Supplement of

Bayesian Inference-Based Estimation of Hourly Primary and Secondary Organic Carbon at Suburban Hong Kong: Multi-temporal Scale Variations and Evolution Characteristics during PM$_{2.5}$ episodes

Shan Wang[1#], Kezheng Liao[2#], Zijing Zhang[1], Yuk Ying Cheng[2], Qiongqiong Wang[3, 2], Hanzhe Chen[1], and Jian Zhen Yu[1,2,*]

[1]Division of Environment and Sustainability, The Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China

15   [2]Department of Chemistry, The Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong, China

[3]School of Environmental Studies, China University of Geosciences, Wuhan, China

[#]These authors contributed equally to this work.

Corresponding to: Jian Zhen Yu (jian.yu@ust.hk)

20

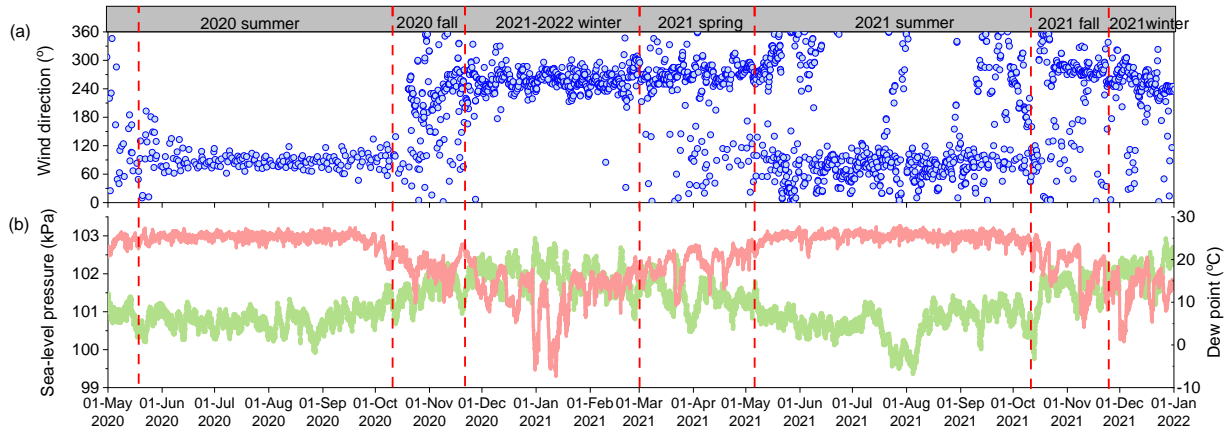
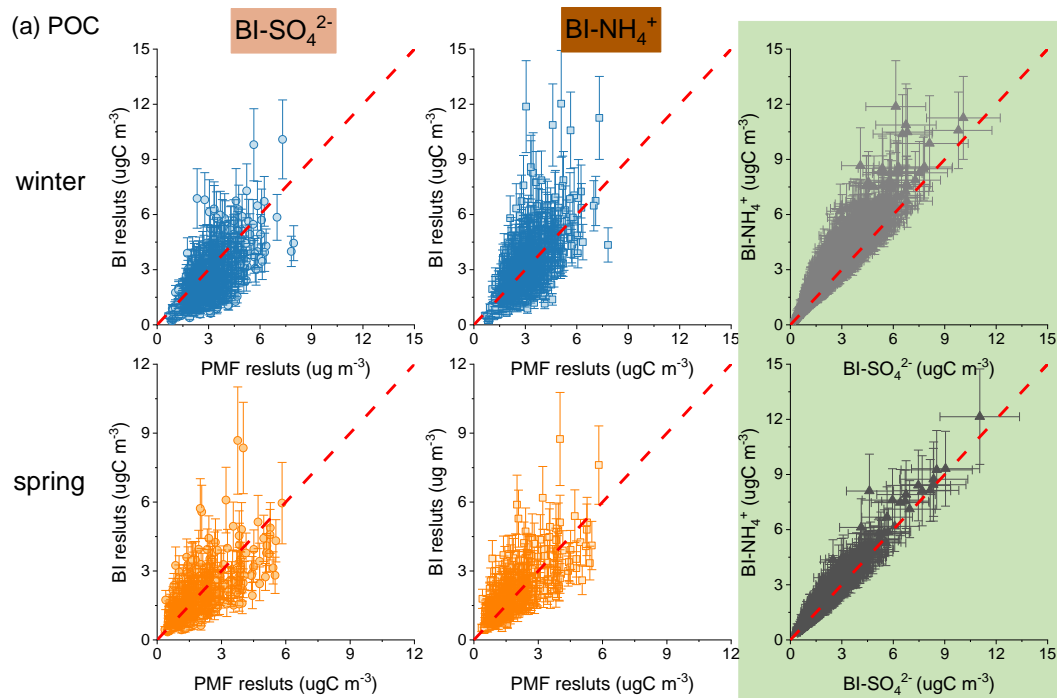



Figure S1. Time series of (a) upper wind direction at 15000 ± 1000 m height, and (b) sea-level pressure and dew point at Hong Kong Observatory station from 1 May 2021 to 31 December 2021.

