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In situ ozone production is highly sensitive to volatile organic compounds in Delhi, India

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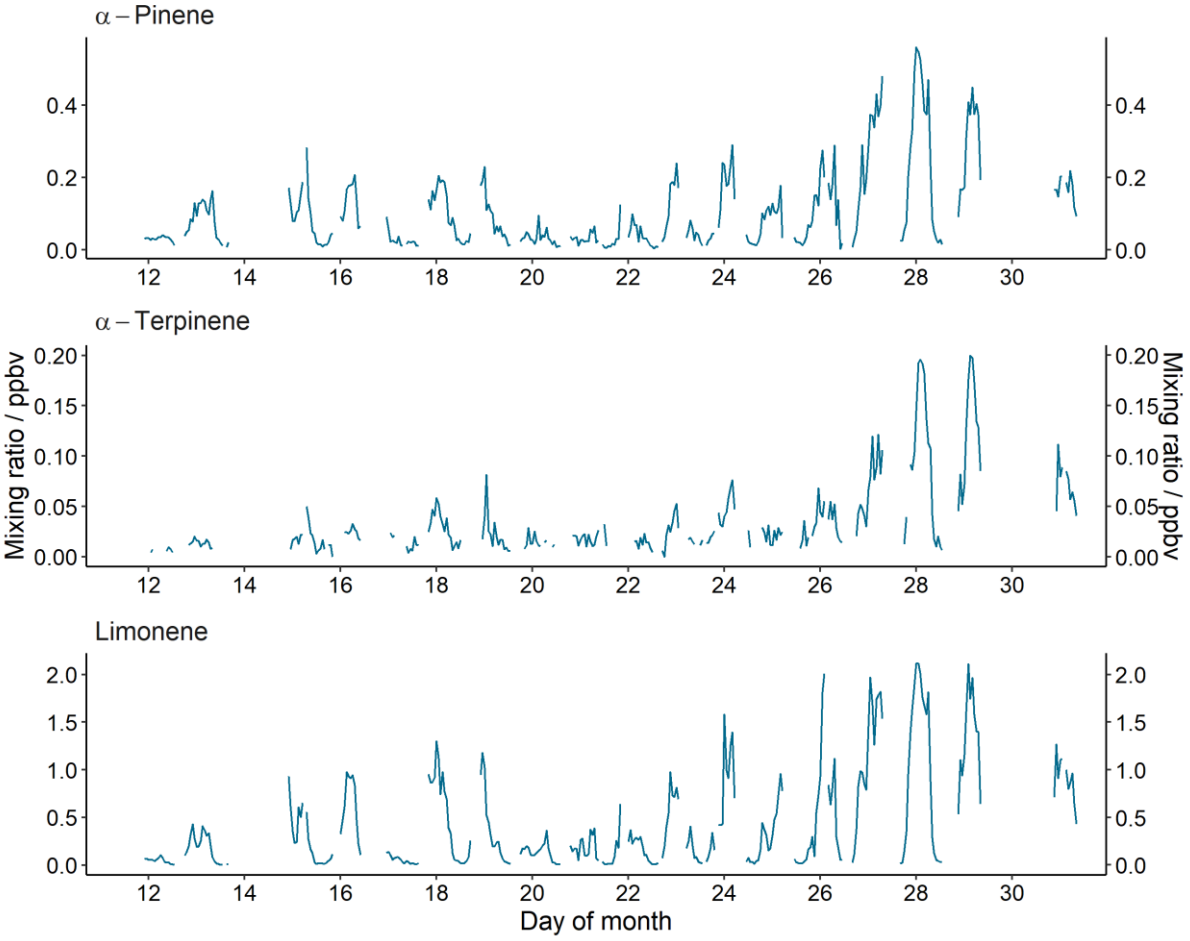

Figure S1: Selected timeseries for monoterpenes measured during October, 2018 at Indira Gandhi Delhi Technical University for Women. Top to bottom: α-pinene, α-terpinene, limonene.

