

Supplementary Materials
for
A Functional Group Oxidation Model (FGOM) for SOA formation and Aging

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1. Statistical fit of compound vapor pressure

We used 1080 “standard molecules” to obtain the parameters in equation (2). There are 35 sets of different combinations of the four functional groups. For each combination, carbon number ranges from 5 to 14. Alkanes are included with the same carbon number range. In addition, the contribution of straight, branching and cyclic structures to the vapor pressure are also considered. In summary, 1080 “standard compounds” are used for the nonlinear fitting. All are listed in Table S1.

2. Development of the functionalization vs. fragmentation channels in the FGOM

Photooxidation of dodecane under high-NO_x conditions illustrates how the functionalization vs. fragmentation channels are developed in the FGOM model. Figure S2 shows the detailed scheme for the formation of 1st generation products, i.e., C₁₂-(ONO₂), C₁₂-(OH + ONO₂), and C₁₂-(C=O + OH), in addition to the formation of 2nd generation products, i.e., C₁₂-(C=O), C₁₂-(2×ONO₂), C₁₂-(OH + ONO₂), C₁₂-(C=O + OH), C₁₂-(OH + 2×ONO₂), and C₁₂-(C=O + OH + ONO₂), from one of the 1st generation products. The specific chemistry underlying the formation of the C₁₂ products in the functionalization channel is discussed in Section 2.1. For the high-NO_x photooxidation of dodecane, the OH reaction rates, the photolysis rate of the –ONO₂ group, together with the branching ratio (obtained from MCM 3.1) for the formation of the RO· radical vs. the –ONO₂ group from the RO₂· + NO pathway, govern the relative abundances of different functional

groups (Figure S2). Note that since the OH concentration generally varies with time over the course of photooxidation, the branching ratios are a function of time. The values shown in Figure S2 correspond to those at the beginning of the photooxidation, when the OH concentration is $\sim 1 \times 10^7$ molecules cm^{-3} .

Once a certain generation of products is formed, an operator P_f , which is a function of the O:C ratio, is applied to each of the products to calculate the fraction of fragmentation that the product undergoes. Take the 2nd generation product $\text{C}_{12}\text{-(OH+2}\times\text{ONO}_2)$ as an example (Figure S3), the best-fit f_v value obtained from the optimization is 0.57, indicating that 26.4% of this product undergoes further functionalization and 73.6% of it fragments, producing a C_1 product, together with a co-product $\text{C}_{11}\text{-(OH+2}\times\text{ONO}_2)$. An operator P_f is subsequently applied to this C_{11} product to calculate its fraction of functionalization, via the same reaction mechanism as $\text{C}_{12}\text{-(OH+2}\times\text{ONO}_2)$, vs. fragmentation, which generates another C_1 product, together with a co-product $\text{C}_{10}\text{-(OH+2}\times\text{ONO}_2)$. Equation (2) in the main text governs the least carbon number for a certain combination of different functional groups that can be produced from the fragmentation channel. Alkoxy ($\text{RO}\cdot$) radical fragmentation mechanisms are not incorporated explicitly in the FGOM model. Instead, the operator P_f , which is indicative of the chemical species, is applied to the stable molecules to govern the probability of fragmentation in an OH-reaction initiated generation.

Table S1. Characteristics of the 1080 “standard molecules”

No.	Structure	Carbon Number	Oxygen Number	Nitrogen Number	Functional Groups	Vapor Pressure (atm @ 298 K)
1	Straight	5	0	0	-	6.4849E-01
2	Straight	6	0	0	-	2.1204E-01
3	Straight	7	0	0	-	6.9332E-02
4	Straight	8	0	0	-	2.2670E-02
5	Straight	9	0	0	-	7.4124E-03
6	Straight	10	0	0	-	2.4237E-03
7	Straight	11	0	0	-	7.9248E-04
8	Straight	12	0	0	-	2.5912E-04
9	Straight	13	0	0	-	8.4726E-05
10	Straight	14	0	0	-	2.7703E-05
11	Straight	5	1	0	1-OH	1.3021E-02
12	Straight	6	1	0	1-OH	4.2574E-03
13	Straight	7	1	0	1-OH	1.3921E-03
14	Straight	8	1	0	1-OH	4.5517E-04
15	Straight	9	1	0	1-OH	1.4883E-04
16	Straight	10	1	0	1-OH	4.8664E-05
17	Straight	11	1	0	1-OH	1.5912E-05
18	Straight	12	1	0	1-OH	5.2028E-06
19	Straight	13	1	0	1-OH	1.7012E-06
20	Straight	14	1	0	1-OH	5.5624E-07
21	Straight	5	2	0	2-OH	3.0091E-05
22	Straight	6	2	0	2-OH	9.8391E-06
23	Straight	7	2	0	2-OH	3.2171E-06
24	Straight	8	2	0	2-OH	1.0519E-06
25	Straight	9	2	0	2-OH	3.4395E-07
26	Straight	10	2	0	2-OH	1.1246E-07
27	Straight	11	2	0	2-OH	3.6773E-08
28	Straight	12	2	0	2-OH	1.2024E-08
29	Straight	13	2	0	2-OH	3.9315E-09
30	Straight	14	2	0	2-OH	1.2855E-09
31	Straight	5	3	0	3-OH	5.1505E-08
32	Straight	6	3	0	3-OH	1.6841E-08
33	Straight	7	3	0	3-OH	5.5065E-09
34	Straight	8	3	0	3-OH	1.8005E-09
35	Straight	9	3	0	3-OH	5.8871E-10
36	Straight	10	3	0	3-OH	1.9249E-10
37	Straight	11	3	0	3-OH	6.2941E-11
38	Straight	12	3	0	3-OH	2.0580E-11
39	Straight	13	3	0	3-OH	6.7292E-12
40	Straight	14	3	0	3-OH	2.2003E-12
41	Straight	5	1	0	1-C=O	4.1382E-02

42	Straight	6	1	0	1FC=O	1.3531EF02
43	Straight	7	1	0	1FC=O	4.4243EF03
44	Straight	8	1	0	1FC=O	1.4466EF03
45	Straight	9	1	0	1FC=O	4.7301EF04
46	Straight	10	1	0	1FC=O	1.5466EF04
47	Straight	11	1	0	1FC=O	5.0570EF05
48	Straight	12	1	0	1FC=O	1.6535EF05
49	Straight	13	1	0	1FC=O	5.4066EF06
50	Straight	14	1	0	1FC=O	1.7678EF06
51	Straight	5	2	0	2FC=O	3.7533EF03
52	Straight	6	2	0	2FC=O	1.2272EF03
53	Straight	7	2	0	2FC=O	4.0128EF04
54	Straight	8	2	0	2FC=O	1.3121EF04
55	Straight	9	2	0	2FC=O	4.2901EF05
56	Straight	10	2	0	2FC=O	1.4028EF05
57	Straight	11	2	0	2FC=O	4.5867EF06
58	Straight	12	2	0	2FC=O	1.4997EF06
59	Straight	13	2	0	2FC=O	4.9037EF07
60	Straight	14	2	0	2FC=O	1.6034EF07
61	Straight	5	3	0	3FC=O	4.9317EF04
62	Straight	6	3	0	3FC=O	1.6125EF04
63	Straight	7	3	0	3FC=O	5.2726EF05
64	Straight	8	3	0	3FC=O	1.7240EF05
65	Straight	9	3	0	3FC=O	5.6371EF06
66	Straight	10	3	0	3FC=O	1.8432EF06
67	Straight	11	3	0	3FC=O	6.0268EF07
68	Straight	12	3	0	3FC=O	1.9706EF07
69	Straight	13	3	0	3FC=O	6.4434EF08
70	Straight	14	3	0	3FC=O	2.1068EF08
71	Straight	5	2	0	1FOOH	9.6145EF04
72	Straight	6	2	0	1FOOH	3.1437EF04
73	Straight	7	2	0	1FOOH	1.0279EF04
74	Straight	8	2	0	1FOOH	3.3610EF05
75	Straight	9	2	0	1FOOH	1.0990EF05
76	Straight	10	2	0	1FOOH	3.5933EF06
77	Straight	11	2	0	1FOOH	1.1749EF06
78	Straight	12	2	0	1FOOH	3.8417EF07
79	Straight	13	2	0	1FOOH	1.2561EF07
80	Straight	14	2	0	1FOOH	4.1073EF08
81	Straight	5	4	0	2FOOH	4.9545EF07
82	Straight	6	4	0	2FOOH	1.6200EF07
83	Straight	7	4	0	2FOOH	5.2969EF08
84	Straight	8	4	0	2FOOH	1.7320EF08
85	Straight	9	4	0	2FOOH	5.6631EF09

86	Straight	10	4	0	2FOOH	1.8517EF09
87	Straight	11	4	0	2FOOH	6.0546EF10
88	Straight	12	4	0	2FOOH	1.9797EF10
89	Straight	13	4	0	2FOOH	6.4731EF11
90	Straight	14	4	0	2FOOH	2.1165EF11
91	Straight	5	6	0	3FOOH	2.1457EF10
92	Straight	6	6	0	3FOOH	7.0157EF11
93	Straight	7	6	0	3FOOH	2.2940EF11
94	Straight	8	6	0	3FOOH	7.5007EF12
95	Straight	9	6	0	3FOOH	2.4525EF12
96	Straight	10	6	0	3FOOH	8.0192EF13
97	Straight	11	6	0	3FOOH	2.6221EF13
98	Straight	12	6	0	3FOOH	8.5735EF14
99	Straight	13	6	0	3FOOH	2.8033EF14
100	Straight	14	6	0	3FOOH	9.1662EF15
101	Straight	5	3	1	1FONO ₂	2.7776EF03
102	Straight	6	3	1	1FONO ₂	9.0821EF04
103	Straight	7	3	1	1FONO ₂	2.9696EF04
104	Straight	8	3	1	1FONO ₂	9.7099EF05
105	Straight	9	3	1	1FONO ₂	3.1749EF05
106	Straight	10	3	1	1FONO ₂	1.0381EF05
107	Straight	11	3	1	1FONO ₂	3.3944EF06
108	Straight	12	3	1	1FONO ₂	1.1099EF06
109	Straight	13	3	1	1FONO ₂	3.6290EF07
110	Straight	14	3	1	1FONO ₂	1.1866EF07
111	Straight	5	6	2	2FONO ₂	1.1897EF05
112	Straight	6	6	2	2FONO ₂	3.8901EF06
113	Straight	7	6	2	2FONO ₂	1.2720EF06
114	Straight	8	6	2	2FONO ₂	4.1590EF07
115	Straight	9	6	2	2FONO ₂	1.3599EF07
116	Straight	10	6	2	2FONO ₂	4.4465EF08
117	Straight	11	6	2	2FONO ₂	1.4539EF08
118	Straight	12	6	2	2FONO ₂	4.7538EF09
119	Straight	13	6	2	2FONO ₂	1.5544EF09
120	Straight	14	6	2	2FONO ₂	5.0824EF10
121	Straight	5	9	3	3FONO ₂	5.0958EF08
122	Straight	6	9	3	3FONO ₂	1.6662EF08
123	Straight	7	9	3	3FONO ₂	5.4481EF09
124	Straight	8	9	3	3FONO ₂	1.7814EF09
125	Straight	9	9	3	3FONO ₂	5.8247EF10