25

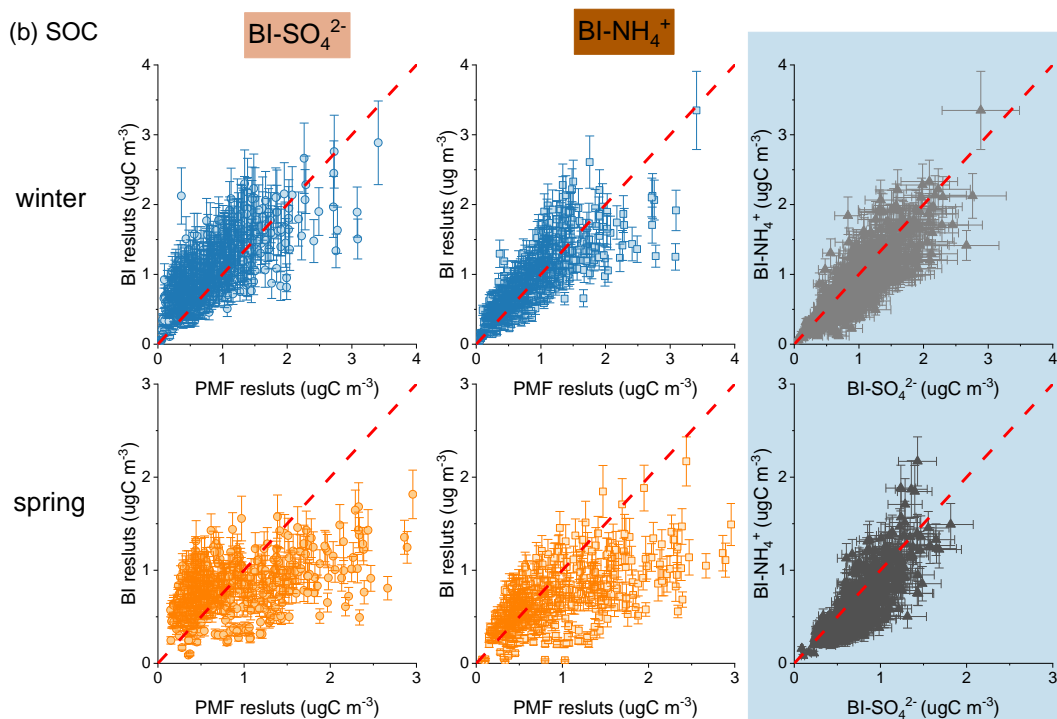



Figure S2. (a) POC and (b) SOC estimations for the HKUST winter (24 November 2020 – 28 February 2021) and spring (1 March -2 May 2021) data. Results comparison between PMF and BI with sulfate and ammonium as tracers for SOC.

30

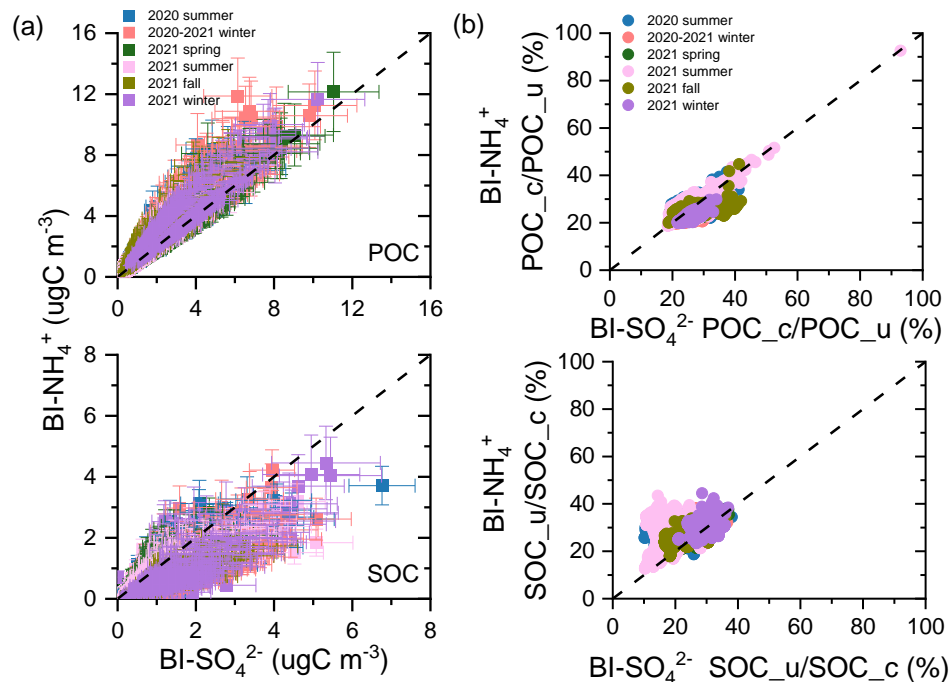



Figure S3. Comparison of (a) absolute concentration and uncertainty and (b) relative uncertainty of POC and SOC between BI with sulfate and ammonium as tracers for SOC.

35   **Table S1. Model performance evaluation metrics (Bayesian Inference Criterion, BIC)[a] for individual seasons using sulfate, nitrate and ammonium as tracers for SOC.**

Tracers / Period	SO_4^{2-}	NO_3^-	NH_4^+
2020 summer	**2247**	3150	2713
2020-2021 winter	**6266**	6768	7065
2021 spring	**10525**	10731	13450
2021 summer	15951	16491	**14511**
2021 fall	**2614**	3793	4117
2021 winter	**2445**	2449	2600
Entire	**40047**	43382	44456

[a]Note: bold numbers are the minimum values, represents the most optimal model performance.