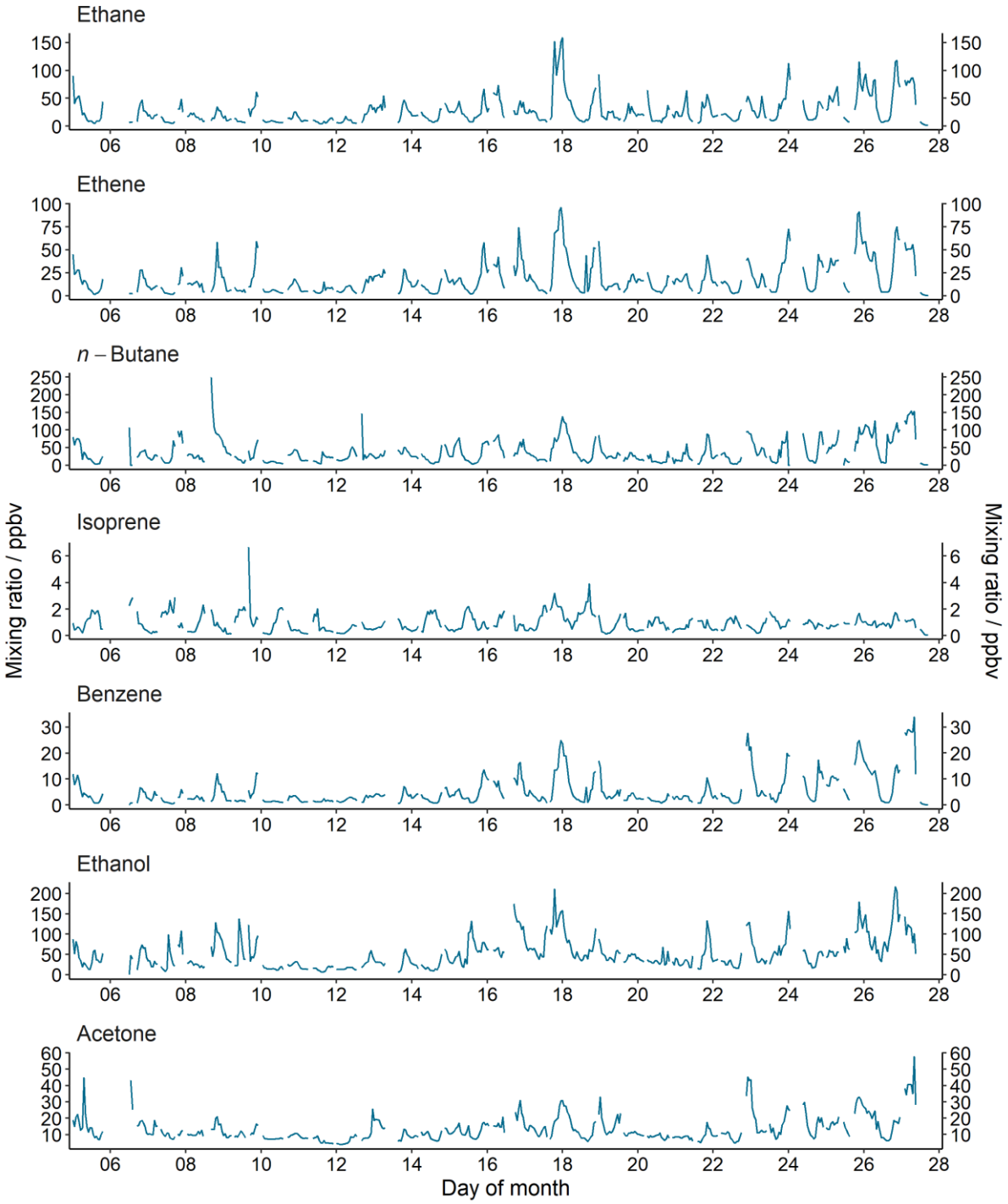

Figure S2: Selected timeseries for VOCs measured during October, 2018 at Indira Gandhi Delhi Technical University for Women. Top to bottom: ethane, ethene, *n*-butane, isoprene, benzene, ethanol, acetone.