126	Straight	10	9	3	3FONO ₂	1.9045EF10
127	Straight	11	9	3	3FONO ₂	6.2273EF11
128	Straight	12	9	3	3FONO ₂	2.0362EF11
129	Straight	13	9	3	3FONO ₂	6.6578EF12
130	Straight	14	9	3	3FONO ₂	2.1769EF12
131	Straight	5	2	0	1FOH+1FC=O	8.3089EF04
132	Straight	6	2	0	1FOH+1FC=O	2.7168EF04
133	Straight	7	2	0	1FOH+1FC=O	8.8832EF05
134	Straight	8	2	0	1FOH+1FC=O	2.9046EF05
135	Straight	9	2	0	1FOH+1FC=O	9.4973EF06
136	Straight	10	2	0	1FOH+1FC=O	3.1054EF06
137	Straight	11	2	0	1FOH+1FC=O	1.0154EF06
138	Straight	12	2	0	1FOH+1FC=O	3.3200EF07
139	Straight	13	2	0	1FOH+1FC=O	1.0856EF07
140	Straight	14	2	0	1FOH+1FC=O	3.5495EF08
141	Straight	5	3	0	1FOH+1FOOH	7.3193EF06
142	Straight	6	3	0	1FOH+1FOOH	2.3932EF06
143	Straight	7	3	0	1FOH+1FOOH	7.8253EF07
144	Straight	8	3	0	1FOH+1FOOH	2.5587EF07
145	Straight	9	3	0	1FOH+1FOOH	8.3662EF08
146	Straight	10	3	0	1FOH+1FOOH	2.7355EF08
147	Straight	11	3	0	1FOH+1FOOH	8.9445EF09
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149	Straight	13	3	0	1FOH+1FOOH	9.5628EF10
150	Straight	14	3	0	1FOH+1FOOH	3.1268EF10
151	Straight	5	4	1	1FOH+1FONO ₂	5.5771EF05
152	Straight	6	4	1	1FOH+1FONO ₂	1.8236EF05
153	Straight	7	4	1	1FOH+1FONO ₂	5.9626EF06
154	Straight	8	4	1	1FOH+1FONO ₂	1.9496EF06
155	Straight	9	4	1	1FOH+1FONO ₂	6.3747EF07
156	Straight	10	4	1	1FOH+1FONO ₂	2.0844EF07
157	Straight	11	4	1	1FOH+1FONO ₂	6.8154EF08
158	Straight	12	4	1	1FOH+1FONO ₂	2.2285EF08
159	Straight	13	4	1	1FOH+1FONO ₂	7.2865EF09
160	Straight	14	4	1	1FOH+1FONO ₂	2.3825EF09
161	Straight	5	3	0	1FC=O+1FOOH	6.1353EF05
162	Straight	6	3	0	1FC=O+1FOOH	2.0061EF05
163	Straight	7	3	0	1FC=O+1FOOH	6.5594EF06
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165	Straight	9	3	0	1FC=O+1FOOH	7.0128EF07
166	Straight	10	3	0	1FC=O+1FOOH	2.2930EF07
167	Straight	11	3	0	1FC=O+1FOOH	7.4976EF08

168	Straight	12	3	0	1FC=O+1FOOH	2.4515EF08
169	Straight	13	3	0	1FC=O+1FOOH	8.0158EF09
170	Straight	14	3	0	1FC=O+1FOOH	2.6210EF09
171	Straight	5	4	1	1FC=O+1FONO ₂	1.7725EF04
172	Straight	6	4	1	1FC=O+1FONO ₂	5.7956EF05
173	Straight	7	4	1	1FC=O+1FONO ₂	1.8950EF05
174	Straight	8	4	1	1FC=O+1FONO ₂	6.1962EF06
175	Straight	9	4	1	1FC=O+1FONO ₂	2.0260EF06
176	Straight	10	4	1	1FC=O+1FONO ₂	6.6245EF07
177	Straight	11	4	1	1FC=O+1FONO ₂	2.1660EF07
178	Straight	12	4	1	1FC=O+1FONO ₂	7.0824EF08
179	Straight	13	4	1	1FC=O+1FONO ₂	2.3158EF08
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182	Straight	6	5	1	1FOOH+1FONO ₂	1.3465EF06
183	Straight	7	5	1	1FOOH+1FONO ₂	4.4028EF07
184	Straight	8	5	1	1FOOH+1FONO ₂	1.4396EF07
185	Straight	9	5	1	1FOOH+1FONO ₂	4.7071EF08
186	Straight	10	5	1	1FOOH+1FONO ₂	1.5391EF08
187	Straight	11	5	1	1FOOH+1FONO ₂	5.0325EF09
188	Straight	12	5	1	1FOOH+1FONO ₂	1.6455EF09
189	Straight	13	5	1	1FOOH+1FONO ₂	5.3804EF10
190	Straight	14	5	1	1FOOH+1FONO ₂	1.7592EF10
191	Straight	5	3	0	2FOH+1FC=O	1.6605EF06
192	Straight	6	3	0	2FOH+1FC=O	5.4293EF07
193	Straight	7	3	0	2FOH+1FC=O	1.7752EF07
194	Straight	8	3	0	2FOH+1FC=O	5.8046EF08
195	Straight	9	3	0	2FOH+1FC=O	1.8980EF08
196	Straight	10	3	0	2FOH+1FC=O	6.2058EF09
197	Straight	11	3	0	2FOH+1FC=O	2.0292EF09
198	Straight	12	3	0	2FOH+1FC=O	6.6348EF10
199	Straight	13	3	0	2FOH+1FC=O	2.1694EF10
200	Straight	14	3	0	2FOH+1FC=O	7.0935EF11
201	Straight	5	4	0	2FOH+1FOOH	1.1194EF08
202	Straight	6	4	0	2FOH+1FOOH	3.6603EF09
203	Straight	7	4	0	2FOH+1FOOH	1.1968EF09
204	Straight	8	4	0	2FOH+1FOOH	3.9133EF10
205	Straight	9	4	0	2FOH+1FOOH	1.2795EF10
206	Straight	10	4	0	2FOH+1FOOH	4.1838EF11
207	Straight	11	4	0	2FOH+1FOOH	1.3680EF11
208	Straight	12	4	0	2FOH+1FOOH	4.4730EF12

209	Straight	13	4	0	2FOH+1FOOH	1.4626EF12
210	Straight	14	4	0	2FOH+1FOOH	4.7822EF13
211	Straight	5	5	1	2FOH+1FONO ₂	1.1145EF07
212	Straight	6	5	1	2FOH+1FONO ₂	3.6442EF08
213	Straight	7	5	1	2FOH+1FONO ₂	1.1916EF08
214	Straight	8	5	1	2FOH+1FONO ₂	3.8961EF09
215	Straight	9	5	1	2FOH+1FONO ₂	1.2739EF09
216	Straight	10	5	1	2FOH+1FONO ₂	4.1655EF10
217	Straight	11	5	1	2FOH+1FONO ₂	1.3620EF10
218	Straight	12	5	1	2FOH+1FONO ₂	4.4534EF11
219	Straight	13	5	1	2FOH+1FONO ₂	1.4561EF11
220	Straight	14	5	1	2FOH+1FONO ₂	4.7612EF12
221	Straight	5	3	0	2FC=O+1FOH	1.3683EF04
222	Straight	6	3	0	2FC=O+1FOH	4.4739EF05
223	Straight	7	3	0	2FC=O+1FOH	1.4629EF05
224	Straight	8	3	0	2FC=O+1FOH	4.7832EF06
225	Straight	9	3	0	2FC=O+1FOH	1.5640EF06
226	Straight	10	3	0	2FC=O+1FOH	5.1138EF07
227	Straight	11	3	0	2FC=O+1FOH	1.6721EF07
228	Straight	12	3	0	2FC=O+1FOH	5.4673EF08
229	Straight	13	3	0	2FC=O+1FOH	1.7877EF08
230	Straight	14	3	0	2FC=O+1FOH	5.8452EF09
231	Straight	5	4	0	2FC=O+1FOOH	1.0103EF05
232	Straight	6	4	0	2FC=O+1FOOH	3.3035EF06
233	Straight	7	4	0	2FC=O+1FOOH	1.0802EF06
234	Straight	8	4	0	2FC=O+1FOOH	3.5319EF07
235	Straight	9	4	0	2FC=O+1FOOH	1.1548EF07
236	Straight	10	4	0	2FC=O+1FOOH	3.7760EF08
237	Straight	11	4	0	2FC=O+1FOOH	1.2347EF08
238	Straight	12	4	0	2FC=O+1FOOH	4.0371EF09
239	Straight	13	4	0	2FC=O+1FOOH	1.3200EF09
240	Straight	14	4	0	2FC=O+1FOOH	4.3161EF10
241	Straight	5	5	1	2FC=O+1FONO ₂	2.9189EF05
242	Straight	6	5	1	2FC=O+1FONO ₂	9.5439EF06
243	Straight	7	5	1	2FC=O+1FONO ₂	3.1206EF06
244	Straight	8	5	1	2FC=O+1FONO ₂	1.0204EF06
245	Straight	9	5	1	2FC=O+1FONO ₂	3.3363EF07
246	Straight	10	5	1	2FC=O+1FONO ₂	1.0909EF07
247	Straight	11	5	1	2FC=O+1FONO ₂	3.5670EF08
248	Straight	12	5	1	2FC=O+1FONO ₂	1.1663EF08
249	Straight	13	5	1	2FC=O+1FONO ₂	3.8135EF09

250	Straight	14	5	1	2FC=O+1FONO ₂	1.2469EF09
251	Straight	5	5	0	2FOOH+1FOH	3.2943EF09
252	Straight	6	5	0	2FOOH+1FOH	1.0772EF09
253	Straight	7	5	0	2FOOH+1FOH	3.5220EF10
254	Straight	8	5	0	2FOOH+1FOH	1.1516EF10
255	Straight	9	5	0	2FOOH+1FOH	3.7655EF11
256	Straight	10	5	0	2FOOH+1FOH	1.2312EF11
257	Straight	11	5	0	2FOOH+1FOH	4.0258EF12
258	Straight	12	5	0	2FOOH+1FOH	1.3163EF12
259	Straight	13	5	0	2FOOH+1FOH	4.3041EF13
260	Straight	14	5	0	2FOOH+1FOH	1.4073EF13
261	Straight	5	5	0	2FOOH+1FC=O	3.1616EF08
262	Straight	6	5	0	2FOOH+1FC=O	1.0338EF08
263	Straight	7	5	0	2FOOH+1FC=O	3.3801EF09
264	Straight	8	5	0	2FOOH+1FC=O	1.1052EF09
265	Straight	9	5	0	2FOOH+1FC=O	3.6138EF10
266	Straight	10	5	0	2FOOH+1FC=O	1.1816EF10
267	Straight	11	5	0	2FOOH+1FC=O	3.8636EF11
268	Straight	12	5	0	2FOOH+1FC=O	1.2633EF11
269	Straight	13	5	0	2FOOH+1FC=O	4.1307EF12
270	Straight	14	5	0	2FOOH+1FC=O	1.3506EF12
271	Straight	5	7	1	2FOOH+1FONO ₂	2.1221EF09
272	Straight	6	7	1	2FOOH+1FONO ₂	6.9388EF10
273	Straight	7	7	1	2FOOH+1FONO ₂	2.2688EF10
274	Straight	8	7	1	2FOOH+1FONO ₂	7.4184EF11
275	Straight	9	7	1	2FOOH+1FONO ₂	2.4256EF11
276	Straight	10	7	1	2FOOH+1FONO ₂	7.9312EF12
277	Straight	11	7	1	2FOOH+1FONO ₂	2.5933EF12
278	Straight	12	7	1	2FOOH+1FONO ₂	8.4795EF13
279	Straight	13	7	1	2FOOH+1FONO ₂	2.7726EF13
280	Straight	14	7	1	2FOOH+1FONO ₂	9.0656EF14
281	Straight	5	7	2	2FONO ₂ +1FOH	2.3888EF07
282	Straight	6	7	2	2FONO ₂ +1FOH	7.8107EF08
283	Straight	7	7	2	2FONO ₂ +1FOH	2.5539EF08
284	Straight	8	7	2	2FONO ₂ +1FOH	8.3506EF09
285	Straight	9	7	2	2FONO ₂ +1FOH	2.7304EF09
286	Straight	10	7	2	2FONO ₂ +1FOH	8.9278EF10
287	Straight	11	7	2	2FONO ₂ +1FOH	2.9192EF10
288	Straight	12	7	2	2FONO ₂ +1FOH	9.5450EF11
289	Straight	13	7	2	2FONO ₂ +1FOH	3.1210EF11
290	Straight	14	7	2	2FONO ₂ +1FOH	1.0205EF11