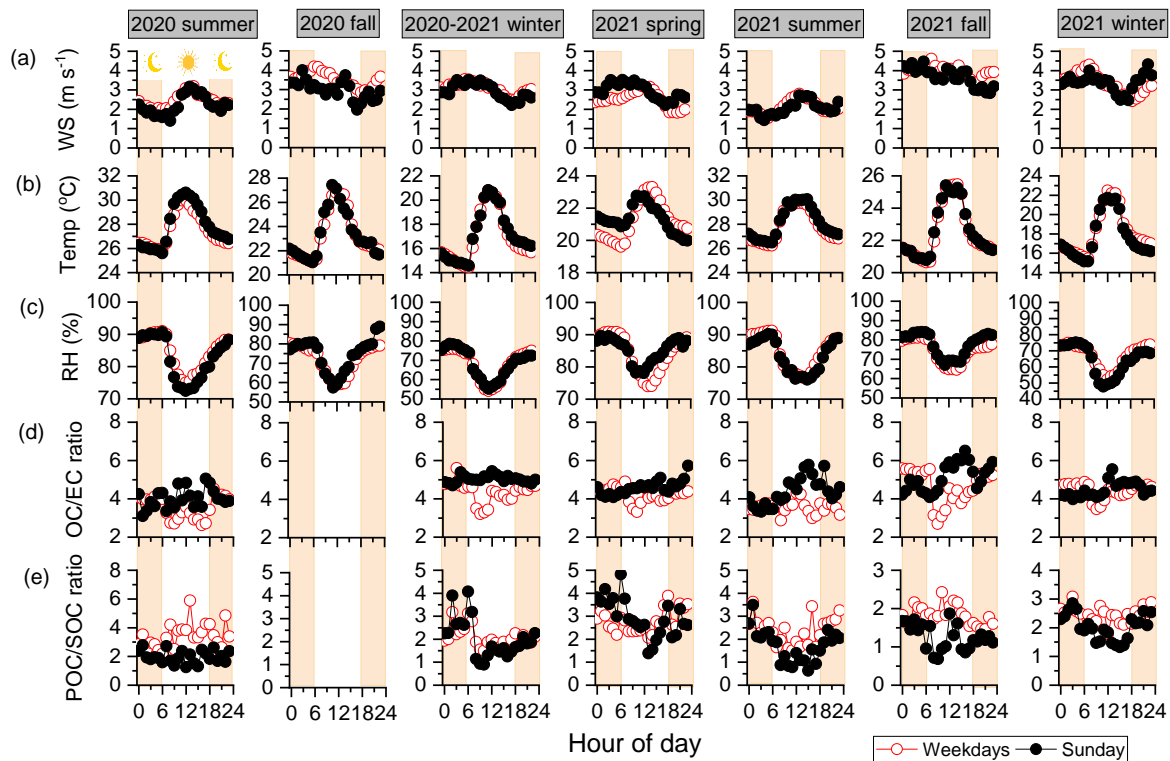



Figure S4. Diurnal variations of (a) wind speed, (b) temperature, (c) RH, and (d) OC/EC ratio and (e) POC/SOC ratio over the entire measurement period. The circles represent the hourly data averaged over weekdays (Monday -Saturday, red) and Sunday (black). The yellow shades represent nighttime periods.

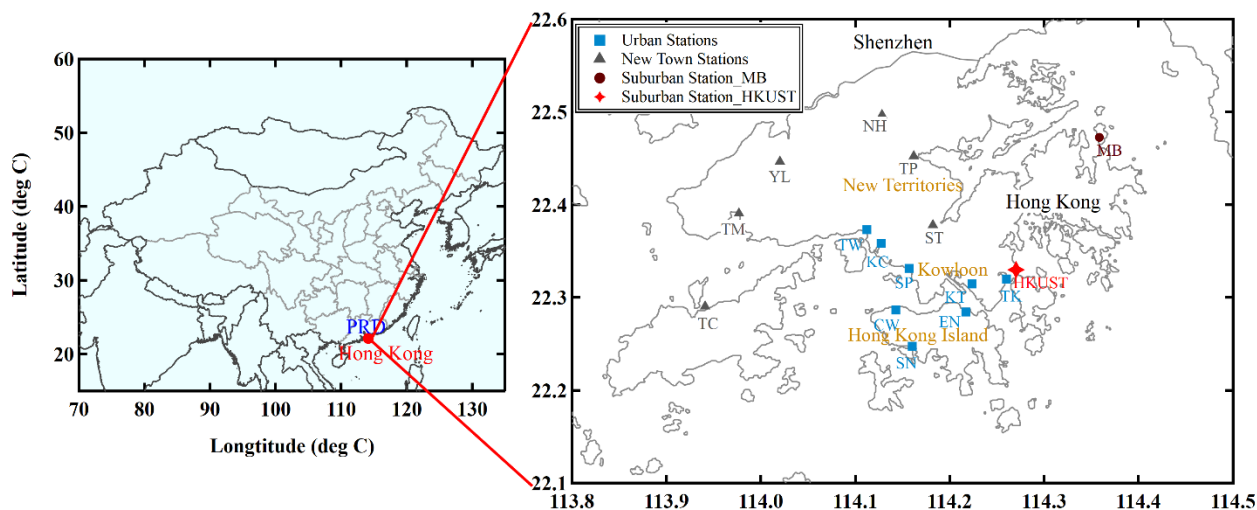



Figure S5. Geographical locations of the 15 HKEPD general air quality monitoring stations and the HKUST supersite.