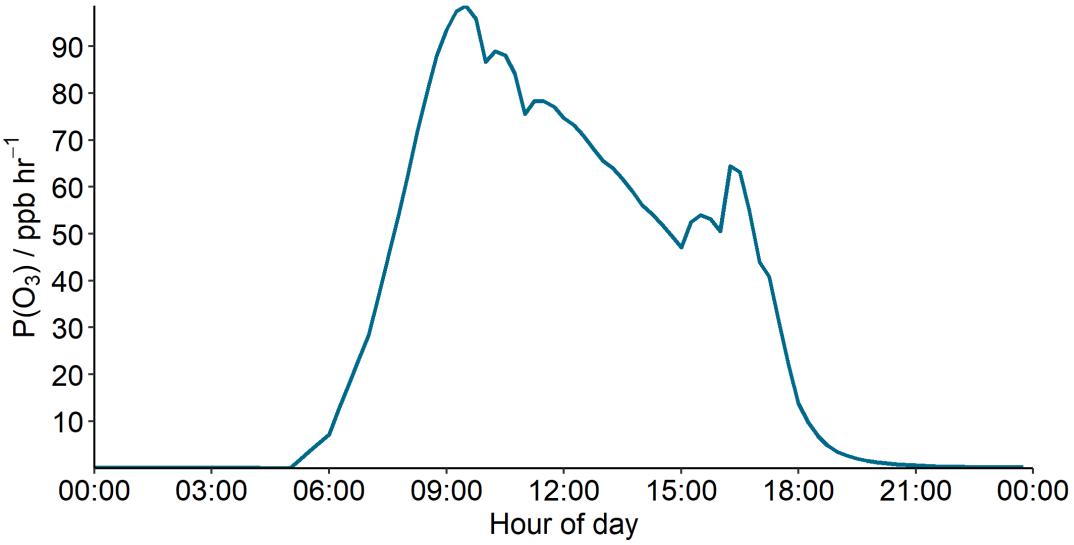

Figure S3: Diel profile of campaign averaged modelled ozone production, $P(O_3)$.

Table S1: List of VOCs included in model, along with campaign averaged mixing ratios and proxy mechanisms for species not found in the master chemical mechanism (MCM). Rate constants for additional species to those in the MCM can be found on the IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation database (http://iupac.pole-ether.fr/, last access: August 2018), originally published in Atkinson et al., 2006, or in Atkinson and Arey, 2003.

Species	Class	Campaign Average Mixing Ratios / ppbv			Proxy Mechanism used for species not in the MCM	Instrument
		Mean	Min.	Max.		
Ethanol	Alcohol	50.98	29.69	92	-	(DC)-GC-FID
Methanol		49.87	21.1	81.71	-	(DC)-GC-FID
Ethane	Alkane	27.09	7.09	51.63	-	(DC)-GC-FID
Isobutane		19.89	5.96	34.95	-	(DC)-GC-FID
Isopentane		15.86	3.97	36	-	(DC)-GC-FID
n-Butane		37.21	6.7	69.21	-	(DC)-GC-FID
n-Decane		1.07	0.2	1.99	-	GC × GC-FID
n-Dodecane		1.09	0.16	1.87	-	GC × GC-FID
n-Heptane		1.18	0.2	2.93	-	(DC)-GC-FID
n-Hexane		1.63	0.3	3.69	-	(DC)-GC-FID