291	Straight	5	7	2	2FONO ₂ +1FC=O	7.5919EF07
292	Straight	6	7	2	2FONO ₂ +1FC=O	2.4824EF07
293	Straight	7	7	2	2FONO ₂ +1FC=O	8.1167EF08
294	Straight	8	7	2	2FONO ₂ +1FC=O	2.6540EF08
295	Straight	9	7	2	2FONO ₂ +1FC=O	8.6778EF09
296	Straight	10	7	2	2FONO ₂ +1FC=O	2.8374EF09
297	Straight	11	7	2	2FONO ₂ +1FC=O	9.2777EF10
298	Straight	12	7	2	2FONO ₂ +1FC=O	3.0336EF10
299	Straight	13	7	2	2FONO ₂ +1FC=O	9.9190EF11
300	Straight	14	7	2	2FONO ₂ +1FC=O	3.2433EF11
301	Straight	5	8	2	2FONO ₂ +1FOOH	1.7639EF08
302	Straight	6	8	2	2FONO ₂ +1FOOH	5.7674EF09
303	Straight	7	8	2	2FONO ₂ +1FOOH	1.8858EF09
304	Straight	8	8	2	2FONO ₂ +1FOOH	6.1661EF10
305	Straight	9	8	2	2FONO ₂ +1FOOH	2.0162EF10
306	Straight	10	8	2	2FONO ₂ +1FOOH	6.5923EF11
307	Straight	11	8	2	2FONO ₂ +1FOOH	2.1555EF11
308	Straight	12	8	2	2FONO ₂ +1FOOH	7.0480EF12
309	Straight	13	8	2	2FONO ₂ +1FOOH	2.3045EF12
310	Straight	14	8	2	2FONO ₂ +1FOOH	7.5352EF13
311	Straight	5	4	0	1FOH+1FC=O+1FOOH	4.6707EF07
312	Straight	6	4	0	1FOH+1FC=O+1FOOH	1.5272EF07
313	Straight	7	4	0	1FOH+1FC=O+1FOOH	4.9936EF08
314	Straight	8	4	0	1FOH+1FC=O+1FOOH	1.6328EF08
315	Straight	9	4	0	1FOH+1FC=O+1FOOH	5.3387EF09
316	Straight	10	4	0	1FOH+1FC=O+1FOOH	1.7456EF09
317	Straight	11	4	0	1FOH+1FC=O+1FOOH	5.7078EF10
318	Straight	12	4	0	1FOH+1FC=O+1FOOH	1.8663EF10
319	Straight	13	4	0	1FOH+1FC=O+1FOOH	6.1023EF11
320	Straight	14	4	0	1FOH+1FC=O+1FOOH	1.9953EF11
321	Straight	5	5	1	1FOH+1FC=O+1FONO ₂	3.5589EF06
322	Straight	6	5	1	1FOH+1FC=O+1FONO ₂	1.1637EF06
323	Straight	7	5	1	1FOH+1FC=O+1FONO ₂	3.8049EF07
324	Straight	8	5	1	1FOH+1FC=O+1FONO ₂	1.2441EF07
325	Straight	9	5	1	1FOH+1FC=O+1FONO ₂	4.0679EF08
326	Straight	10	5	1	1FOH+1FC=O+1FONO ₂	1.3301EF08
327	Straight	11	5	1	1FOH+1FC=O+1FONO ₂	4.3491EF09
328	Straight	12	5	1	1FOH+1FC=O+1FONO ₂	1.4220EF09
329	Straight	13	5	1	1FOH+1FC=O+1FONO ₂	4.6497EF10
330	Straight	14	5	1	1FOH+1FC=O+1FONO ₂	1.5203EF10

331	Straight	5	6	1	1FOH+1FOOH+1FONO ₂	3.1350EF08
332	Straight	6	6	1	1FOH+1FOOH+1FONO ₂	1.0251EF08
333	Straight	7	6	1	1FOH+1FOOH+1FONO ₂	3.3518EF09
334	Straight	8	6	1	1FOH+1FOOH+1FONO ₂	1.0959EF09
335	Straight	9	6	1	1FOH+1FOOH+1FONO ₂	3.5834EF10
336	Straight	10	6	1	1FOH+1FOOH+1FONO ₂	1.1717EF10
337	Straight	11	6	1	1FOH+1FOOH+1FONO ₂	3.8311EF11
338	Straight	12	6	1	1FOH+1FOOH+1FONO ₂	1.2527EF11
339	Straight	13	6	1	1FOH+1FOOH+1FONO ₂	4.0960EF12
340	Straight	14	6	1	1FOH+1FOOH+1FONO ₂	1.3393EF12
341	Straight	5	6	1	1FC=O+1FOOH+1FONO ₂	2.6279EF07
342	Straight	6	6	1	1FC=O+1FOOH+1FONO ₂	8.5925EF08
343	Straight	7	6	1	1FC=O+1FOOH+1FONO ₂	2.8095EF08
344	Straight	8	6	1	1FC=O+1FOOH+1FONO ₂	9.1865EF09
345	Straight	9	6	1	1FC=O+1FOOH+1FONO ₂	3.0037EF09
346	Straight	10	6	1	1FC=O+1FOOH+1FONO ₂	9.8215EF10
347	Straight	11	6	1	1FC=O+1FOOH+1FONO ₂	3.2114EF10
348	Straight	12	6	1	1FC=O+1FOOH+1FONO ₂	1.0500EF10
349	Straight	13	6	1	1FC=O+1FOOH+1FONO ₂	3.4334EF11
350	Straight	14	6	1	1FC=O+1FOOH+1FONO ₂	1.1226EF11
351	Straight	5	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	2.0006EF09
352	Straight	6	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	6.5413EF10
353	Straight	7	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	2.1389EF10
354	Straight	8	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	6.9935EF11
355	Straight	9	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	2.2867EF11
356	Straight	10	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	7.4769EF12
357	Straight	11	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	2.4448EF12
358	Straight	12	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	7.9938EF13
359	Straight	13	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	2.6138EF13
360	Straight	14	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	8.5463EF14
361	Branching	5	0	0	F	1.0263E+00
362	Branching	6	0	0	F	3.3557EF01
363	Branching	7	0	0	F	1.0972EF01
364	Branching	8	0	0	F	3.5877EF02
365	Branching	9	0	0	F	1.1731EF02
366	Branching	10	0	0	F	3.8357EF03
367	Branching	11	0	0	F	1.2542EF03
368	Branching	12	0	0	F	4.1008EF04
369	Branching	13	0	0	F	1.3409EF04
370	Branching	14	0	0	F	4.3843EF05

371	Branching	5	1	0	1FOH	2.0607EF02
372	Branching	6	1	0	1FOH	6.7378EF03
373	Branching	7	1	0	1FOH	2.2031EF03
374	Branching	8	1	0	1FOH	7.2036EF04
375	Branching	9	1	0	1FOH	2.3554EF04
376	Branching	10	1	0	1FOH	7.7015EF05
377	Branching	11	1	0	1FOH	2.5182EF05
378	Branching	12	1	0	1FOH	8.2339EF06
379	Branching	13	1	0	1FOH	2.6923EF06
380	Branching	14	1	0	1FOH	8.8030EF07
381	Branching	5	2	0	2FOH	4.7622EF05
382	Branching	6	2	0	2FOH	1.5571EF05
383	Branching	7	2	0	2FOH	5.0914EF06
384	Branching	8	2	0	2FOH	1.6648EF06
385	Branching	9	2	0	2FOH	5.4434EF07
386	Branching	10	2	0	2FOH	1.7798EF07
387	Branching	11	2	0	2FOH	5.8197EF08
388	Branching	12	2	0	2FOH	1.9029EF08
389	Branching	13	2	0	2FOH	6.2219EF09
390	Branching	14	2	0	2FOH	2.0344EF09
391	Branching	5	3	0	3FOH	8.1511EF08
392	Branching	6	3	0	3FOH	2.6652EF08
393	Branching	7	3	0	3FOH	8.7146EF09
394	Branching	8	3	0	3FOH	2.8494EF09
395	Branching	9	3	0	3FOH	9.3170EF10
396	Branching	10	3	0	3FOH	3.0464EF10
397	Branching	11	3	0	3FOH	9.9610EF11
398	Branching	12	3	0	3FOH	3.2570EF11
399	Branching	13	3	0	3FOH	1.0650EF11
400	Branching	14	3	0	3FOH	3.4821EF12
401	Branching	5	1	0	1FC=O	6.5491EF02
402	Branching	6	1	0	1FC=O	2.1414EF02
403	Branching	7	1	0	1FC=O	7.0018EF03
404	Branching	8	1	0	1FC=O	2.2894EF03
405	Branching	9	1	0	1FC=O	7.4858EF04
406	Branching	10	1	0	1FC=O	2.4477EF04
407	Branching	11	1	0	1FC=O	8.0033EF05
408	Branching	12	1	0	1FC=O	2.6169EF05
409	Branching	13	1	0	1FC=O	8.5565EF06
410	Branching	14	1	0	1FC=O	2.7978EF06
411	Branching	5	2	0	2FC=O	5.9400EF03
412	Branching	6	2	0	2FC=O	1.9422EF03
413	Branching	7	2	0	2FC=O	6.3506EF04
414	Branching	8	2	0	2FC=O	2.0765EF04

415	Branching	9	2	0	2FC=O	6.7896EF05
416	Branching	10	2	0	2FC=O	2.2200EF05
417	Branching	11	2	0	2FC=O	7.2589EF06
418	Branching	12	2	0	2FC=O	2.3735EF06
419	Branching	13	2	0	2FC=O	7.7607EF07
420	Branching	14	2	0	2FC=O	2.5375EF07
421	Branching	5	3	0	3FC=O	7.8049EF04
422	Branching	6	3	0	3FC=O	2.5520EF04
423	Branching	7	3	0	3FC=O	8.3444EF05
424	Branching	8	3	0	3FC=O	2.7284EF05
425	Branching	9	3	0	3FC=O	8.9213EF06
426	Branching	10	3	0	3FC=O	2.9170EF06
427	Branching	11	3	0	3FC=O	9.5379EF07
428	Branching	12	3	0	3FC=O	3.1187EF07
429	Branching	13	3	0	3FC=O	1.0197EF07
430	Branching	14	3	0	3FC=O	3.3342EF08
431	Branching	5	2	0	1FOOH	1.5216EF03
432	Branching	6	2	0	1FOOH	4.9752EF04
433	Branching	7	2	0	1FOOH	1.6268EF04
434	Branching	8	2	0	1FOOH	5.3191EF05
435	Branching	9	2	0	1FOOH	1.7392EF05
436	Branching	10	2	0	1FOOH	5.6868EF06
437	Branching	11	2	0	1FOOH	1.8594EF06
438	Branching	12	2	0	1FOOH	6.0799EF07
439	Branching	13	2	0	1FOOH	1.9880EF07
440	Branching	14	2	0	1FOOH	6.5002EF08
441	Branching	5	4	0	2FOOH	7.8409EF07
442	Branching	6	4	0	2FOOH	2.5638EF07
443	Branching	7	4	0	2FOOH	8.3829EF08
444	Branching	8	4	0	2FOOH	2.7410EF08
445	Branching	9	4	0	2FOOH	8.9624EF09
446	Branching	10	4	0	2FOOH	2.9305EF09
447	Branching	11	4	0	2FOOH	9.5819EF10
448	Branching	12	4	0	2FOOH	3.1331EF10
449	Branching	13	4	0	2FOOH	1.0244EF10
450	Branching	14	4	0	2FOOH	3.3496EF11
451	Branching	5	6	0	3FOOH	3.3957EF10
452	Branching	6	6	0	3FOOH	1.1103EF10
453	Branching	7	6	0	3FOOH	3.6304EF11
454	Branching	8	6	0	3FOOH	1.1871EF11
455	Branching	9	6	0	3FOOH	3.8814EF12
456	Branching	10	6	0	3FOOH	1.2691EF12
457	Branching	11	6	0	3FOOH	4.1497EF13
458	Branching	12	6	0	3FOOH	1.3568EF13