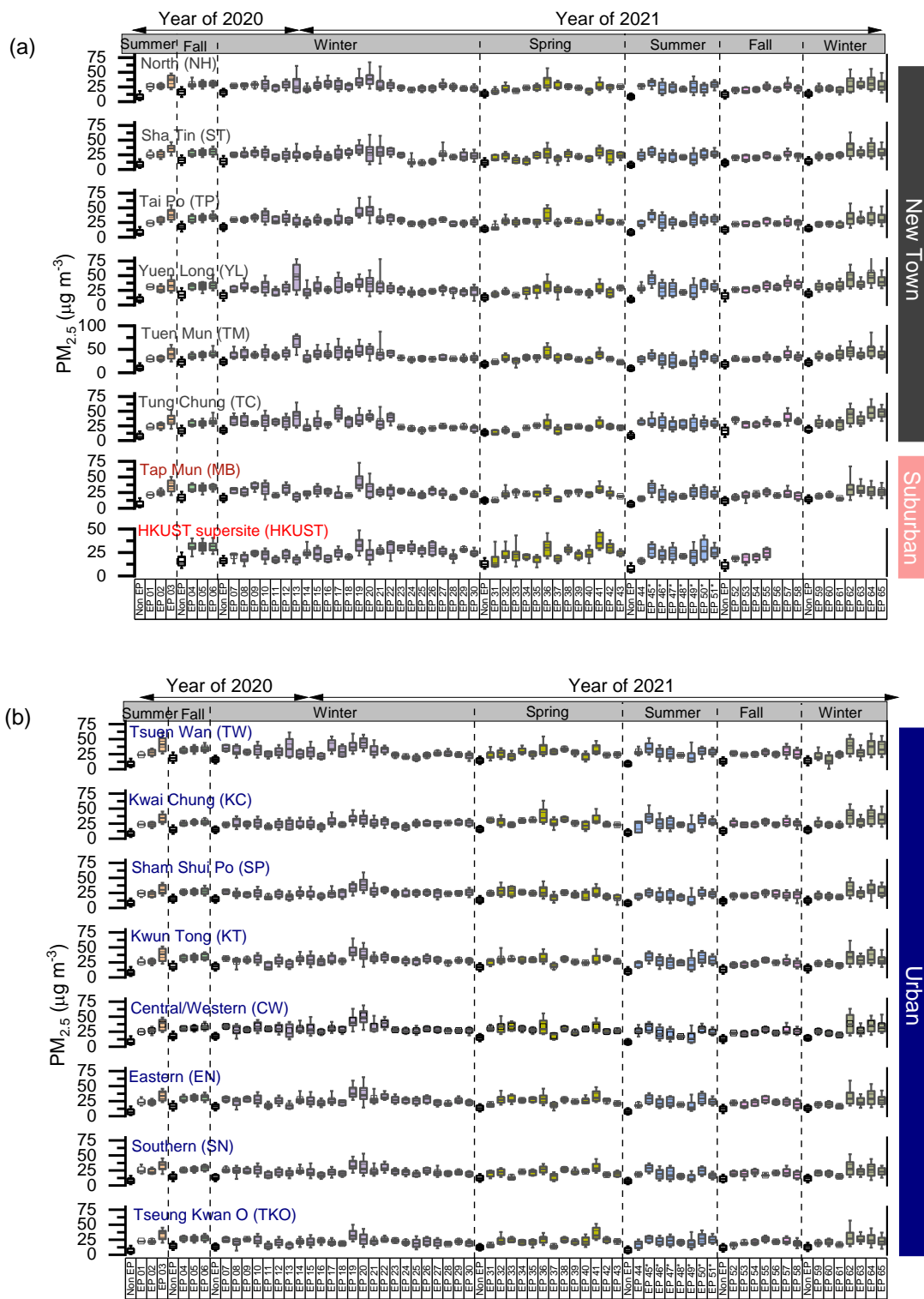



Figure S6. The average concentrations of PM$_{2.5}$ during individual episodes (solid pattern) and those during the non-episode hours in the same season (blank pattern) in the 15 HKEPD general air quality monitoring stations and the HKUST supersite in HK.

Table S2. Statistical summary of PM$_{2.5}$ at 15 Hong Kong EPD general air quality monitoring stations and the HKUST supersite during the 65 episodes and the remaining non-episode hours for the period from 16 July 2020 to 31 December 2021. Meteorological parameters and gas pollutant data are from the HKUST supersite. The NO$_x$ and O$_3$ at MB station were used as reference during the missing period.