n-Nonane		1.35	0.24	2.67	-	GC × GC-FID
n-Octane		0.54	0.09	1.33	-	(DC)-GC-FID
n-Pentane		6.05	1.4	13.48	-	(DC)-GC-FID
n-Tetradecane		1.42	0.41	2.28	*n*-Dodecane	GC × GC-FID
n-Tridecane		2.93	0.52	4.67	*n*-Dodecane	GC × GC-FID
n-Undecane		0.54	0.09	0.95	-	GC × GC-FID
Propane		39.12	9.84	68.95	-	(DC)-GC-FID
1,2-Butadiene	Alkene	0.28	0.07	0.45	1,3-Butadiene	(DC)-GC-FID
1,3-Butadiene		0.7	0.07	1.65	-	(DC)-GC-FID
But-1-ene		1.47	0.21	3.02	-	(DC)-GC-FID
cis-But-2-ene		1.03	0.2	2.19	-	(DC)-GC-FID
Ethene		18.34	3.14	39.82	-	(DC)-GC-FID
Isopropene		2.22	0.32	4.65	-	(DC)-GC-FID
Pent-1-ene		0.34	0.06	0.77	-	(DC)-GC-FID
Propene		5.26	0.64	11.3	-	(DC)-GC-FID
trans-But-2-ene		1.07	0.16	2.36	-	(DC)-GC-FID
trans-Pent-2-ene		0.53	0.09	1.4	-	(DC)-GC-FID
Acetylene	Alkyne	8.91	2.16	20.2	-	(DC)-GC-FID
Propyne		0.38	0.09	0.82	Acetylene	(DC)-GC-FID
1,2,3,4-Tetramethylbenzene	Aromatic	0.21	0.01	0.5	1,2,3-Trimethylbenzene	GC × GC-FID
1,2,3,5-Tetramethylbenzene		0.28	0.02	0.64	1,2,3-Trimethylbenzene	GC × GC-FID
1,2,3-Trimethylbenzene		0.64	0.06	1.48	-	GC × GC-FID
1,2,4,5-Tetramethylbenzene		0.16	0.02	0.32	1,2,4-Trimethylbenzene	GC × GC-FID
1,2,4-Trimethylbenzene		1.86	0.2	4.3	-	GC × GC-FID
1,2-Diethylbenzene		0.18	0.02	0.39	*o*-Ethyltoluene	GC × GC-FID
1,2-Dimethyl-4-ethylbenzene		0.35	0.02	0.84	3,5-Dimethyl-1-ethylbenzene	GC × GC-FID
1,3,5-Trimethylbenzene		0.61	0.05	1.41	-	GC × GC-FID
1,3-Diethyl-2-ethylbenzene		0.1	0.02	0.21	3,5-Dimethyl-1-ethylbenzene	GC × GC-FID
1,3-Diethylbenzene		0.2	0.02	0.44	*m*-Ethyltoluene	GC × GC-FID
1,4-Diethylbenzene		0.51	0.04	1.20	*p*-Ethyltoluene	GC × GC-FID
1-Methyl-3-propylbenzene		0.10	0.01	0.21	Propylbenzene	GC × GC-FID