459	Branching	13	6	0	3FOOH	4.4365EF14
460	Branching	14	6	0	3FOOH	1.4506EF14
461	Branching	5	3	1	1FONO ₂	4.3959EF03
462	Branching	6	3	1	1FONO ₂	1.4373EF03
463	Branching	7	3	1	1FONO ₂	4.6997EF04
464	Branching	8	3	1	1FONO ₂	1.5367EF04
465	Branching	9	3	1	1FONO ₂	5.0246EF05
466	Branching	10	3	1	1FONO ₂	1.6429EF05
467	Branching	11	3	1	1FONO ₂	5.3719EF06
468	Branching	12	3	1	1FONO ₂	1.7565EF06
469	Branching	13	3	1	1FONO ₂	5.7433EF07
470	Branching	14	3	1	1FONO ₂	1.8779EF07
471	Branching	5	6	2	2FONO ₂	1.8828EF05
472	Branching	6	6	2	2FONO ₂	6.1564EF06
473	Branching	7	6	2	2FONO ₂	2.0130EF06
474	Branching	8	6	2	2FONO ₂	6.5820EF07
475	Branching	9	6	2	2FONO ₂	2.1521EF07
476	Branching	10	6	2	2FONO ₂	7.0370EF08
477	Branching	11	6	2	2FONO ₂	2.3009EF08
478	Branching	12	6	2	2FONO ₂	7.5234EF09
479	Branching	13	6	2	2FONO ₂	2.4600EF09
480	Branching	14	6	2	2FONO ₂	8.0435EF10
481	Branching	5	9	3	3FONO ₂	8.0646EF08
482	Branching	6	9	3	3FONO ₂	2.6369EF08
483	Branching	7	9	3	3FONO ₂	8.6221EF09
484	Branching	8	9	3	3FONO ₂	2.8192EF09
485	Branching	9	9	3	3FONO ₂	9.2181EF10
486	Branching	10	9	3	3FONO ₂	3.0141EF10
487	Branching	11	9	3	3FONO ₂	9.8553EF11
488	Branching	12	9	3	3FONO ₂	3.2224EF11
489	Branching	13	9	3	3FONO ₂	1.0537EF11
490	Branching	14	9	3	3FONO ₂	3.4452EF12
491	Branching	5	2	0	1FOH+1FC=O	1.3150EF03
492	Branching	6	2	0	1FOH+1FC=O	4.2996EF04
493	Branching	7	2	0	1FOH+1FC=O	1.4059EF04
494	Branching	8	2	0	1FOH+1FC=O	4.5968EF05
495	Branching	9	2	0	1FOH+1FC=O	1.5030EF05
496	Branching	10	2	0	1FOH+1FC=O	4.9146EF06
497	Branching	11	2	0	1FOH+1FC=O	1.6069EF06
498	Branching	12	2	0	1FOH+1FC=O	5.2543EF07

499	Branching	13	2	0	1FOH+1FC=O	1.7180EF07
500	Branching	14	2	0	1FOH+1FC=O	5.6175EF08
501	Branching	5	3	0	1FOH+1FOOH	1.1584EF05
502	Branching	6	3	0	1FOH+1FOOH	3.7875EF06
503	Branching	7	3	0	1FOH+1FOOH	1.2384EF06
504	Branching	8	3	0	1FOH+1FOOH	4.0494EF07
505	Branching	9	3	0	1FOH+1FOOH	1.3240EF07
506	Branching	10	3	0	1FOH+1FOOH	4.3293EF08
507	Branching	11	3	0	1FOH+1FOOH	1.4156EF08
508	Branching	12	3	0	1FOH+1FOOH	4.6285EF09
509	Branching	13	3	0	1FOH+1FOOH	1.5134EF09
510	Branching	14	3	0	1FOH+1FOOH	4.9485EF10
511	Branching	5	4	1	1FOH+1FONO ₂	8.8262EF05
512	Branching	6	4	1	1FOH+1FONO ₂	2.8860EF05
513	Branching	7	4	1	1FOH+1FONO ₂	9.4363EF06
514	Branching	8	4	1	1FOH+1FONO ₂	3.0854EF06
515	Branching	9	4	1	1FOH+1FONO ₂	1.0089EF06
516	Branching	10	4	1	1FOH+1FONO ₂	3.2987EF07
517	Branching	11	4	1	1FOH+1FONO ₂	1.0786EF07
518	Branching	12	4	1	1FOH+1FONO ₂	3.5268EF08
519	Branching	13	4	1	1FOH+1FONO ₂	1.1532EF08
520	Branching	14	4	1	1FOH+1FONO ₂	3.7705EF09
521	Branching	5	3	0	1FC=O+1FOOH	9.7097EF05
522	Branching	6	3	0	1FC=O+1FOOH	3.1748EF05
523	Branching	7	3	0	1FC=O+1FOOH	1.0381EF05
524	Branching	8	3	0	1FC=O+1FOOH	3.3943EF06
525	Branching	9	3	0	1FC=O+1FOOH	1.1098EF06
526	Branching	10	3	0	1FC=O+1FOOH	3.6289EF07
527	Branching	11	3	0	1FC=O+1FOOH	1.1866EF07
528	Branching	12	3	0	1FC=O+1FOOH	3.8798EF08
529	Branching	13	3	0	1FC=O+1FOOH	1.2686EF08
530	Branching	14	3	0	1FC=O+1FOOH	4.1480EF09
531	Branching	5	4	1	1FC=O+1FONO ₂	2.8051EF04
532	Branching	6	4	1	1FC=O+1FONO ₂	9.1721EF05
533	Branching	7	4	1	1FC=O+1FONO ₂	2.9990EF05
534	Branching	8	4	1	1FC=O+1FONO ₂	9.8061EF06
535	Branching	9	4	1	1FC=O+1FONO ₂	3.2063EF06
536	Branching	10	4	1	1FC=O+1FONO ₂	1.0484EF06
537	Branching	11	4	1	1FC=O+1FONO ₂	3.4280EF07
538	Branching	12	4	1	1FC=O+1FONO ₂	1.1209EF07
539	Branching	13	4	1	1FC=O+1FONO ₂	3.6649EF08

540	Branching	14	4	1	1FC=O+1FONO ₂	1.1983EF08
541	Branching	5	5	1	1FOOH+1FONO ₂	6.5173EF06
542	Branching	6	5	1	1FOOH+1FONO ₂	2.1310EF06
543	Branching	7	5	1	1FOOH+1FONO ₂	6.9678EF07
544	Branching	8	5	1	1FOOH+1FONO ₂	2.2783EF07
545	Branching	9	5	1	1FOOH+1FONO ₂	7.4494EF08
546	Branching	10	5	1	1FOOH+1FONO ₂	2.4358EF08
547	Branching	11	5	1	1FOOH+1FONO ₂	7.9644EF09
548	Branching	12	5	1	1FOOH+1FONO ₂	2.6042EF09
549	Branching	13	5	1	1FOOH+1FONO ₂	8.5149EF10
550	Branching	14	5	1	1FOOH+1FONO ₂	2.7842EF10
551	Branching	5	3	0	2FOH+1FC=O	2.6278EF06
552	Branching	6	3	0	2FOH+1FC=O	8.5924EF07
553	Branching	7	3	0	2FOH+1FC=O	2.8095EF07
554	Branching	8	3	0	2FOH+1FC=O	9.1864EF08
555	Branching	9	3	0	2FOH+1FC=O	3.0037EF08
556	Branching	10	3	0	2FOH+1FC=O	9.8214EF09
557	Branching	11	3	0	2FOH+1FC=O	3.2113EF09
558	Branching	12	3	0	2FOH+1FC=O	1.0500EF09
559	Branching	13	3	0	2FOH+1FC=O	3.4333EF10
560	Branching	14	3	0	2FOH+1FC=O	1.1226EF10
561	Branching	5	4	0	2FOH+1FOOH	1.7716EF08
562	Branching	6	4	0	2FOH+1FOOH	5.7927EF09
563	Branching	7	4	0	2FOH+1FOOH	1.8941EF09
564	Branching	8	4	0	2FOH+1FOOH	6.1932EF10
565	Branching	9	4	0	2FOH+1FOOH	2.0250EF10
566	Branching	10	4	0	2FOH+1FOOH	6.6213EF11
567	Branching	11	4	0	2FOH+1FOOH	2.1650EF11
568	Branching	12	4	0	2FOH+1FOOH	7.0790EF12
569	Branching	13	4	0	2FOH+1FOOH	2.3146EF12
570	Branching	14	4	0	2FOH+1FOOH	7.5683EF13
571	Branching	5	5	1	2FOH+1FONO ₂	1.7639EF07
572	Branching	6	5	1	2FOH+1FONO ₂	5.7674EF08
573	Branching	7	5	1	2FOH+1FONO ₂	1.8858EF08
574	Branching	8	5	1	2FOH+1FONO ₂	6.1660EF09
575	Branching	9	5	1	2FOH+1FONO ₂	2.0161EF09
576	Branching	10	5	1	2FOH+1FONO ₂	6.5922EF10
577	Branching	11	5	1	2FOH+1FONO ₂	2.1555EF10
578	Branching	12	5	1	2FOH+1FONO ₂	7.0479EF11
579	Branching	13	5	1	2FOH+1FONO ₂	2.3045EF11
580	Branching	14	5	1	2FOH+1FONO ₂	7.5351EF12

581	Branching	5	3	0	2FC=O+1FOH	2.1654EF04
582	Branching	6	3	0	2FC=O+1FOH	7.0804EF05
583	Branching	7	3	0	2FC=O+1FOH	2.3151EF05
584	Branching	8	3	0	2FC=O+1FOH	7.5699EF06
585	Branching	9	3	0	2FC=O+1FOH	2.4752EF06
586	Branching	10	3	0	2FC=O+1FOH	8.0931EF07
587	Branching	11	3	0	2FC=O+1FOH	2.6462EF07
588	Branching	12	3	0	2FC=O+1FOH	8.6526EF08
589	Branching	13	3	0	2FC=O+1FOH	2.8292EF08
590	Branching	14	3	0	2FC=O+1FOH	9.2507EF09
591	Branching	5	4	0	2FC=O+1FOOH	1.5990EF05
592	Branching	6	4	0	2FC=O+1FOOH	5.2282EF06
593	Branching	7	4	0	2FC=O+1FOOH	1.7095EF06
594	Branching	8	4	0	2FC=O+1FOOH	5.5896EF07
595	Branching	9	4	0	2FC=O+1FOOH	1.8277EF07
596	Branching	10	4	0	2FC=O+1FOOH	5.9760EF08
597	Branching	11	4	0	2FC=O+1FOOH	1.9540EF08
598	Branching	12	4	0	2FC=O+1FOOH	6.3891EF09
599	Branching	13	4	0	2FC=O+1FOOH	2.0891EF09
600	Branching	14	4	0	2FC=O+1FOOH	6.8307EF10
601	Branching	5	5	1	2FC=O+1FONO ₂	4.6194EF05
602	Branching	6	5	1	2FC=O+1FONO ₂	1.5104EF05
603	Branching	7	5	1	2FC=O+1FONO ₂	4.9387EF06
604	Branching	8	5	1	2FC=O+1FONO ₂	1.6148EF06
605	Branching	9	5	1	2FC=O+1FONO ₂	5.2801EF07
606	Branching	10	5	1	2FC=O+1FONO ₂	1.7265EF07
607	Branching	11	5	1	2FC=O+1FONO ₂	5.6451EF08
608	Branching	12	5	1	2FC=O+1FONO ₂	1.8458EF08
609	Branching	13	5	1	2FC=O+1FONO ₂	6.0353EF09
610	Branching	14	5	1	2FC=O+1FONO ₂	1.9734EF09
611	Branching	5	5	0	2FOOH+1FOH	5.2136EF09
612	Branching	6	5	0	2FOOH+1FOH	1.7047EF09
613	Branching	7	5	0	2FOOH+1FOH	5.5740EF10
614	Branching	8	5	0	2FOOH+1FOH	1.8226EF10
615	Branching	9	5	0	2FOOH+1FOH	5.9593EF11
616	Branching	10	5	0	2FOOH+1FOH	1.9485EF11
617	Branching	11	5	0	2FOOH+1FOH	6.3712EF12
618	Branching	12	5	0	2FOOH+1FOH	2.0832EF12
619	Branching	13	5	0	2FOOH+1FOH	6.8116EF13
620	Branching	14	5	0	2FOOH+1FOH	2.2272EF13
621	Branching	5	5	0	2FOOH+1FC=O	5.0035EF08
622	Branching	6	5	0	2FOOH+1FC=O	1.6360EF08