Episode	Season	Time period (date, time)	Duration (h)	Wind speed (m s^{-1})	T (ºC)	RH (%)	O$_3$ (ppb)	NOx (ppb)	Mean PM$_{2.5}$ concentrations			
									City-wide	Min	Max	Max-to-min
EP01	2020 summer	21 Aug, 09:00-22 Aug, 22:00	38	1.71	28.9	78.6	33.4	4.8	24.9	21.1	31.0	1.5
EP02	2020 summer	29 Aug, 10:00-31 Aug, 23:00	38	1.64	29.4	76.2	58.7	5.4	25.7	22.1	30.1	1.4
EP03	2020 summer	01 Sep, 12:00-04 Sep, 23:00	84	1.36	29.5	79.2	60.2	7.1	36.0	30.9	41.7	1.3
Non-EP	2020 summer	16 July, 00:00-7 Oct, 23:00	1841	2.47	27.4	84.5	53.8	4.9	8.50	7.10	10.6	1.5
EP04	2020 fall	29 Oct, 19:00-30 Oct, 20:00	26	2.39	22.6	82.3	38.2	7.9	29.4	25.4	35.2	1.4
EP05	2020 fall	02 Nov, 09:00-04 Nov, 21:00	61	3.91	23.2	65.5	57.8	8.9	30.5	26.7	37.7	1.4
EP06	2020 fall	06 Nov, 11:00-10 Nov, 23:00	109	3.38	24.2	57.1	68.9	11	32.7	28.2	40.6	1.4
Non-EP	2020 fall	08 Oct, 00:00-23 Nov, 23:00	932	3.46	23.2	74.3	52.8	6.6	17.1	14.4	22.8	1.6
EP07	2020-2021 winter	24 Nov, 08:00-19:00	11	3.24	23.5	73.2	48.5	14	29.4	23.2	38.3	1.7
EP08	2020-2021 winter	26 Nov, 10:00-27 Nov, 03:00	18	2.01	23.2	79.1	59.8	8.0	27.7	20.2	38.8	1.9
EP09	2020-2021 winter	02 Dec, 19:00-03 Dec, 11:00	17	5.55	16.5	66.2	28.9	9.2	28.5	22.4	37.3	1.7
EP10	2020-2021 winter	05 Dec, 00:00-14 Dec 00:00	239	2.59	18.6	74.1	42.4	11	30.8	24.2	43.2	1.8
EP11	2020-2021 winter	17 Dec, 11:00-23:00	13	2.90	15.0	66.3	6.60	25	23.0	14.5	35.1	2.4
EP12	2020-2021 winter	19 Dec, 13:00-25 Dec 23:00	155	3.63	16.3	68.5	37.8	8.9	28.3	20.6	41.5	2.0
EP13	2020-2021 winter	27 Dec, 11:00-28 Dec, 11:00	25	1.89	20.5	58.0	61.5	5.1	29.3	15.6	65.8	4.2
EP14	2020-2021 winter	29 Dec, 00:00-30 Dec, 05:00	30	2.67	19.2	73.5	43.0	10	25.5	21.7	32.0	1.5
EP15	2020-2021 winter	03 Jan, 03:00-08 Jan, 23:00	141	3.44	14.4	64.0	45.6	8.1	29.1	22.6	42.2	1.9
EP16	2020-2021 winter	12 Jan, 00:00-23:00	24	5.52	11.4	22.0	40.4	10	25.1	17.2	41.5	2.4
EP17	2020-2021 winter	14 Jan, 05:00-23:00	19	1.81	15.0	45.7	64.7	12	30.5	20.4	47.8	2.3
EP18	2020-2021 winter	15 Jan, 15:00-16 Jan, 12:00	22	1.74	15.9	61.5	78.0	6.6	26.8	18.7	41.2	2.2
EP19	2020-2021 winter	16 Jan, 22:00-19 Jan, 11:00	62	3.57	14.0	56.7	54.6	7.7	39.2	33.1	49.2	1.5
EP20	2020-2021 winter	21 Jan, 22:00-24 Jan, 08:00	59	1.81	20.2	73.1	39.1	14	38.1	27.7	51.5	1.9
EP21	2020-2021 winter	25 Jan, 04:00-27 Jan, 21:00	66	1.76	17.6	78.5	56.2	9.3	30.9	22.7	44.1	1.9
EP22	2020-2021 winter	28 Jan, 08:00-23:00	16	3.16	20.3	55.1	60.0	7.9	31.7	25.2	41.1	1.6
EP23	2020-2021 winter	29 Jan, 21:00-30 Jan, 16:00	20	3.21	14.8	70.1	59.2	4.2	25.8	22.3	31.6	1.4
EP24	2020-2021 winter	02 Feb, 18:00-03 Feb, 11:00	18	3.78	16.3	78.2	57.8	3.7	22.4	12.8	28.5	2.2
EP25	2020-2021 winter	06 Feb, 10:00-08 Feb, 14:00	53	2.03	19.2	73.2	56.3	8.8	22.9	17.5	30.0	1.7
EP26	2020-2021 winter	09 Feb, 01:00-18:00	18	4.29	16.3	82.7	56.8	2.5	24.8	13.7	31.1	2.3
EP27	2020-2021 winter	14 Feb, 17:00-15 Feb, 13:00	21	1.51	20.6	60.9	51.8	9.5	25.9	19.7	32.1	1.6
EP28	2020-2021 winter	16 Feb, 20:00-17 Feb, 07:00	12	2.65	17.3	72.1	49.1	3.8	23.1	17.3	29.9	1.7
EP29	2020-2021 winter	17 Feb, 22:00-18 Feb, 23:00	26	3.06	16.6	68.6	49.5	3.7	24.8	21.7	29.9	1.4
EP30	2020-2021 winter	20 Feb, 12:00-22 Feb, 13:00	50	1.68	18.8	76.9	68.0	5.2	24.1	18.8	31.3	1.7
Non-EP	2020-2021 winter	24 Nov, 00:00-28 Feb, 23:00	1192	3.24	16.6	67.8	43.6	6.9	16.3	13.2	23.4	1.8
EP31	2021 spring	01 Mar, 20:00-02 Mar, 06:00	11	2.32	19.6	89.5	37.2	13	21.4	13.7	30.9	2.3
EP32	2021 spring	04 Mar, 20:00-05 Mar, 23:00	39	1.74	17.8	95.8	31.8	7.3	26.1	17.6	33.5	1.9
EP33	2021 spring	06 Mar, 09:00-20:00	12	1.34	18.9	99.9	34.5	5.5	22.6	9.60	34.1	3.6