1-Methyl-4-propylbenzene		0.14	0.01	0.33	Propylbenzene	GC × GC-FID
1-Methylpropylbenzene		0.17	0.02	0.36	Propylbenzene	GC × GC-FID
2,3-Dimethyl-1-ethylbenzene		0.09	0.01	0.22	3,5-Dimethyl-1-ethylbenzene	GC × GC-FID
2,4-Dimethyl-1-ethylbenzene		0.17	0.02	0.4	3,5-Dimethyl-1-ethylbenzene	GC × GC-FID
2-Methylpropylbenzene		0.16	0.02	0.36	Propylbenzene	GC × GC-FID
Benzene		5.26	1.15	10.05	-	(DC)-GC-FID
Ethylbenzene		2.09	0.36	4.88	-	(DC)-GC-FID
Isoproylbenzene		0.29	0.03	0.72	-	GC × GC-FID
m-Xylene		2.19	0.32	6.02	-	(DC)-GC-FID
n-Butylbenzene		0.51	0.04	1.2	Propylbenzene	GC × GC-FID
o-Ethyltoluene		0.65	0.08	1.47	-	GC × GC-FID
o-Xylene		1.85	0.3	4.86	-	(DC)-GC-FID
p-Ethyltoluene		1.78	0.27	4.13	-	GC × GC-FID
Propylbenzene		0.39	0.06	0.87	-	GC × GC-FID
p-Xylene		2.19	0.32	6.02	-	(DC)-GC-FID
Styrene		0.9	0.06	1.69	-	GC × GC-FID
Toluene		14.09	2.62	30.09	-	(DC)-GC-FID
Acetaldehyde	Carbonyl	8.3	2.93	11.89	-	PTR-QiTOF-MS
Acetone		13.24	7.44	18.64	-	(DC)-GC-FID
Cyclohexane		0.35	0.12	0.55	-	PTR-QiTOF-MS
Ethylacetate		8.48	2.04	14.14	-	GC × GC-FID
Formaldehyde		14.29	8.69	18.25	-	PTR-QiTOF-MS
Hexan-2-one		0.48	0.15	0.67	-	PTR-QiTOF-MS
Hexan-3-one		0.48	0.15	0.67	-	PTR-QiTOF-MS
Methacrolein		1.01	0.49	1.46	-	PTR-QiTOF-MS
Methyl isobutyl ketone		0.48	0.15	0.67	-	PTR-QiTOF-MS
Methyl propyl ketone		1.64	0.73	2.28	-	PTR-QiTOF-MS
Methyl vinyl ketone		3.59	1.2	5.29	-	PTR-QiTOF-MS
Isoprene	Isoprene	0.94	0.44	1.57	-	(DC)-GC-FID
α-Phellandrene	Monoterpene	0.09	0.02	0.15	α-Pinene	GC × GC-FID
3-Carene		0.08	0.02	0.15	α-Pinene	GC × GC-FID

Camphene		0.09	0.01	0.16	β-Pinene	GC × GC-FID
Limonene		0.38	0.02	0.79	-	GC × GC-FID
m-Cymene		0.53	0.04	1.03	*m*-Ethyltoluene	GC × GC-FID
Myrcene		0.08	0.01	0.14	Limonene	GC × GC-FID
o-Cymene		0.06	0.01	0.11	*o*-Ethyltoluene	GC × GC-FID
p-Cymene		0.53	0.04	1.03	*p*-Ethyltoluene	GC × GC-FID
Sabinene		0.06	0.02	0.13	β-Pinene	GC × GC-FID
Terpinolene		0.07	0	0.15	β-Pinene	GC × GC-FID
α-Pinene		0.09	0.01	0.18	-	GC × GC-FID
α-Terpinene		0.03	0.01	0.06	α-Pinene	GC × GC-FID
β-Ocimene		0.31	0.02	0.67	Limonene	GC × GC-FID
β-Pinene		0.05	0.01	0.09	-	GC × GC-FID
γ-terpinene		0.05	0.01	0.1	α-Pinene	GC × GC-FID