623	Branching	7	5	0	2FOOH+1FC=O	5.3494EF09
624	Branching	8	5	0	2FOOH+1FC=O	1.7491EF09
625	Branching	9	5	0	2FOOH+1FC=O	5.7192EF10
626	Branching	10	5	0	2FOOH+1FC=O	1.8700EF10
627	Branching	11	5	0	2FOOH+1FC=O	6.1145EF11
628	Branching	12	5	0	2FOOH+1FC=O	1.9993EF11
629	Branching	13	5	0	2FOOH+1FC=O	6.5372EF12
630	Branching	14	5	0	2FOOH+1FC=O	2.1375EF12
631	Branching	5	7	1	2FOOH+1FONO ₂	3.3584EF09
632	Branching	6	7	1	2FOOH+1FONO ₂	1.0981EF09
633	Branching	7	7	1	2FOOH+1FONO ₂	3.5906EF10
634	Branching	8	7	1	2FOOH+1FONO ₂	1.1740EF10
635	Branching	9	7	1	2FOOH+1FONO ₂	3.8388EF11
636	Branching	10	7	1	2FOOH+1FONO ₂	1.2552EF11
637	Branching	11	7	1	2FOOH+1FONO ₂	4.1042EF12
638	Branching	12	7	1	2FOOH+1FONO ₂	1.3420EF12
639	Branching	13	7	1	2FOOH+1FONO ₂	4.3879EF13
640	Branching	14	7	1	2FOOH+1FONO ₂	1.4347EF13
641	Branching	5	7	2	2FONO ₂ +1FOH	3.7805EF07
642	Branching	6	7	2	2FONO ₂ +1FOH	1.2361EF07
643	Branching	7	7	2	2FONO ₂ +1FOH	4.0418EF08
644	Branching	8	7	2	2FONO ₂ +1FOH	1.3216EF08
645	Branching	9	7	2	2FONO ₂ +1FOH	4.3212EF09
646	Branching	10	7	2	2FONO ₂ +1FOH	1.4129EF09
647	Branching	11	7	2	2FONO ₂ +1FOH	4.6199EF10
648	Branching	12	7	2	2FONO ₂ +1FOH	1.5106EF10
649	Branching	13	7	2	2FONO ₂ +1FOH	4.9392EF11
650	Branching	14	7	2	2FONO ₂ +1FOH	1.6150EF11
651	Branching	5	7	2	2FONO ₂ +1FC=O	1.2015EF06
652	Branching	6	7	2	2FONO ₂ +1FC=O	3.9286EF07
653	Branching	7	7	2	2FONO ₂ +1FC=O	1.2846EF07
654	Branching	8	7	2	2FONO ₂ +1FC=O	4.2002EF08
655	Branching	9	7	2	2FONO ₂ +1FC=O	1.3733EF08
656	Branching	10	7	2	2FONO ₂ +1FC=O	4.4905EF09
657	Branching	11	7	2	2FONO ₂ +1FC=O	1.4683EF09
658	Branching	12	7	2	2FONO ₂ +1FC=O	4.8009EF10
659	Branching	13	7	2	2FONO ₂ +1FC=O	1.5698EF10
660	Branching	14	7	2	2FONO ₂ +1FC=O	5.1328EF11
661	Branching	5	8	2	2FONO ₂ +1FOOH	2.7915EF08
662	Branching	6	8	2	2FONO ₂ +1FOOH	9.1275EF09

663	Branching	7	8	2	2FONO ₂ +1FOOH	2.9845EF09
664	Branching	8	8	2	2FONO ₂ +1FOOH	9.7584EF10
665	Branching	9	8	2	2FONO ₂ +1FOOH	3.1908EF10
666	Branching	10	8	2	2FONO ₂ +1FOOH	1.0433EF10
667	Branching	11	8	2	2FONO ₂ +1FOOH	3.4113EF11
668	Branching	12	8	2	2FONO ₂ +1FOOH	1.1154EF11
669	Branching	13	8	2	2FONO ₂ +1FOOH	3.6471EF12
670	Branching	14	8	2	2FONO ₂ +1FOOH	1.1925EF12
671	Branching	5	4	0	1FOH+1FC=O+1FOOH	7.3918EF07
672	Branching	6	4	0	1FOH+1FC=O+1FOOH	2.4169EF07
673	Branching	7	4	0	1FOH+1FC=O+1FOOH	7.9028EF08
674	Branching	8	4	0	1FOH+1FC=O+1FOOH	2.5840EF08
675	Branching	9	4	0	1FOH+1FC=O+1FOOH	8.4491EF09
676	Branching	10	4	0	1FOH+1FC=O+1FOOH	2.7626EF09
677	Branching	11	4	0	1FOH+1FC=O+1FOOH	9.0331EF10
678	Branching	12	4	0	1FOH+1FC=O+1FOOH	2.9536EF10
679	Branching	13	4	0	1FOH+1FC=O+1FOOH	9.6575EF11
680	Branching	14	4	0	1FOH+1FC=O+1FOOH	3.1578EF11
681	Branching	5	5	1	1FOH+1FC=O+1FONO ₂	5.6323EF06
682	Branching	6	5	1	1FOH+1FC=O+1FONO ₂	1.8416EF06
683	Branching	7	5	1	1FOH+1FC=O+1FONO ₂	6.0216EF07
684	Branching	8	5	1	1FOH+1FC=O+1FONO ₂	1.9689EF07
685	Branching	9	5	1	1FOH+1FC=O+1FONO ₂	6.4379EF08
686	Branching	10	5	1	1FOH+1FC=O+1FONO ₂	2.1050EF08
687	Branching	11	5	1	1FOH+1FC=O+1FONO ₂	6.8829EF09
688	Branching	12	5	1	1FOH+1FC=O+1FONO ₂	2.2505EF09
689	Branching	13	5	1	1FOH+1FC=O+1FONO ₂	7.3587EF10
690	Branching	14	5	1	1FOH+1FC=O+1FONO ₂	2.4061EF10
691	Branching	5	6	1	1FOH+1FOOH+1FONO ₂	4.9615EF08
692	Branching	6	6	1	1FOH+1FOOH+1FONO ₂	1.6223EF08
693	Branching	7	6	1	1FOH+1FOOH+1FONO ₂	5.3045EF09
694	Branching	8	6	1	1FOH+1FOOH+1FONO ₂	1.7344EF09
695	Branching	9	6	1	1FOH+1FOOH+1FONO ₂	5.6711EF10
696	Branching	10	6	1	1FOH+1FOOH+1FONO ₂	1.8543EF10
697	Branching	11	6	1	1FOH+1FOOH+1FONO ₂	6.0632EF11
698	Branching	12	6	1	1FOH+1FOOH+1FONO ₂	1.9825EF11
699	Branching	13	6	1	1FOH+1FOOH+1FONO ₂	6.4823EF12
700	Branching	14	6	1	1FOH+1FOOH+1FONO ₂	2.1195EF12
701	Branching	5	6	1	1FC=O+1FOOH+1FONO ₂	4.1589EF07
702	Branching	6	6	1	1FC=O+1FOOH+1FONO ₂	1.3598EF07

703	Branching	7	6	1	1FC=O+1FOOH+1FONO ₂	4.4464EF08
704	Branching	8	6	1	1FC=O+1FOOH+1FONO ₂	1.4538EF08
705	Branching	9	6	1	1FC=O+1FOOH+1FONO ₂	4.7537EF09
706	Branching	10	6	1	1FC=O+1FOOH+1FONO ₂	1.5543EF09
707	Branching	11	6	1	1FC=O+1FOOH+1FONO ₂	5.0823EF10
708	Branching	12	6	1	1FC=O+1FOOH+1FONO ₂	1.6618EF10
709	Branching	13	6	1	1FC=O+1FOOH+1FONO ₂	5.4336EF11
710	Branching	14	6	1	1FC=O+1FOOH+1FONO ₂	1.7767EF11
711	Branching	5	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	3.1661EF09
712	Branching	6	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	1.0352EF09
713	Branching	7	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	3.3849EF10
714	Branching	8	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	1.1068EF10
715	Branching	9	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	3.6189EF11
716	Branching	10	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	1.1833EF11
717	Branching	11	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	3.8691EF12
718	Branching	12	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	1.2651EF12
719	Branching	13	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	4.1365EF13
720	Branching	14	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	1.3525EF13
721	Cyclo	5	0	0	F	4.0976EF01
722	Cyclo	6	0	0	F	1.3398EF01
723	Cyclo	7	0	0	F	4.3809EF02
724	Cyclo	8	0	0	F	1.4324EF02
725	Cyclo	9	0	0	F	4.6837EF03
726	Cyclo	10	0	0	F	1.5315EF03
727	Cyclo	11	0	0	F	5.0075EF04
728	Cyclo	12	0	0	F	1.6373EF04
729	Cyclo	13	0	0	F	5.3536EF05
730	Cyclo	14	0	0	F	1.7505EF05
731	Cyclo	5	1	0	1FOH	8.2274EF03
732	Cyclo	6	1	0	1FOH	2.6902EF03
733	Cyclo	7	1	0	1FOH	8.7961EF04
734	Cyclo	8	1	0	1FOH	2.8761EF04
735	Cyclo	9	1	0	1FOH	9.4042EF05
736	Cyclo	10	1	0	1FOH	3.0749EF05
737	Cyclo	11	1	0	1FOH	1.0054EF05
738	Cyclo	12	1	0	1FOH	3.2875EF06
739	Cyclo	13	1	0	1FOH	1.0749EF06
740	Cyclo	14	1	0	1FOH	3.5147EF07
741	Cyclo	5	2	0	2FOH	1.9014EF05
742	Cyclo	6	2	0	2FOH	6.2171EF06
743	Cyclo	7	2	0	2FOH	2.0328EF06