EP34	2021 spring	14 Mar, 10:00-23:00	14	2.11	19.2	85.3	67.7	5.7	25.4	15.0	32.5	2.2
EP35	2021 spring	21 Mar, 07:00-14:00	8	4.57	20.3	74.0	18.6	12	25.8	20.8	32.5	1.6
EP36	2021 spring	22 Mar, 16:00-25 Mar, 23:00	80	2.60	19.0	64.6	45.7	14	31.7	25.8	41.9	1.6
EP37	2021 spring	04 Apr, 10:00-23:00	14	2.64	21.7	97.5	46.1	5.8	21.1	13.9	30.8	2.2
EP38	2021 spring	05 Apr, 19:00-07 Apr, 21:00	32	2.31	21.3	85.2	67.9	5.4	27.7	23.0	33.9	1.5
EP39	2021 spring	09 Apr, 21:00-10 Apr, 09:00	13	4.07	19.2	76.7	50.6	5.1	24.3	21.2	28.1	1.3
EP40	2021 spring	17 Apr, 10:00-21:00	12	1.80	21.1	93.3	53.4	7.3	22.6	18.0	29.3	1.6
EP41	2021 spring	18 Apr, 11:00-19 Apr, 16:00	30	4.67	20.9	72.2	80.1	5.5	31.6	26.8	39.1	1.5
EP42	2021 spring	23 Apr, 08:00-22:00	15	1.91	28.1	69.0	48.7	32	24.1	17.9	32.1	1.8
EP43	2021 spring	02 May, 00:00-12:00	13	1.26	25.1	78.4	46.0	13	23.0	16.6	29.4	1.8
Non-EP	2021 spring	01 Mar, 00:00-02 May, 23:00	1219	2.52	21.5	85.5	40.9	7.6	14.0	12.0	18.0	1.5
EP44	2021 summer	05 May, 14:00-23:00	10	2.18	26.0	81.5	70.3	19	23.0	15.2	31.0	2.0
EP45	2021 summer	05 June, 14:00-06 June, 23:00	34	1.65	27.2	73.3	81.4	18	32.8	25.3	44.5	1.8
EP46	2021 summer	23 July, 13:00-25 July, 16:00	52	1.50	29.7	78.2	71.3	17	24.0	19.6	29.3	1.5
EP47	2021 summer	27 July, 10:00-28 July, 17:00	32	1.15	30.4	78.6	43.9	19	23.1	18.6	27.2	1.5
EP48	2021 summer	06 Aug, 09:00-07 Aug, 13:00	20	1.49	28.0	87.7	26.5	25	21.1	16.0	26.9	1.7
EP49	2021 summer	11 Sep, 15:00-13 Sep, 18:00	52	1.35	31.0	76.5	51.4	16	21.6	13.4	29.8	2.2
EP50	2021 summer	17 Sep, 08:00-18 Sep, 03:00	20	1.67	28.9	83.5	79.6	7.7	28.8	21.8	36.5	1.7
EP51	2021 summer	27 Sep, 14:00-02 Oct, 03:00	110	1.43	28.7	81.2	55.3	11	26.7	16.1	31.8	2.0
Non-EP	2021 summer	03 May, 00:00-07 Oct, 23:00	3462	2.16	27.8	85.0	28.0	9.9	8.40	6.60	10.2	1.6
EP52	2021 fall	23 Oct, 15:00-23:00	9	3.44	19.8	75.6	20.4	21	22.8	16.0	35.6	2.2
EP53	2021 fall	27 Oct, 12:00-22:00	11	2.40	24.2	79.7	66.1	10	21.9	18.2	28.2	1.5
EP54	2021 fall	28 Oct, 12:00-29 Oct, 21:00	34	3.16	23.8	81.6	66.2	6.6	23.4	19.7	29.1	1.5
EP55	2021 fall	30 Oct, 10:00-01 Nov, 20:00	59	2.95	23.2	79.1	58.5	9.7	27.5	17.2	33.5	1.9
EP56	2021 fall	03 Nov, 10:00-04 Nov, 09:00	24	3.01	23.8	80.5	63.6	6.1	23.6	19.5	30.0	1.5
EP57	2021 fall	15 Nov, 22:00-18 Nov, 04:00	55	2.67	21.7	73.9	39.2	8.7	28.3	20.8	39.8	1.9
EP58	2021 fall	18 Nov, 17:00-20 Nov, 07:00	39	2.15	21.5	79.1	43.1	6.5	24.3	17.4	34.5	2.0
Non-EP	2021 fall	08 Oct, 00:00-24 Nov, 23:00	897	4.23	22.5	74.1	35.1	5.6	13.2	11.3	18.0	1.6
EP59	2021 winter	24 Nov, 14:00-27 Nov, 06:00	65	2.56	19.9	61.8	38.9	10	24.0	19.1	35.1	1.8
EP60	2021 winter	27 Nov, 18:00-01 Dec, 04:00	83	3.82	20.5	61.6	39.9	8.5	23.0	16.6	32.7	2.0
EP61	2021 winter	09 Dec, 14:00-10 Dec, 11:00	21	2.34	18.6	75.8	36.3	7.3	22.4	15.0	39.5	2.6
EP62	2021 winter	11 Dec, 15:00-15 Dec, 02:00	84	2.45	19.4	72.5	44.9	8.4	36.6	30.0	46.4	1.6
EP63	2021 winter	18 Dec, 19:00-20 Dec, 16:00	64	4.43	15.9	58.0	34.6	8.4	29.3	23.3	37.9	1.6
EP64	2021 winter	23 Dec, 19:00-26 Dec, 19:00	73	3.08	17.0	81.2	22.4	11	36.9	26.6	54.4	2.0
EP65	2021 winter	27 Dec, 12:00-31 Dec, 23:00	108	2.72	15.9	75.3	24.5	13	32.7	23.6	48.2	2.0
Non-EP	2021 winter	25 Nov, 00:00-31 Dec, 23:00	414	3.63	18.1	63.2	36.2	7.2	15.0	11.9	21.7	1.8

