylfuran [22]
125	Cyclopentene dimethyl-1, methylcyclohexene	C_6H_{10}	67.4	NIST - considered same as cyclohexene
126	4-methylpentanenitrile	$C_6H_{11}N$	11.0	* From hexane [6]
127	2-Methanol furanone	$C_5H_6O_2$	13.6	* From furan
128	Methylcyclopentanone, cyclohexanone, hexanones	$C_6H_{10}O$	6.4	[23] cyclohexanone
129	Dihydrofuranodione	$C_4H_4O_3$	20.0	* From butadione, furan
130	Methyl methacrylate, other hydrocarbon	$C_5H_8O_2$	30.3	[22]
131	Hexanals, hexanones	$C_6H_{12}O$	18.6	[23] average C_6 carbonyls

132	Acetic anhydride	$C_4H_6O_3$	43.0	* From methylmethacrylate
133	Benzonitrile	C_7H_5N	1.0	[22]
134	Styrene	C_8H_8	58.0	[23]
135	Benzaldehyde	C_7H_6O	12.0	[23]
136	Dimethyl + ethyl pyridine, heptyl nitriles	C_7H_9N	3.2	NIST Database
137	Quinone	$C_6H_4O_2$	4.6	NIST Database
138	Cresol, anisole	C_7H_8O	26.2	NIST Database
139	Methyl furfural, benzene diols, 2-acetyl furan	$C_6H_6O_2$	80.1	NIST Database; *from furfural
140	C_3 Substituted furans, other compounds	$C_7H_{10}O$	23.3	* From furan
141	5-Hydroxy 2-furfural, 2-furanoic acid	$C_5H_4O_3$	49.0	* From 3-furfural
142	2-Hydroxy-3-methyl-2-cclopenten-1-one	$C_6H_8O_2$	57.0	* From methylfuran
143	Nitrofuran	$C_4H_3NO_3$	40.0	* From furan
144	5-Hydroxymethyl-2[3H]-furanone	$C_5H_6O_3$	100.0	* From furan, furanone
145	C_6 diketone isomers, C_6 esters	$C_6H_{10}O_2$	20.0	NIST Database average
146	Heptanal, 2,4-dimethyl-3-pentanone, heptanone	$C_7H_{14}O$	21.4	[23]
147	5-Hydroxymethyl tetrahydro 2-furanone, 5-hydroxy tetrahydro 2-furfural	$C_5H_8O_3$	5.0	* From dimethylfuran, cyclopentane, cyclopentadiene
148	Benzene acetonitrile	C_8H_7N	1.2	* From benzene
149	Benzofuran	C_8H_6O	37.0	NIST Database

150	Methyl styrene, propenyl benzene + methyl ethynyl benzene, indane	C_9H_{10}	50.4	[23]
151	Tolualdehyde	C_8H_8O	16.0	Atkinson 2003 average tolualdehydes
152	Salicylaldehyde	$C_7H_6O_2$	38.0	* From phenol, benzaldehyde
153	Ethylphenol + dimethyl phenol, methyl anidiol	$C_8H_{10}O$	46.6	NIST Database C_2 phenols, *anisol
154	Hydroxybenzoquinone	$C_6H_4O_3$	4.6	* From benzoquinone
155	Guaiacol	$C_7H_8O_2$	75.0	NIST Database
156	5-Hydroxymethyl 2-furfural	$C_6H_6O_3$	100.0	* From furfural, dimethylfuran
157	Naphthalene	$C_6H_8O_3$	132.0	* From dimethylfuran
158	Methyl benzene acetonitrile	C_9H_9N	5.6	* From toluene
159	Methylbenzofurans	C_9H_8O	37.0	[22]
160	Methylacetephenone	$C_9H_{10}O$	4.5	NIST Database
161	C_{10} aromatics	$C_{10}H_{14}$	9.5	Atkinson 2003 average C_{10} aromatics
162	Methylbenzoic aicd	$C_8H_8O_2$	12.0	* From benzaldehyde
163	Methylguiacol	$C_8H_{10}O_2$	100.0	NIST Database
164	3-Methylcatechol	$C_7H_8O_3$	5	Estimated as same as benzene diols [22]
165	Methylnaphthalene	$C_{11}H_{10}$	50.0	NIST Database
166	Levoglucosan pyrolysis product	$C_6H_8O_4$	4.6	* From benzoquinone
167	Dimethyl benzo furan, ethyl benzo furan	$C_{10}H_{10}O$	37.0	* From benzofuran
168	Estragole	$C_{10}H_{12}O$	50.0	NIST Database: 1-methoxy-4-(2-propenyl) benzene
169	C_{11} aromatics	$C_{11}H_{16}$	50.0	* From C_{10}, C_{12} aromatics

170	Vinyl guaiacol	$C_9H_{10}O_2$	100.0	* From methylguaiacol
171	Vanilin	C_8H8_{O3}	85.0	* From guaiacol, benzaldehyde
172	Syringol	$C_8H_{10}O_3$	100.0	* From methylguaiacol
173	Dimethylnaphthalene	$C_{12}H_{12}$	60.0	NIST Database
174	C_{12} aromatics	$C_{12}H_{18}$	113.0	Hexamethylbenzene[23]
175	Eugenol, isoeugenol	$C_{10}H_{12}O_2$	100.0	* From methylguaiacol

[a] Not included in final calculation due to sensitivity being too different from the NMVOCs used to build the transmission curve but included in table to show that low-rate constant likely has little influence on OH reactivity.

ESI10 – Toxicity equivalence factors

Table S5. TEF values used for individual PAHs in calculation of fuel toxicity.

Compound	TEF	Ref
Naphthalene	0.001	[24]
Methylnaphthalene	0.001	[24]
Dimethylnapthalene	0.001	*
Biphenyl	0.001	*
9-Fluorenone	0.001	*
Acenaphthylene	0.001	[24]
Acenapthene	0.001	[24]
Dibenzofuran	0.001	
Fluorene	0.0005	[25]
Phenanthrene	0.0005	[25]
Anthracene	0.0005	[25]
Carbazole	0.001	*
Fluoranthene	0.05	[25]
Pyrene	0.001	[25]
Benzo[a]anthracene	0.082	[25]
Chrysene	0.017	[25]
Benzo[b]fluoranthene	0.25	[25]
Benzo[k]fluoranthene	0.11	[25]
Benzo[a]pyrene	1	[25]
Indeno[1,2,3-cd]pyrene	0.1	[25]
Dibenzo[a,h]anthracene	1.1	[25]
Benzo[g,h,i]perylene	0.02	[25]

* = lower limit value used equivalent to TEF for naphthalene as TEF values for these PAHs not found in literature.

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