744	Cyclo	8	2	0	2FOH	6.6468EF07
745	Cyclo	9	2	0	2FOH	2.1733EF07
746	Cyclo	10	2	0	2FOH	7.1063EF08
747	Cyclo	11	2	0	2FOH	2.3236EF08
748	Cyclo	12	2	0	2FOH	7.5975EF09
749	Cyclo	13	2	0	2FOH	2.4842EF09
750	Cyclo	14	2	0	2FOH	8.1227EF10
751	Cyclo	5	3	0	3FOH	3.2544EF08
752	Cyclo	6	3	0	3FOH	1.0641EF08
753	Cyclo	7	3	0	3FOH	3.4794EF09
754	Cyclo	8	3	0	3FOH	1.1377EF09
755	Cyclo	9	3	0	3FOH	3.7199EF10
756	Cyclo	10	3	0	3FOH	1.2163EF10
757	Cyclo	11	3	0	3FOH	3.9771EF11
758	Cyclo	12	3	0	3FOH	1.3004EF11
759	Cyclo	13	3	0	3FOH	4.2520EF12
760	Cyclo	14	3	0	3FOH	1.3903EF12
761	Cyclo	5	1	0	1FC=O	2.6148EF02
762	Cyclo	6	1	0	1FC=O	8.5498EF03
763	Cyclo	7	1	0	1FC=O	2.7956EF03
764	Cyclo	8	1	0	1FC=O	9.1408EF04
765	Cyclo	9	1	0	1FC=O	2.9888EF04
766	Cyclo	10	1	0	1FC=O	9.7726EF05
767	Cyclo	11	1	0	1FC=O	3.1954EF05
768	Cyclo	12	1	0	1FC=O	1.0448EF05
769	Cyclo	13	1	0	1FC=O	3.4163EF06
770	Cyclo	14	1	0	1FC=O	1.1170EF06
771	Cyclo	5	2	0	2FC=O	2.3716EF03
772	Cyclo	6	2	0	2FC=O	7.7546EF04
773	Cyclo	7	2	0	2FC=O	2.5355EF04
774	Cyclo	8	2	0	2FC=O	8.2906EF05
775	Cyclo	9	2	0	2FC=O	2.7108EF05
776	Cyclo	10	2	0	2FC=O	8.8637EF06
777	Cyclo	11	2	0	2FC=O	2.8982EF06
778	Cyclo	12	2	0	2FC=O	9.4764EF07
779	Cyclo	13	2	0	2FC=O	3.0985EF07
780	Cyclo	14	2	0	2FC=O	1.0131EF07
781	Cyclo	5	3	0	3FC=O	3.1162EF04
782	Cyclo	6	3	0	3FC=O	1.0189EF04
783	Cyclo	7	3	0	3FC=O	3.3316EF05
784	Cyclo	8	3	0	3FC=O	1.0894EF05
785	Cyclo	9	3	0	3FC=O	3.5619EF06
786	Cyclo	10	3	0	3FC=O	1.1647EF06
787	Cyclo	11	3	0	3FC=O	3.8081EF07

788	Cyclo	12	3	0	3FC=O	1.2452EF07
789	Cyclo	13	3	0	3FC=O	4.0714EF08
790	Cyclo	14	3	0	3FC=O	1.3312EF08
791	Cyclo	5	2	0	1FOOH	6.0751EF04
792	Cyclo	6	2	0	1FOOH	1.9864EF04
793	Cyclo	7	2	0	1FOOH	6.4951EF05
794	Cyclo	8	2	0	1FOOH	2.1237EF05
795	Cyclo	9	2	0	1FOOH	6.9440EF06
796	Cyclo	10	2	0	1FOOH	2.2705EF06
797	Cyclo	11	2	0	1FOOH	7.4240EF07
798	Cyclo	12	2	0	1FOOH	2.4275EF07
799	Cyclo	13	2	0	1FOOH	7.9372EF08
800	Cyclo	14	2	0	1FOOH	2.5953EF08
801	Cyclo	5	4	0	2FOOH	3.1306EF07
802	Cyclo	6	4	0	2FOOH	1.0236EF07
803	Cyclo	7	4	0	2FOOH	3.3470EF08
804	Cyclo	8	4	0	2FOOH	1.0944EF08
805	Cyclo	9	4	0	2FOOH	3.5784EF09
806	Cyclo	10	4	0	2FOOH	1.1700EF09
807	Cyclo	11	4	0	2FOOH	3.8257EF10
808	Cyclo	12	4	0	2FOOH	1.2509EF10
809	Cyclo	13	4	0	2FOOH	4.0902EF11
810	Cyclo	14	4	0	2FOOH	1.3374EF11
811	Cyclo	5	6	0	3FOOH	1.3558EF10
812	Cyclo	6	6	0	3FOOH	4.4331EF11
813	Cyclo	7	6	0	3FOOH	1.4495EF11
814	Cyclo	8	6	0	3FOOH	4.7395EF12
815	Cyclo	9	6	0	3FOOH	1.5497EF12
816	Cyclo	10	6	0	3FOOH	5.0671EF13
817	Cyclo	11	6	0	3FOOH	1.6568EF13
818	Cyclo	12	6	0	3FOOH	5.4174EF14
819	Cyclo	13	6	0	3FOOH	1.7713EF14
820	Cyclo	14	6	0	3FOOH	5.7919EF15
821	Cyclo	5	3	1	1FONO ₂	1.7551EF03
822	Cyclo	6	3	1	1FONO ₂	5.7387EF04
823	Cyclo	7	3	1	1FONO ₂	1.8764EF04
824	Cyclo	8	3	1	1FONO ₂	6.1354EF05
825	Cyclo	9	3	1	1FONO ₂	2.0061EF05
826	Cyclo	10	3	1	1FONO ₂	6.5595EF06
827	Cyclo	11	3	1	1FONO ₂	2.1448EF06
828	Cyclo	12	3	1	1FONO ₂	7.0130EF07
829	Cyclo	13	3	1	1FONO ₂	2.2931EF07

830	Cyclo	14	3	1	1FONO ₂	7.4978EF08
831	Cyclo	5	6	2	2FONO ₂	7.5175EF06
832	Cyclo	6	6	2	2FONO ₂	2.4580EF06
833	Cyclo	7	6	2	2FONO ₂	8.0371EF07
834	Cyclo	8	6	2	2FONO ₂	2.6279EF07
835	Cyclo	9	6	2	2FONO ₂	8.5927EF08
836	Cyclo	10	6	2	2FONO ₂	2.8096EF08
837	Cyclo	11	6	2	2FONO ₂	9.1867EF09
838	Cyclo	12	6	2	2FONO ₂	3.0038EF09
839	Cyclo	13	6	2	2FONO ₂	9.8217EF10
840	Cyclo	14	6	2	2FONO ₂	3.2115EF10
841	Cyclo	5	9	3	3FONO ₂	3.2199EF08
842	Cyclo	6	9	3	3FONO ₂	1.0528EF08
843	Cyclo	7	9	3	3FONO ₂	3.4425EF09
844	Cyclo	8	9	3	3FONO ₂	1.1256EF09
845	Cyclo	9	9	3	3FONO ₂	3.6805EF10
846	Cyclo	10	9	3	3FONO ₂	1.2034EF10
847	Cyclo	11	9	3	3FONO ₂	3.9349EF11
848	Cyclo	12	9	3	3FONO ₂	1.2866EF11
849	Cyclo	13	9	3	3FONO ₂	4.2069EF12
850	Cyclo	14	9	3	3FONO ₂	1.3755EF12
851	Cyclo	5	2	0	1FOH+1FC=O	5.2502EF04
852	Cyclo	6	2	0	1FOH+1FC=O	1.7167EF04
853	Cyclo	7	2	0	1FOH+1FC=O	5.6131EF05
854	Cyclo	8	2	0	1FOH+1FC=O	1.8353EF05
855	Cyclo	9	2	0	1FOH+1FC=O	6.0011EF06
856	Cyclo	10	2	0	1FOH+1FC=O	1.9622EF06
857	Cyclo	11	2	0	1FOH+1FC=O	6.4159EF07
858	Cyclo	12	2	0	1FOH+1FC=O	2.0978EF07
859	Cyclo	13	2	0	1FOH+1FC=O	6.8594EF08
860	Cyclo	14	2	0	1FOH+1FC=O	2.2429EF08
861	Cyclo	5	3	0	1FOH+1FOOH	4.6249EF06
862	Cyclo	6	3	0	1FOH+1FOOH	1.5122EF06
863	Cyclo	7	3	0	1FOH+1FOOH	4.9446EF07
864	Cyclo	8	3	0	1FOH+1FOOH	1.6168EF07
865	Cyclo	9	3	0	1FOH+1FOOH	5.2864EF08
866	Cyclo	10	3	0	1FOH+1FOOH	1.7285EF08
867	Cyclo	11	3	0	1FOH+1FOOH	5.6518EF09
868	Cyclo	12	3	0	1FOH+1FOOH	1.8480EF09
869	Cyclo	13	3	0	1FOH+1FOOH	6.0425EF10
870	Cyclo	14	3	0	1FOH+1FOOH	1.9757EF10

871	Cyclo	5	4	1	1FOH+1FONO ₂	3.5240EF05
872	Cyclo	6	4	1	1FOH+1FONO ₂	1.1523EF05
873	Cyclo	7	4	1	1FOH+1FONO ₂	3.7676EF06
874	Cyclo	8	4	1	1FOH+1FONO ₂	1.2319EF06
875	Cyclo	9	4	1	1FOH+1FONO ₂	4.0280EF07
876	Cyclo	10	4	1	1FOH+1FONO ₂	1.3171EF07
877	Cyclo	11	4	1	1FOH+1FONO ₂	4.3065EF08
878	Cyclo	12	4	1	1FOH+1FONO ₂	1.4081EF08
879	Cyclo	13	4	1	1FOH+1FONO ₂	4.6041EF09
880	Cyclo	14	4	1	1FOH+1FONO ₂	1.5054EF09
881	Cyclo	5	3	0	1FC=O+1FOOH	3.8767EF05
882	Cyclo	6	3	0	1FC=O+1FOOH	1.2676EF05
883	Cyclo	7	3	0	1FC=O+1FOOH	4.1447EF06
884	Cyclo	8	3	0	1FC=O+1FOOH	1.3552EF06
885	Cyclo	9	3	0	1FC=O+1FOOH	4.4312EF07
886	Cyclo	10	3	0	1FC=O+1FOOH	1.4489EF07
887	Cyclo	11	3	0	1FC=O+1FOOH	4.7375EF08
888	Cyclo	12	3	0	1FC=O+1FOOH	1.5490EF08
889	Cyclo	13	3	0	1FC=O+1FOOH	5.0650EF09
890	Cyclo	14	3	0	1FC=O+1FOOH	1.6561EF09
891	Cyclo	5	4	1	1FC=O+1FONO ₂	1.1200EF04
892	Cyclo	6	4	1	1FC=O+1FONO ₂	3.6621EF05
893	Cyclo	7	4	1	1FC=O+1FONO ₂	1.1974EF05
894	Cyclo	8	4	1	1FC=O+1FONO ₂	3.9152EF06
895	Cyclo	9	4	1	1FC=O+1FONO ₂	1.2802EF06
896	Cyclo	10	4	1	1FC=O+1FONO ₂	4.1858EF07
897	Cyclo	11	4	1	1FC=O+1FONO ₂	1.3687EF07
898	Cyclo	12	4	1	1FC=O+1FONO ₂	4.4752EF08
899	Cyclo	13	4	1	1FC=O+1FONO ₂	1.4633EF08
900	Cyclo	14	4	1	1FC=O+1FONO ₂	4.7845EF09
901	Cyclo	5	5	1	1FOOH+1FONO ₂	2.6021EF06
902	Cyclo	6	5	1	1FOOH+1FONO ₂	8.5083EF07
903	Cyclo	7	5	1	1FOOH+1FONO ₂	2.7820EF07
904	Cyclo	8	5	1	1FOOH+1FONO ₂	9.0964EF08
905	Cyclo	9	5	1	1FOOH+1FONO ₂	2.9743EF08
906	Cyclo	10	5	1	1FOOH+1FONO ₂	9.7252EF09
907	Cyclo	11	5	1	1FOOH+1FONO ₂	3.1799EF09
908	Cyclo	12	5	1	1FOOH+1FONO ₂	1.0397EF09
909	Cyclo	13	5	1	1FOOH+1FONO ₂	3.3997EF10
910	Cyclo	14	5	1	1FOOH+1FONO ₂	1.1116EF10