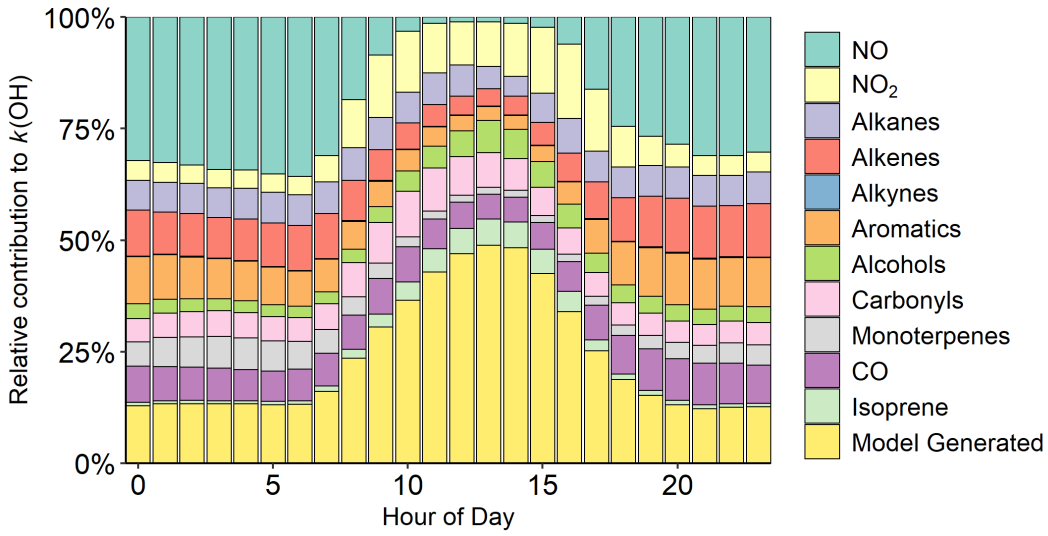

Figure S3: Relative contributions of NO, NO_2, CO, VOC classes and model generated species to *k*(OH) per hour.

Table S2: $\Delta P(O_3)_{increm}$ for 77 VOCs, averaged between 08:00 and 12:00. The 10 highest values are shown in **bold**.

Species	$\Delta P(O_3)_{increm}$ / ppb hr^{-1}
α-Phellandrene	**0.30**
α-Pinene	0.02
α-Terpinene	**0.66**
1,2-Butadiene	0.02
Benzene	0.02
β-Ocimene	**0.26**
β-Pinene	0.00
But-1-ene	0.12
Ethyne	0.00
Ethene	**0.40**
Ethanol	**0.30**
Ethane	0.01
Propyne	0.00
Propene	**0.35**
Propane	0.07
1,3-Butadiene	0.07
Isoprene	**0.94**
3-Carene	0.03
Cis-But-2-ene	0.19
Methanol	0.08
Camphene	0.01
CO	**0.28**
1,2-Diethylbenzene	0.01
1,3-Diethylbenzene	0.02
1,4-Diethylbenzene	0.02
1,2-Dimethyl-4-ethylbenzene	0.06
1,3-Dimethyl-2-ethylbenzene	0.03
2,3-Dimethyl-1-ethylbenezne	0.02
2,4-Dimethyl-1-ethylbenzene	0.03
Ethylbenzene	0.06

γ-Terpinene	0.03
Hex-2-one	0.00
Hex-3-one	0.00
Isobutane	0.15
Isopentane	0.14
Isopropylbenzene	0.01
Limonene	0.09
m-Cymene	0.03
1-Methyl-3-propylbenzene	0.00
1-Methyl-4-propylbenzene	0.00
1-Methylpropylbenzene	0.00
2-Methylpropylbenzene	0.00
Methylpropene	0.23
m-Xylene	0.21
Myrcene	0.08
n-Butylbenzene	0.02
n-Decane	0.01
n-Undecane	0.00
n-Dodecane	0.01
n-Tridecane	0.05
n-Tetradecane	0.04
n-Butane	0.21
n-Pentane	0.07
n-Hexane	0.01
n-Heptane	0.01
n-Octane	0.00
n-Nonane	0.01
o-Cymene	0.00
o-Ethyltoluene	0.04
o-Xylene	0.14
Propylbenzene	0.01
p-Cymene	0.02
Pent-1-ene	0.03

p-Ethyltoluene	0.08
p-Xylene	0.13
Sabinene	0.01
Styrene	0.01
trans-But-2-ene	0.22
1,2,3,4-Tetramethylbenzene	0.04
1,2,3,5-Tetramethylbenzene	0.06
1,2,4,5-Tetramethylbenzene	0.04
1,2,3-Trimethylbenzene	0.09
1,2,4-Trimethylbenzene	**0.29**
1,3,5-Trimethylbenzene	0.12
Toluene	**0.37**
trans-Pent-2-ene	0.11
Terpinolene	0.03

Table S3: Description of source sectors using in section 3.8. IPCC 1996 codes and descriptions taken from IPCC, 1996.

