

Supplemental Material

Classifying Organic Materials by Oxygen-to-Carbon Elemental Ratio to Predict the Activation Regime of Cloud Condensation Nuclei (CCN)

by

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Table S1 Effective density ρ_{eff} of particles generated by homogeneous nucleation. The values of ρ_{eff} were measured using a DMA-APM system.

Compound	d_p (nm)	ρ_{eff} (kg m ⁻³)
adipic acid	250	990
	280	890
pimelic acid	100	1040
	120	1030
	160	1090

Table S2 The results of CCN activity measurements of pure crystalline organic particles. The values of κ (spherical shape assumption) were calculated using the set point mobility diameter of the DMA. Particle shapes were corrected using ρ_{eff} quantified using the DMA-APM system, obtaining volume equivalent diameters.

compound	$S(\%)$	d_p (nm)	κ (spherical shape assumption)	κ (non-spherical shape)
adipic acid	0.54	287	0.002	0.003 ^a
	0.74	246	0.002	0.002 ^a
	1.04	200	0.002	0.002 ^a
pimelic acid	0.16	165	0.12	0.15 ^b
	0.30	111	0.11	0.14 ^b
	0.37	91	0.13	0.16 ^b
suberic acid	0.96	240	0.001	NA
azelaic acid	0.13	299	0.03	NA
	0.73	113	0.02	NA
	1	78	0.03	NA
pinonic acid	0.54	165	0.01	NA
	0.70	135	0.02	NA

^a ρ_{eff} was assumed as 950 kg m⁻³, based on DMA-APM measurement.

^b ρ_{eff} was assumed as 1050 kg m⁻³, based on DMA-APM measurement.

Table S3 The list of parameters of each compound employed in developing Table 3. The values of C_{sat} are taken from Petters et al (2009).

Category	Compound	Formula	MW	O:C	H:C	ρ (kg m ⁻³)	C_{sat} (v/v) ^a	κ	Source
Dicarboxylic acids	Oxalic acid	C ₂ H ₂ O ₄	90	2.000	1.000	1900	1.3	0.315	(Kumar et al., 2003)
	Malonic acid	C ₃ H ₄ O ₄	104	1.333	1.333	1630	9.9×10 ⁻¹	0.223	(Kumar et al., 2003)
	Succinic acid	C ₄ H ₆ O ₄	118	1.000	1.500	1552	5.7×10 ⁻²	0.22	(Corrigan and Novakov, 1999)
	Malic acid	C ₄ H ₆ O ₅	134	1.250	1.500	1595	9.1×10 ⁻¹	0.236	(Hori et al., 2003)
	Glutaric acid	C ₅ H ₈ O ₄	132	0.800	1.600	1429	8.1×10 ⁻¹	0.173	(Kumar et al., 2003)
	Adipic acid	C ₆ H ₁₀ O ₄	146	0.667	1.667	1362	1.8×10 ⁻²	0.002	This study
	Pimelic acid	C ₇ H ₁₂ O ₄	160	0.571	1.714	1321	5.1×10 ⁻²	0.15	This study
	Suberic acid	C ₈ H ₁₄ O ₄	174	0.500	1.750	1272	1.9×10 ⁻³	0.001	This study
Azelaic acid	C ₉ H ₁₆ O ₄	188	0.444	1.778	1251	4.0×10 ⁻³	0.025	This study	
Benzoic acids	2-acetylbenzoic acid	C ₉ H ₈ O ₃	164	0.333	0.889	1362	2.9×10 ⁻³	0.035	(Hartz et al., 2006)
	Homophthalic acid	C ₉ H ₈ O ₄	180	0.444	0.889	1410	3.3×10 ⁻⁴	0.037	(Hartz et al., 2006)
	Isophthalic acid	C ₈ H ₆ O ₄	166	0.500	0.750	1530	5.2×10 ⁻⁵	0.001 ^b	(Hartz et al., 2006)
	Phthalic acid	C ₈ H ₆ O ₄	166	0.500	0.750	1593	2.6×10 ⁻³	0.007	(Hartz et al., 2006)
	4-methylphthalic acid	C ₉ H ₈ O ₄	180	0.444	0.889	1410	2.8×10 ⁻³	0.046	(Hartz et al., 2006)
	Salicylic acid	C ₇ H ₆ O ₃	138	0.429	0.857	1443	1.8×10 ⁻³	0.008	(Hartz et al., 2006)