911	Cyclo	5	3	0	2FOH+1FC=O	1.05EF06
912	Cyclo	6	3	0	2FOH+1FC=O	3.43EF07
913	Cyclo	7	3	0	2FOH+1FC=O	1.12EF07
914	Cyclo	8	3	0	2FOH+1FC=O	3.67EF08
915	Cyclo	9	3	0	2FOH+1FC=O	1.20EF08
916	Cyclo	10	3	0	2FOH+1FC=O	3.92EF09
917	Cyclo	11	3	0	2FOH+1FC=O	1.28EF09
918	Cyclo	12	3	0	2FOH+1FC=O	4.19EF10
919	Cyclo	13	3	0	2FOH+1FC=O	1.37EF10
920	Cyclo	14	3	0	2FOH+1FC=O	4.48EF11
921	Cyclo	5	4	0	2FOH+1FOOH	7.07EF09
922	Cyclo	6	4	0	2FOH+1FOOH	2.31EF09
923	Cyclo	7	4	0	2FOH+1FOOH	7.56EF10
924	Cyclo	8	4	0	2FOH+1FOOH	2.47EF10
925	Cyclo	9	4	0	2FOH+1FOOH	8.09EF11
926	Cyclo	10	4	0	2FOH+1FOOH	2.64EF11
927	Cyclo	11	4	0	2FOH+1FOOH	8.64EF12
928	Cyclo	12	4	0	2FOH+1FOOH	2.83EF12
929	Cyclo	13	4	0	2FOH+1FOOH	9.24EF13
930	Cyclo	14	4	0	2FOH+1FOOH	3.02EF13
931	Cyclo	5	5	1	2FOH+1FONO ₂	7.04EF08
932	Cyclo	6	5	1	2FOH+1FONO ₂	2.30EF08
933	Cyclo	7	5	1	2FOH+1FONO ₂	7.53EF09
934	Cyclo	8	5	1	2FOH+1FONO ₂	2.46EF09
935	Cyclo	9	5	1	2FOH+1FONO ₂	8.05EF10
936	Cyclo	10	5	1	2FOH+1FONO ₂	2.63EF10
937	Cyclo	11	5	1	2FOH+1FONO ₂	8.61EF11
938	Cyclo	12	5	1	2FOH+1FONO ₂	2.81EF11
939	Cyclo	13	5	1	2FOH+1FONO ₂	9.20EF12
940	Cyclo	14	5	1	2FOH+1FONO ₂	3.01EF12
941	Cyclo	5	3	0	2FC=O+1FOH	8.65EF05
942	Cyclo	6	3	0	2FC=O+1FOH	2.83EF05
943	Cyclo	7	3	0	2FC=O+1FOH	9.24EF06
944	Cyclo	8	3	0	2FC=O+1FOH	3.02EF06
945	Cyclo	9	3	0	2FC=O+1FOH	9.88EF07
946	Cyclo	10	3	0	2FC=O+1FOH	3.23EF07
947	Cyclo	11	3	0	2FC=O+1FOH	1.06EF07
948	Cyclo	12	3	0	2FC=O+1FOH	3.45EF08
949	Cyclo	13	3	0	2FC=O+1FOH	1.13EF08
950	Cyclo	14	3	0	2FC=O+1FOH	3.69EF09
951	Cyclo	5	4	0	2FC=O+1FOOH	6.38EF06
952	Cyclo	6	4	0	2FC=O+1FOOH	2.09EF06

953	Cyclo	7	4	0	2FC=O+1FOOH	6.83EF07
954	Cyclo	8	4	0	2FC=O+1FOOH	2.23EF07
955	Cyclo	9	4	0	2FC=O+1FOOH	7.30EF08
956	Cyclo	10	4	0	2FC=O+1FOOH	2.39EF08
957	Cyclo	11	4	0	2FC=O+1FOOH	7.80EF09
958	Cyclo	12	4	0	2FC=O+1FOOH	2.55EF09
959	Cyclo	13	4	0	2FC=O+1FOOH	8.34EF10
960	Cyclo	14	4	0	2FC=O+1FOOH	2.73EF10
961	Cyclo	5	5	1	2FC=O+1FONO ₂	1.84EF05
962	Cyclo	6	5	1	2FC=O+1FONO ₂	6.03EF06
963	Cyclo	7	5	1	2FC=O+1FONO ₂	1.97EF06
964	Cyclo	8	5	1	2FC=O+1FONO ₂	6.45EF07
965	Cyclo	9	5	1	2FC=O+1FONO ₂	2.11EF07
966	Cyclo	10	5	1	2FC=O+1FONO ₂	6.89EF08
967	Cyclo	11	5	1	2FC=O+1FONO ₂	2.25EF08
968	Cyclo	12	5	1	2FC=O+1FONO ₂	7.37EF09
969	Cyclo	13	5	1	2FC=O+1FONO ₂	2.41EF09
970	Cyclo	14	5	1	2FC=O+1FONO ₂	7.88EF10
971	Cyclo	5	5	0	2FOOH+1FOH	2.08EF09
972	Cyclo	6	5	0	2FOOH+1FOH	6.81EF10
973	Cyclo	7	5	0	2FOOH+1FOH	2.23EF10
974	Cyclo	8	5	0	2FOOH+1FOH	7.28EF11
975	Cyclo	9	5	0	2FOOH+1FOH	2.38EF11
976	Cyclo	10	5	0	2FOOH+1FOH	7.78EF12
977	Cyclo	11	5	0	2FOOH+1FOH	2.54EF12
978	Cyclo	12	5	0	2FOOH+1FOH	8.32EF13
979	Cyclo	13	5	0	2FOOH+1FOH	2.72EF13
980	Cyclo	14	5	0	2FOOH+1FOH	8.89EF14
981	Cyclo	5	5	0	2FOOH+1FC=O	2.00EF08
982	Cyclo	6	5	0	2FOOH+1FC=O	6.53EF09
983	Cyclo	7	5	0	2FOOH+1FC=O	2.14EF09
984	Cyclo	8	5	0	2FOOH+1FC=O	6.98EF10
985	Cyclo	9	5	0	2FOOH+1FC=O	2.28EF10
986	Cyclo	10	5	0	2FOOH+1FC=O	7.47EF11
987	Cyclo	11	5	0	2FOOH+1FC=O	2.44EF11
988	Cyclo	12	5	0	2FOOH+1FC=O	7.98EF12
989	Cyclo	13	5	0	2FOOH+1FC=O	2.61EF12
990	Cyclo	14	5	0	2FOOH+1FC=O	8.53EF13
991	Cyclo	5	7	1	2FOOH+1FONO ₂	1.34EF09
992	Cyclo	6	7	1	2FOOH+1FONO ₂	4.38EF10
993	Cyclo	7	7	1	2FOOH+1FONO ₂	1.43EF10
994	Cyclo	8	7	1	2FOOH+1FONO ₂	4.69EF11

995	Cyclo	9	7	1	2FOOH+1FONO ₂	1.53EF11
996	Cyclo	10	7	1	2FOOH+1FONO ₂	5.01EF12
997	Cyclo	11	7	1	2FOOH+1FONO ₂	1.64EF12
998	Cyclo	12	7	1	2FOOH+1FONO ₂	5.36EF13
999	Cyclo	13	7	1	2FOOH+1FONO ₂	1.75EF13
1000	Cyclo	14	7	1	2FOOH+1FONO ₂	5.73EF14
1001	Cyclo	5	7	2	2FONO ₂ +1FOH	1.51EF07
1002	Cyclo	6	7	2	2FONO ₂ +1FOH	4.94EF08
1003	Cyclo	7	7	2	2FONO ₂ +1FOH	1.61EF08
1004	Cyclo	8	7	2	2FONO ₂ +1FOH	5.28EF09
1005	Cyclo	9	7	2	2FONO ₂ +1FOH	1.73EF09
1006	Cyclo	10	7	2	2FONO ₂ +1FOH	5.64EF10
1007	Cyclo	11	7	2	2FONO ₂ +1FOH	1.84EF10
1008	Cyclo	12	7	2	2FONO ₂ +1FOH	6.03EF11
1009	Cyclo	13	7	2	2FONO ₂ +1FOH	1.97EF11
1010	Cyclo	14	7	2	2FONO ₂ +1FOH	6.45EF12
1011	Cyclo	5	7	2	2FONO ₂ +1FC=O	4.80EF07
1012	Cyclo	6	7	2	2FONO ₂ +1FC=O	1.57EF07
1013	Cyclo	7	7	2	2FONO ₂ +1FC=O	5.13EF08
1014	Cyclo	8	7	2	2FONO ₂ +1FC=O	1.68EF08
1015	Cyclo	9	7	2	2FONO ₂ +1FC=O	5.48EF09
1016	Cyclo	10	7	2	2FONO ₂ +1FC=O	1.79EF09
1017	Cyclo	11	7	2	2FONO ₂ +1FC=O	5.86EF10
1018	Cyclo	12	7	2	2FONO ₂ +1FC=O	1.92EF10
1019	Cyclo	13	7	2	2FONO ₂ +1FC=O	6.2675EF11
1020	Cyclo	14	7	2	2FONO ₂ +1FC=O	2.0493EF11
1021	Cyclo	5	8	2	2FONO ₂ +1FOOH	1.1145EF08
1022	Cyclo	6	8	2	2FONO ₂ +1FOOH	3.6443EF09
1023	Cyclo	7	8	2	2FONO ₂ +1FOOH	1.1916EF09
1024	Cyclo	8	8	2	2FONO ₂ +1FOOH	3.8962EF10
1025	Cyclo	9	8	2	2FONO ₂ +1FOOH	1.2740EF10
1026	Cyclo	10	8	2	2FONO ₂ +1FOOH	4.1655EF11
1027	Cyclo	11	8	2	2FONO ₂ +1FOOH	1.3620EF11
1028	Cyclo	12	8	2	2FONO ₂ +1FOOH	4.4535EF12
1029	Cyclo	13	8	2	2FONO ₂ +1FOOH	1.4562EF12
1030	Cyclo	14	8	2	2FONO ₂ +1FOOH	4.7613EF13
1031	Cyclo	5	4	0	1FOH+1FC=O+1FOOH	2.9513EF07
1032	Cyclo	6	4	0	1FOH+1FC=O+1FOOH	9.6500EF08
1033	Cyclo	7	4	0	1FOH+1FC=O+1FOOH	3.1553EF08

1034	Cyclo	8	4	0	1FOH+1FC=O+1FOOH	1.0317EF08
1035	Cyclo	9	4	0	1FOH+1FC=O+1FOOH	3.3734EF09
1036	Cyclo	10	4	0	1FOH+1FC=O+1FOOH	1.1030EF09
1037	Cyclo	11	4	0	1FOH+1FC=O+1FOOH	3.6066EF10
1038	Cyclo	12	4	0	1FOH+1FC=O+1FOOH	1.1793EF10
1039	Cyclo	13	4	0	1FOH+1FC=O+1FOOH	3.8559EF11
1040	Cyclo	14	4	0	1FOH+1FC=O+1FOOH	1.2608EF11
1041	Cyclo	5	5	1	1FOH+1FC=O+1FONO ₂	2.2488EF06
1042	Cyclo	6	5	1	1FOH+1FC=O+1FONO ₂	7.3529EF07
1043	Cyclo	7	5	1	1FOH+1FC=O+1FONO ₂	2.4042EF07
1044	Cyclo	8	5	1	1FOH+1FC=O+1FONO ₂	7.8611EF08
1045	Cyclo	9	5	1	1FOH+1FC=O+1FONO ₂	2.5704EF08
1046	Cyclo	10	5	1	1FOH+1FC=O+1FONO ₂	8.4046EF09
1047	Cyclo	11	5	1	1FOH+1FC=O+1FONO ₂	2.7481EF09
1048	Cyclo	12	5	1	1FOH+1FC=O+1FONO ₂	8.9855EF10
1049	Cyclo	13	5	1	1FOH+1FC=O+1FONO ₂	2.9380EF10
1050	Cyclo	14	5	1	1FOH+1FC=O+1FONO ₂	9.6066EF11
1051	Cyclo	5	6	1	1FOH+1FOOH+1FONO ₂	1.9809EF08
1052	Cyclo	6	6	1	1FOH+1FOOH+1FONO ₂	6.4772EF09
1053	Cyclo	7	6	1	1FOH+1FOOH+1FONO ₂	2.1179EF09
1054	Cyclo	8	6	1	1FOH+1FOOH+1FONO ₂	6.9249EF10
1055	Cyclo	9	6	1	1FOH+1FOOH+1FONO ₂	2.2643EF10
1056	Cyclo	10	6	1	1FOH+1FOOH+1FONO ₂	7.4036EF11
1057	Cyclo	11	6	1	1FOH+1FOOH+1FONO ₂	2.4208EF11
1058	Cyclo	12	6	1	1FOH+1FOOH+1FONO ₂	7.9154EF12
1059	Cyclo	13	6	1	1FOH+1FOOH+1FONO ₂	2.5881EF12
1060	Cyclo	14	6	1	1FOH+1FOOH+1FONO ₂	8.4625EF13
1061	Cyclo	5	6	1	1FC=O+1FOOH+1FONO ₂	1.6605EF07
1062	Cyclo	6	6	1	1FC=O+1FOOH+1FONO ₂	5.4294EF08
1063	Cyclo	7	6	1	1FC=O+1FOOH+1FONO ₂	1.7753EF08
1064	Cyclo	8	6	1	1FC=O+1FOOH+1FONO ₂	5.8047EF09
1065	Cyclo	9	6	1	1FC=O+1FOOH+1FONO ₂	1.8980EF09
1066	Cyclo	10	6	1	1FC=O+1FOOH+1FONO ₂	6.2059EF10
1067	Cyclo	11	6	1	1FC=O+1FOOH+1FONO ₂	2.0292EF10
1068	Cyclo	12	6	1	1FC=O+1FOOH+1FONO ₂	6.6349EF11
1069	Cyclo	13	6	1	1FC=O+1FOOH+1FONO ₂	2.1694EF11
1070	Cyclo	14	6	1	1FC=O+1FOOH+1FONO ₂	7.0935EF12
1071	Cyclo	5	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	1.2641EF09
1072	Cyclo	6	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	4.1333EF10