Source	**IPCC code (1996)**		**Description**
Road Transport (RT)	1A3b	1A3b	All combustion and evaporative emissions from fuel use in road vehicles, including agricultural vehicles on highways.
		i	Cars: automobiles designed primary for transport of persons, with a capacity of 12 or fewer. Gross vehicle weight rating of 3900 kg or less. Includes passenger vehicles with and without 3-way catalysts.
		ii	Light duty trucks: Vehicles with a gross vehicle weight of 3900 kg or less, designed primarily for the transportation of light-weight cargo or equipped with special features such as four-wheel drive for off-road operation. Includes light duty trucks with and without 3-way catalysts.
		iii	Heavy Duty trucks and buses: Any vehicle rated at more than 3900 kg gross vehicle weight or designed to carry more than 12 persons at a time.

		iv	Motorcycles: Any motor vehicle designed to travel with not more than three wheels in contact with the ground, and weighing less than 680 kg.
		v	Evaporative emissions from vehicles.
Railways, Pipelines and Off-Road Transport (RPORT)	1A3c+1A3e	1A3c	Fuel combustion emissions from railways, including both freight and passenger traffic routes.
		1A3e	Combustion emissions from all remaining transport activities including pipeline transportation, ground activities in airports and harbours, and off-road activities not reported under agriculture or manufacturing industries and construction.
Energy for Buildings (EB)	1A4	1A4a	Emissions from fuel combustion in commercial and institutional buildings.
		1A4b	All emissions from residential fuel combustion in households.
		1A4c	Emissions from fuel combustion in agriculture, forestry or domestic inland coastal and deep-sea fishing. Includes traction vehicles, pump fuel use, grain drying, horticultural greenhouse and other agriculture, forestry or fishing related fuel use.
Combustion for Manufacturing (CM)	1A2	1A2	Emissions from combustion of fuels in industry including combustion for the generation of electricity and heat.
		1A2a	Iron and steel.
		1A2b	Non-ferrous metals.
		1A2c	Chemicals.
		1A2d	Pulp, paper and print.
		1A2e	Food processing, beverages and tobacco.
		1A2f	Other emissions from fuel combustion in industry, including from the construction branch.
Process emissions (PE)	2	2A	Emissions from industrial processes: mineral products.
		2A1	Cement production.
		2A2	Lime production.
		2A3	Limestone and dolomite use.
		2A4	Soda ash production and use.
		2A5	Asphalt roofing.
		2A6	Road paving with asphalt.

		2A7	Other.
		2B	Emissions from chemical industry.
		2B1	Ammonia production.
		2B2	Nitric acid production.
		2B3	Adipic acid production.
		2B4	Carbide production.
		2B5	Other.
		2C	Emissions from metal production industry.
		2C1	Iron and steel production.
		2C2	Ferroalloys production.
		2C3	Aluminium production.
		2C4	SF_6 used in aluminium and magnesium foundries.
		2C5	Other.
		2D	Emissions from other production industries.
		2D1	Pulp and paper.
		2D2	Food and drink.
		2E	Production of halocarbons and sulfur hexafluoride.
		2E1	By-product emissions.
		2E2	Fugitive emissions.
		2E3	Other.
		2F	Consumption of halocarbons and sulfur hexafluoride.
		2F1	Refrigeration and air conditioning equipment.
		2F2	Foam blowing.
		2F3	Fire extinguishers.
		2F4	Aerosols.
		2F5	Solvents.
		2F5	Other.
		2G	Other emissions from industrial processes.
	3		Solvent and other product use. This category mainly covers volatile organic compound (VOC) emissions from solvents and other products containing VOCs.
		3A	Paint application.

		3B	Degreasing and dry cleaning.
		3C	Chemical products, manufacturing and processing.
		3D	Other, including the use of N_2O as a carrier gas, anaesthetic and propellant.

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