Carbohydrates	Erythritol	C ₄ H ₁₀ O ₄	122	1.000	2.500	1451	4.4×10 ⁻¹	0.165	(Petters et al., 2009)
	Threitol	C ₄ H ₁₀ O ₄	122	1.000	2.500	1451	4.4×10 ⁻¹	0.14	(Petters et al., 2009)
	Erythronic acid γ lactone	C ₄ H ₆ O ₄	118	1.000	1.500	N/A	>1.0×10 ⁻¹	0.125	(Petters et al., 2009)
	Xylitol	C ₅ H ₁₂ O ₅	152	1.000	2.400	1525	>1.0×10 ⁻¹	0.165	(Petters et al., 2009)
	Lyxose	C ₅ H ₁₀ O ₅	150	1.000	2.000	N/A	>1.0×10 ⁻¹	0.155	(Petters et al., 2009)
	Ribonic acid γ lactone	C ₅ H ₈ O ₅	148	1.000	1.600	N/A	>1.0×10 ⁻¹	0.205	(Petters et al., 2009)
	Mannitol	C ₆ H ₁₄ O ₆	182	1.000	2.333	1489	>1.0×10 ⁻¹	0.1	(Petters et al., 2009)
	Fructose	C ₆ H ₁₂ O ₆	180	1.000	2.000	1600	2.6×10 ¹	0.17	(Rosenorn et al., 2006).
	Glucose	C ₆ H ₁₂ O ₆	180	1.000	2.000	1566	5.8×10 ⁻¹	0.17	(Rosenorn et al., 2006).
	Mannose	C ₆ H ₁₂ O ₆	180	1.000	2.000	1539	1.6×10 ¹	0.17	(Rosenorn et al., 2006).
	Levoglucofan	C ₆ H ₁₀ O ₅	162	0.833	1.667	1618	>1.0×10 ⁻¹	0.185	(Rosenorn et al., 2006).
	Seduheptulose	C ₇ H ₁₄ O ₇	210	1.000	2.000	N/A	>1.0×10 ⁻¹	0.135	(Petters et al., 2009)
	Methyl- α glucose pyranoside	C ₇ H ₁₄ O ₆	194	0.857	2.000	N/A	>1.0×10 ⁻¹	0.14	(Petters et al., 2009)
	Sucrose	C ₁₂ H ₂₂ O ₁₁	342	0.917	1.833	1538	1.3	0.095	(Petters et al., 2009)
	Maltose	C ₁₂ H ₂₂ O ₁₁	342	0.917	1.833	N/A	6.1×10 ⁻²	0.055	(Rosenorn et al., 2006).
Fatty acids	Myristic acid	C ₁₄ H ₂₈ O ₂	228	0.143	2.000	866	2.3×10 ⁻⁵	0.001 ^b	(Raymond and Pandis, 2002)
	Palmitic acid	C ₁₆ H ₃₂ O ₂	256	0.125	2.000	853	8.2×10 ⁻⁶	0.001 ^b	(Raymond and Pandis,

