

Supplemental information for “Secondary organic aerosol yields of 12-carbon alkanes”

C. L. Loza, J. S. Craven, L. D. Yee, M. M. Coggon, R. H. Schwantes, M. Shiraiwa, X. Zhang, K. A. Schilling, N. L. Ng, M. R. Canagaratna, P. J. Ziemann, R. C. Flagan, and J. H. Seinfeld

Contains Tables S1-5 and Figure S1.

Table S1: CO⁺-to-CO₂⁺ ratios calculated from “W-mode” used in HR-AMS fragmentation table.

Expt.	CO ⁺ /CO ₂ ⁺	Change in CO ⁺ from CO ⁺ = CO ₂ ⁺ (%)
ML1	1.0	0
ML2	1.0	0
ML3	N/A ^a	N/A
DL1	N/A ^a	N/A
DL2	1.0	0
HL1	1.0	0
HL2	1.7	4-8
CL1	1.0	0
CL2	2.3	10-15
CL3	2.6	10-15
DH1	0.45	-(5-10)
DH2	1.0 ^b	0
DH3	1.0 ^b	0
MH1	3.5	30
MH2	1.4	3-7
HH1	1.3	4-5
HH2	1.3	3-5
CH1	1.9	10-15
CH2	2.4	10-15

^aThe AMS was not run on this experiment.

^bThe AMS was run in “V-mode” only. A ratio of unity was used.

Table S2: Low-NO_x experimental details for combined experiments.

Expt.	Irradiation (h)	Alkane	Seed vol. (μm ³ cm ⁻³)	HC _o (ppbv)
ML2a	18	2-methylundecane	16.7 ± 5.0	27.3 ± 0.9
ML2b	36	2-methylundecane	15.5 ± 4.5	29.8 ± 1.0
DL2a	18	dodecane	12.1 ± 3.6	33.0 ± 1.1
DL2b	36	dodecane	13.1 ± 3.9	34.9 ± 1.1
HL1a	18	hexylcyclohexane	11.2 ± 3.4	16.2 ± 0.5
HL2b	36	hexylcyclohexane	4.2 ± 1.3	14.9 ± 0.5
CL2a	18	cyclododecane	15.3 ± 4.6	9.8 ± 0.3
CL2b	36	cyclododecane	15.8 ± 4.7	11.0 ± 0.4

Table S3: Mass-to-charge ratios (m/z) monitored using the CIMS, and their proposed chemical assignments.

m/z	Ion	Molecular Wt.	Formula	Family
123	[R·F] ⁻	104	C ₄ H ₈ O ₃	C _n H _{2n} O ₃
135	[R·F] ⁻	116	C ₆ H ₁₂ O ₂	C _n H _{2n} O ₂
149	[R·F] ⁻	130	C ₇ H ₁₄ O ₂	C _n H _{2n} O ₂
151	[R·F] ⁻	132	C ₆ H ₁₂ O ₃	C _n H _{2n} O ₃
163	[R·F] ⁻	144	C ₈ H ₁₆ O ₂	C _n H _{2n} O ₂
165	[R·F] ⁻	146	C ₇ H ₁₄ O ₃	C _n H _{2n} O ₃
177	[R·F] ⁻	158	C ₉ H ₁₈ O ₂	C _n H _{2n} O ₂
191	[R·F] ⁻	172	C ₁₀ H ₂₀ O ₂	C _n H _{2n} O ₂
204	[R·CF ₃ O] ⁻	119	C ₃ H ₅ NO ₄	C _n H _{2n-1} NO ₄
205	[R·F] ⁻	186	C ₁₁ H ₂₂ O ₂	C _n H _{2n} O ₂
206	[R·CF ₃ O] ⁻	121	C ₃ H ₇ NO ₄	C _n H _{2n+1} NO ₄
218	[R·CF ₃ O] ⁻	133	C ₄ H ₇ NO ₄	C _n H _{2n-1} NO ₄
220	[R·CF ₃ O] ⁻	135	C ₄ H ₉ NO ₄	C _n H _{2n+1} NO ₄
232	[R·CF ₃ O] ⁻	147	C ₅ H ₉ NO ₄	C _n H _{2n-1} NO ₄
246	[R·CF ₃ O] ⁻	161	C ₆ H ₁₁ NO ₄	C _n H _{2n-1} NO ₄
248	[R·CF ₃ O] ⁻	163	C ₆ H ₁₃ NO ₄	C _n H _{2n+1} NO ₄
260	[R·CF ₃ O] ⁻	175	C ₇ H ₁₃ NO ₄	C _n H _{2n-1} NO ₄
262	[R·CF ₃ O] ⁻	177	C ₇ H ₁₅ NO ₄	C _n H _{2n+1} NO ₄
276	[R·CF ₃ O] ⁻	191	C ₈ H ₁₇ NO ₄	C _n H _{2n+1} NO ₄
288	[R·CF ₃ O] ⁻	203	C ₉ H ₁₇ NO ₄	C _n H _{2n-1} NO ₄
290	[R·CF ₃ O] ⁻	205	C ₉ H ₁₉ NO ₄	C _n H _{2n+1} NO ₄
302	[R·CF ₃ O] ⁻	217	C ₁₀ H ₁₉ NO ₄	C _n H _{2n-1} NO ₄
304	[R·CF ₃ O] ⁻	219	C ₁₀ H ₂₁ NO ₄	C _n H _{2n+1} NO ₄

Table S4: Pearson's correlation coefficients for SOA yield and mass fraction of familyCH ions with 9-12 carbons.

NO _x condition	Yield bound	C ₉	C ₁₀	C ₁₁	C ₁₂
High	Lower	0.907	0.900	0.853	0.835
High	Upper	0.768	0.763	0.690	0.669
Low	Lower	0.732	0.774	0.732	0.802
Low	Upper	0.860	0.887	0.852	0.763

Table S5: Pearson's correlation coefficients for SOA yield and mass fraction of family CHO1 ions with 9-12 carbons.

NO_x condition	Yield bound	C_9	C_{10}	C_{11}	C_{12}
High	Lower	0.748	0.871	0.907	0.671
High	Upper	0.603	0.740	0.762	0.526
Low	Lower	0.709	0.809	0.707	0.792
Low	Upper	0.761	0.850	0.845	0.575

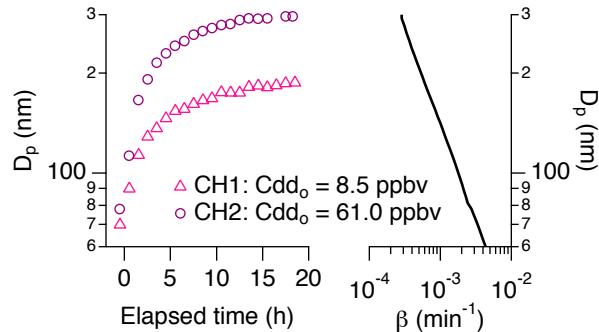


Figure S1: Comparison of size distribution peak diameter for two cyclododecane high- NO_x experiments (left panel). Also shown is the size-dependent particle wall loss rate constant, β , measured in a separate calibration experiment (right panel).