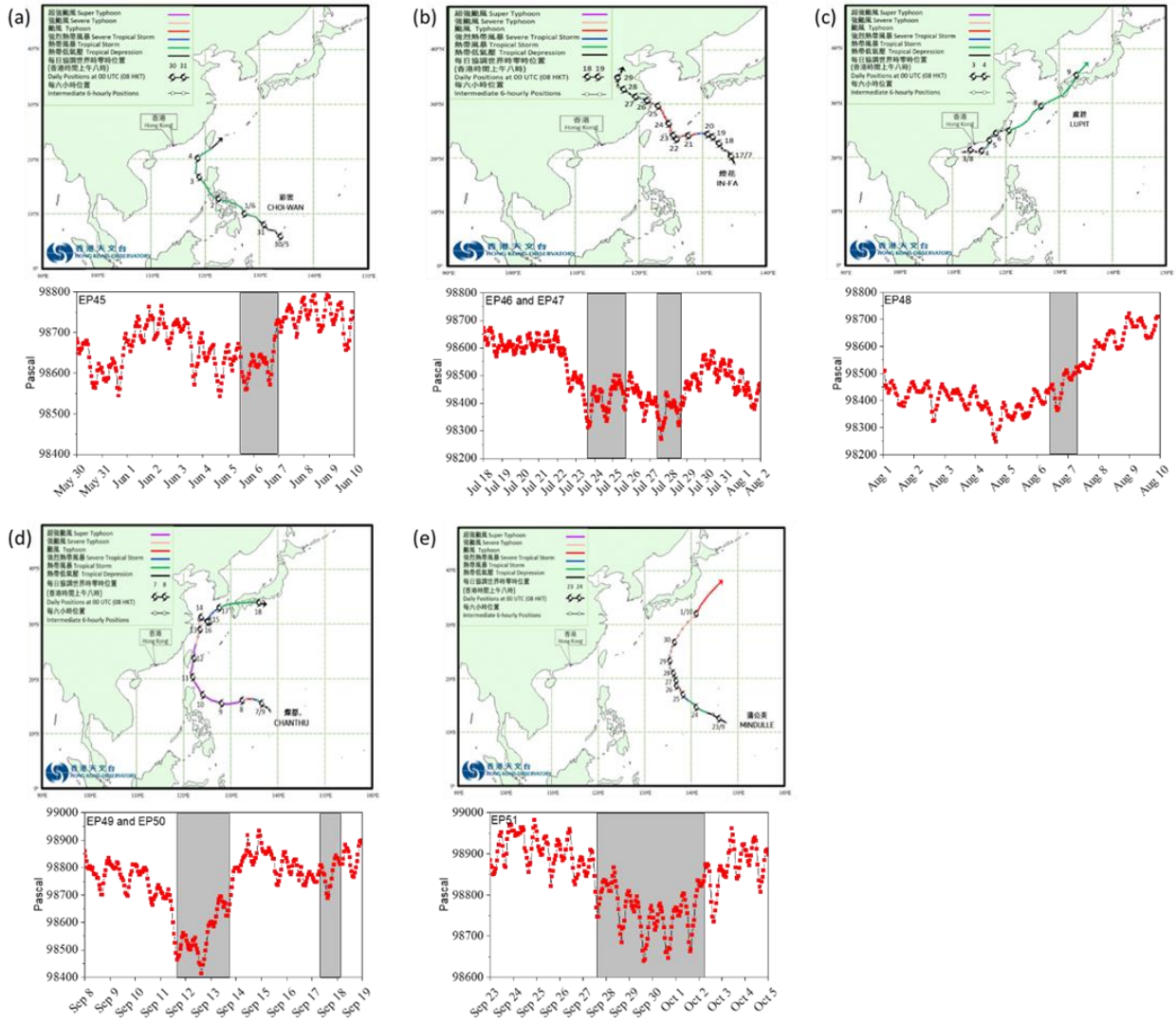



Figure S7. The provisional tropical cyclone tracks of (a) Chaiwan, (b) Infa, (c) Lupit, (d) Chanthu and (e) Mindule together with the corresponding atmospheric pressure (pascal) at the HKUST supersite. The episode period is indicated by the grey area. The tropical cyclone tracks are downloaded from Hong Kong Observatory website.