	Oleic acid	$C_{18}H_{34}O_2$	282	0.111	1.889	890	N/A	0.0007 _b	2002) (Shilling et al., 2007)
	Stearic acid	$C_{18}H_{36}O_2$	284	0.111	2.000	847	3.5×10^{-6}	0.001 _b	(Raymond and Pandis, 2002)
Water-soluble polymers	Triethylene glycol	$C_6H_{14}O_4$	150	0.667	2.333	1100	∞ (miscible)	0.24	(Petters et al., 2009)
	Tetraethylene glycol	$C_8H_{18}O_5$	194	0.625	2.250	1250	∞ (miscible)	0.17	(Petters et al., 2009)
	Pentaethylene glycol	$C_{10}H_{22}O_6$	238	0.600	2.200	1250	∞ (miscible)	0.059	(Petters et al., 2009)
	Hexaethylene glycol	$C_{12}H_{26}O_7$	282	0.583	2.167	1270	∞ (miscible)	0.079	(Petters et al., 2009)
	Polyethylene glycol	$(C_2H_4O)_n$	400	0.500	2.000	1230	∞ (miscible)	0.078	(Petters et al., 2009)
	Polyethylene glycol	$(C_2H_4O)_n$	1000	0.500	2.000	1230	∞ (miscible)	0.049	(Petters et al., 2009)
	Polyethylene glycol	$(C_2H_4O)_n$	2050	0.500	2.000	1230	∞ (miscible)	0.048	(Petters et al., 2009)
	Polyacrylic acid	$(C_3H_4O_2)_n$	2000	0.667	1.333	1540	∞ (miscible)	0.054	(Petters et al., 2009)
Other	Pinonic acid	$C_{10}H_{16}O_3$	184	0.300	1.600	1169	6.1×10^{-3}	0.01	This study
	Hexadecane	$C_{16}H_{34}$	226	0.000	2.125	773	1.2×10^{-9}	0.001 _b	(Raymond and Pandis, 2002)

Hexadecanol	C ₁₆ H ₃₄ O	242	0.063	2.125	830	3.6×10 ⁻⁸	0.001 ^b	(Raymond and Pandis, 2002)
Cholesterol	C ₂₇ H ₄₆ O	387	0.037	1.704	1030	9.7×10 ⁻⁷	0.001 ^b	(Hartz et al., 2006)

^a The values of C for some compounds are not accurately known. In developing Figure 3, C was assumed as 1×10^{-1} for some carbohydrates, following Petters et al. (2009). Soluble polymers are miscible with water; C of those compounds were assumed as unity in Figure 3 for presentation purpose.

^b CCN activation was not observed. Those values correspond to the maximum estimation.

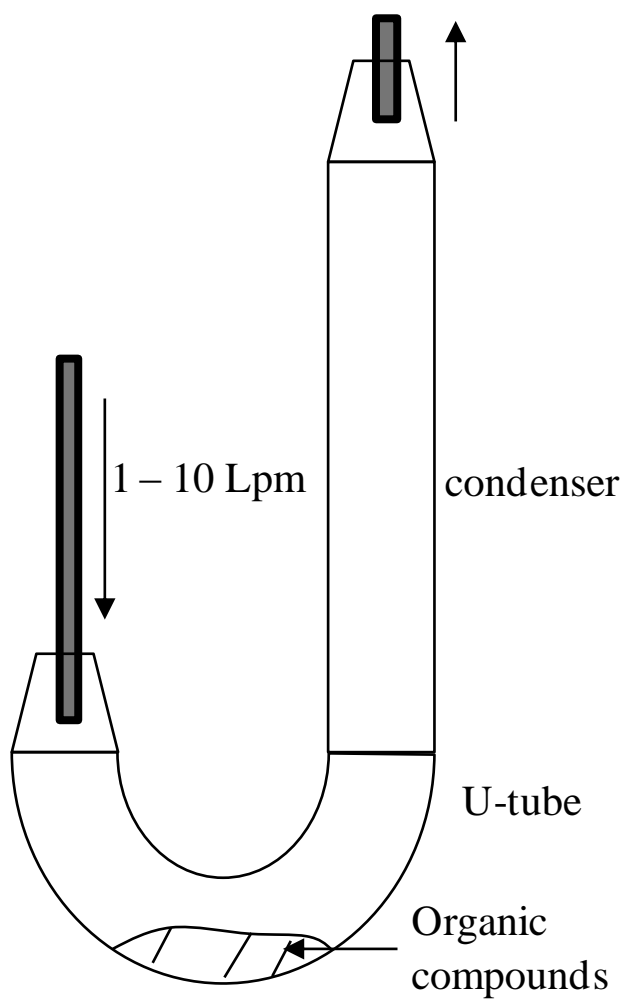


Figure S1 Homogeneous nucleation particle generator employed to generate particles of pure organic compounds.