1073	Cyclo	7	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	1.3515EF10
1074	Cyclo	8	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	4.4190EF11
1075	Cyclo	9	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	1.4449EF11
1076	Cyclo	10	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	4.7245EF12
1077	Cyclo	11	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	1.5448EF12
1078	Cyclo	12	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	5.0510EF13
1079	Cyclo	13	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	1.6516EF13
1080	Cyclo	14	7	1	1FOH+1FC=O+1FOOH+1FONO ₂	5.4002EF14

Table S2. Values of best-fit parameters in Equation (2).

Best-fit parameters	Values
n_C^0	2.6212e+01
b_C	4.3909e-01
b_O	1.4606e+00
b_{CO}	1.8457e-02
$b_{(-OH)}$	6.1623e-01
$b_{(-C=O)}$	-6.0560e-01
$b_{(-OOH)}$	-4.7798e-03
$b_{(-ONO2)}$	-2.3032e+00

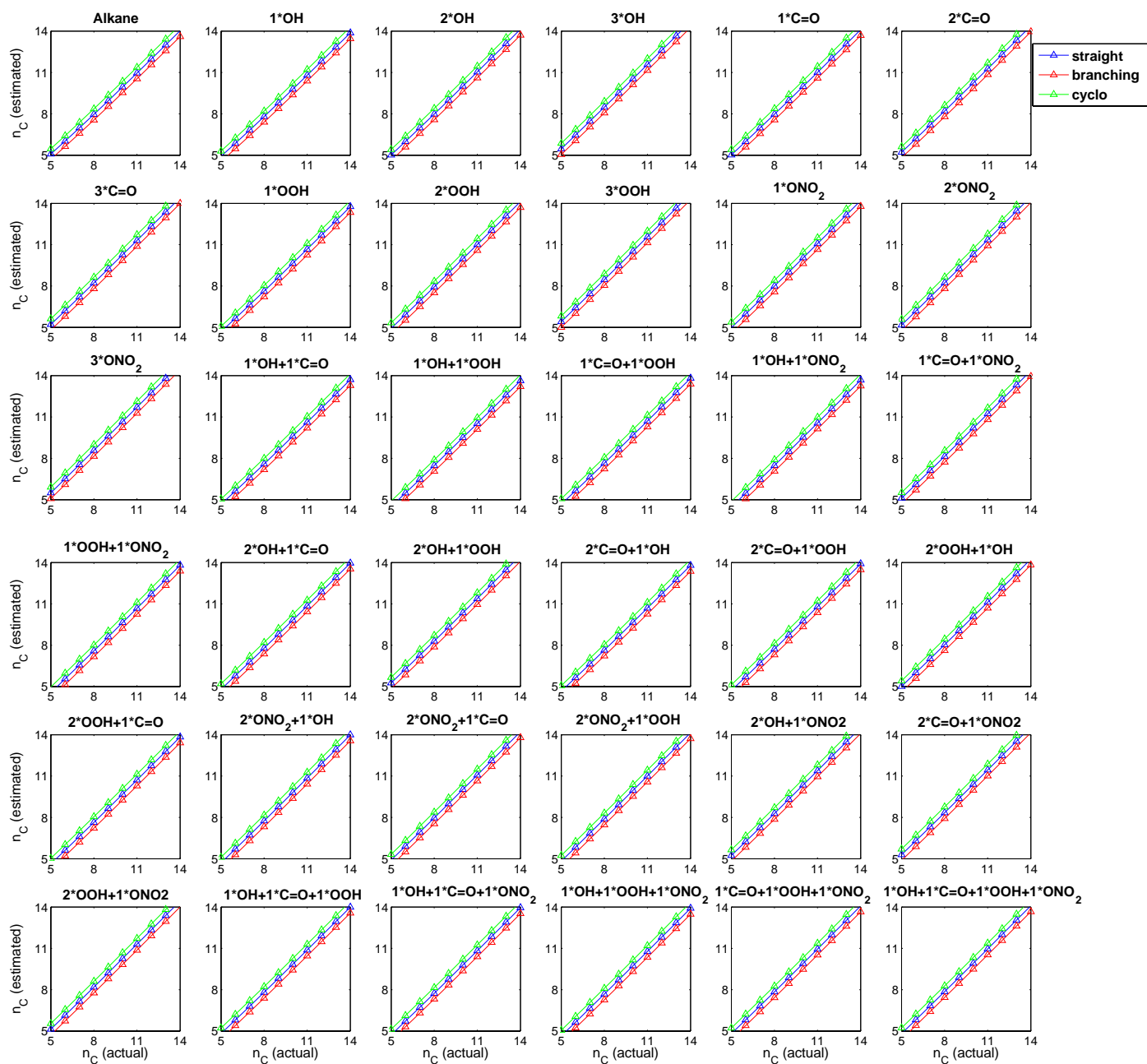


Figure S1. Estimated vs. Actual carbon numbers for 1080 standards.

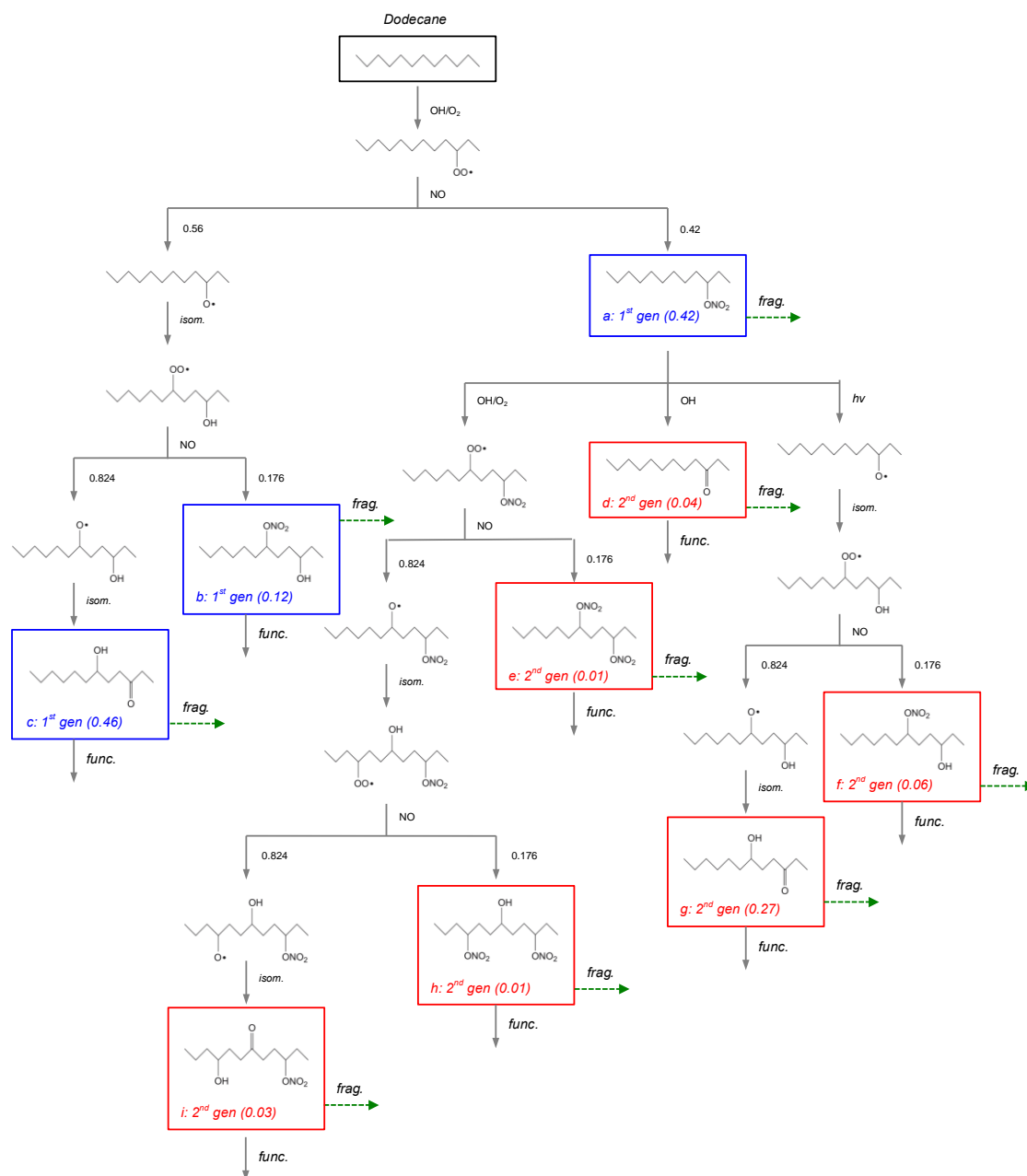


Figure S2. Development of the functionalization vs. fragmentation channels in the FGOM model, using the high-NO_x photooxidation of dodecane as an example.

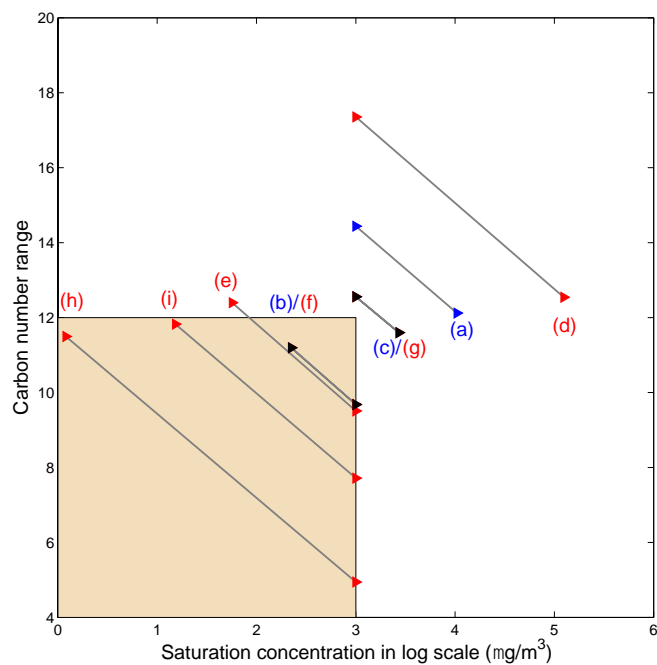


Figure S3. Carbon number range for 1st and 2nd generation products of OH oxidation of dodecane under high-NO_x conditions. For illustration, the shaded region ($C^* \leq 1000 \mu\text{g}/\text{m}^3$) is taken to represent the combination of carbon number and volatility for which a molecule can appreciably partition to the particle phase.