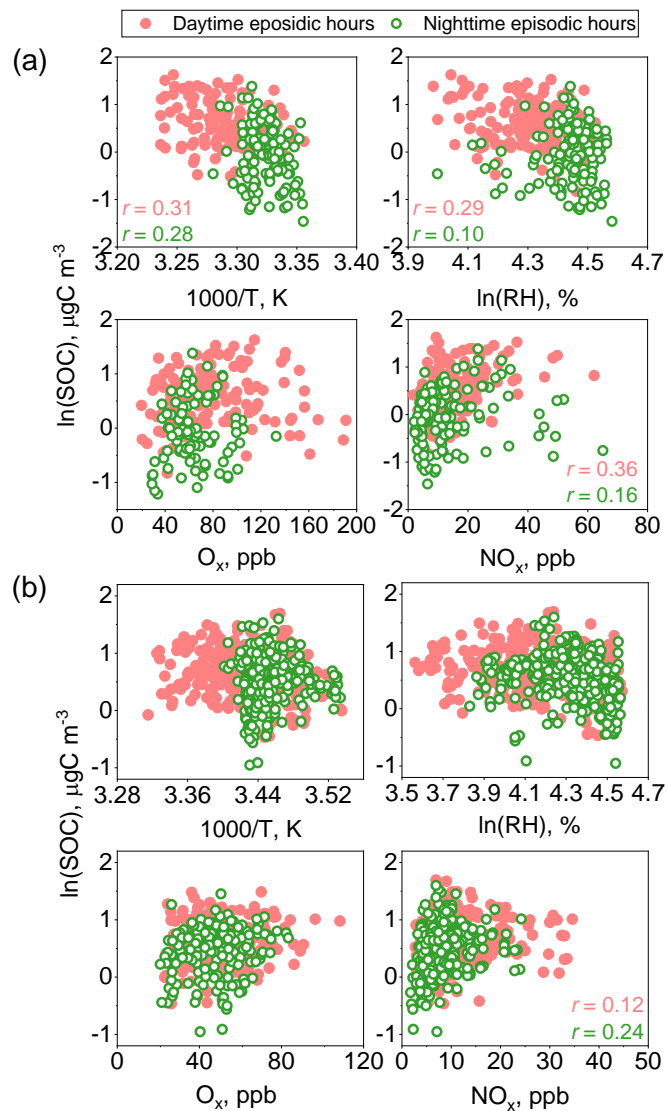



Figure S8. Scatter plot of SOC with meteorological parameters (i.e., temperature and RH), and oxidants (i.e., O_x and NO_x) during the episodic hours in (a) summer typhoon episodes and (b) winter haze episodes. The solid red circle represents daytime hours, blank green circle represents nighttime hours.

Table S3. Statistical summary of aerosol water content and [H⁺] during the summer typhoon episodes and winter haze episodes during the daytime and nighttime, respectively.

Episodes	Day/night	AWC ($\mu g\ m^{-3}$)	[H⁺] ($mol\ m^{-3}$)
Summer typhoon episodes	Day	12.5 ± 8.34	1.70 ± 1.20 E-10
Summer typhoon episodes	Night	23.1 ± 23.4	1.49 ± 1.00 E-10
Winter haze episodes	Day	6.36 ± 6.60	7.51 ± 1.80 E-11
Winter haze episodes	Night	8.86 ± 8.47	1.54 ± 9.72 E-10

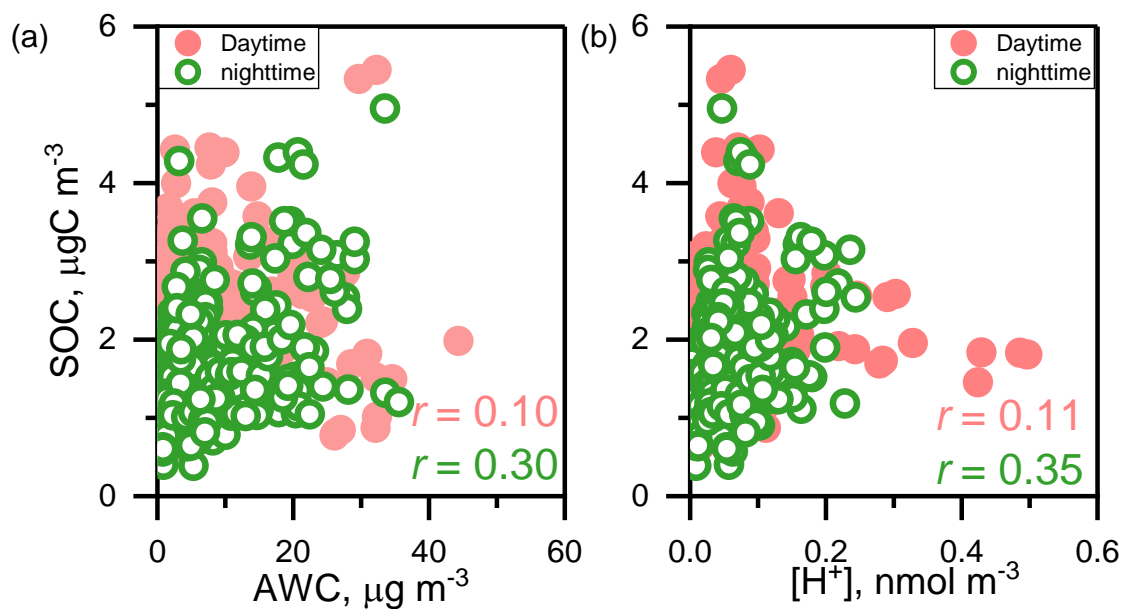



Figure S9. Scatter plot of SOC with (a) aerosol water contents (AWC) and (b) [H⁺] during the winter haze episodes. The solid red circle represents daytime hours, blank green circle represents nighttime hours.