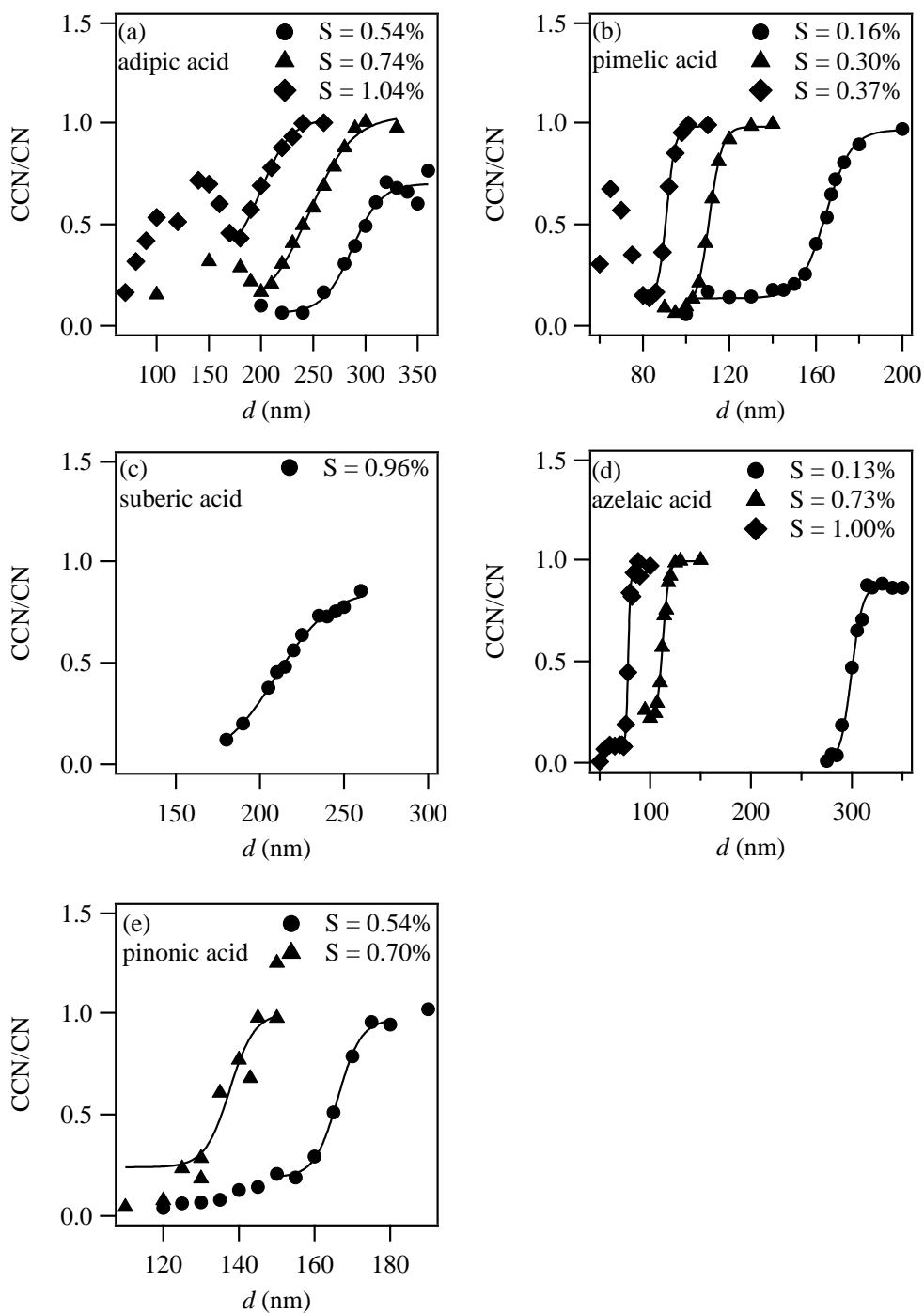


Figure S2 CCN activation curves measured for the pure compounds.

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