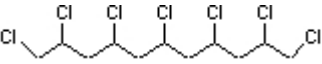


## Supplementary Information for

### The OH-initiated Chemical Transformation of 1,2,4,6,8,10,11-heptachloroundecane in the Atmosphere

Ruirui Liu,<sup>a</sup> Chenxi Zhang,<sup>b</sup> Lingyan Kang,<sup>a</sup> Xiaomin Sun,<sup>\*a</sup> Yan Zhao<sup>c</sup>

**S1 The structures and energies of all the 170 mono-substituted C<sub>11</sub>H<sub>17</sub>Cl<sub>7</sub> isomers** (for mono-substituted C<sub>11</sub>H<sub>17</sub>Cl<sub>7</sub>, there are only 4 C atoms which have no Cl atom attached. All the C atoms are numbered from 1 to 11, and the numbers listed in the table indicate the non-attached C atoms. For example, atom numbers 3,5,7,9 means the structure . All the energies were calculated at b3lyp/6-31+g(d) level.)

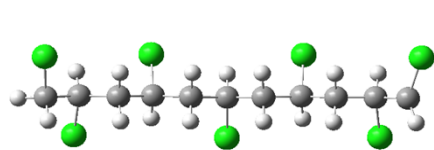
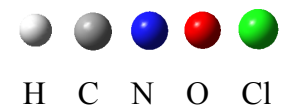
molecule numbers	Energy (- Hartree)	atom numbers	molecule numbers	Energy (- Hartree)	atom numbers	molecule numbers	Energy (- Hartree)	atom numbers
1	3650.8070	1,2,3,4	58	3650.8178	1,3,7,11	115	3650.8230	2,3,5,10
2	3650.8013	1,2,3,5	59	3650.8278	1,3,8,9	116	3650.8140	2,3,6,7
3	3650.7968	1,2,3,6	60	3650.8244	1,3,8,10	117	3650.8238	2,3,6,8
4	3650.8057	1,2,3,7	61	3650.8245	1,3,8,11	118	3650.8309	2,3,6,9
5	3650.8148	1,2,3,8	62	3650.8184	1,3,9,10	119	3650.8337	2,3,6,10
6	3650.8038	1,2,3,9	63	3650.8135	1,3,9,11	120	3650.8104	2,3,7,8
7	3650.8049	1,2,3,10	64	3650.8056	1,4,5,6	121	3650.8233	2,3,7,9
8	3650.8012	1,2,3,11	65	3650.8198	1,4,5,7	122	3650.8222	2,3,7,10
9	3650.7997	1,2,4,5	66	3650.8234	1,4,5,8	123	3650.8139	2,3,8,9

10	3650.8041	1,2,4,6	67	3650.8226	1,4,5,9	124	3650.8222	2,3,8,10
11	3650.8171	1,2,4,7	68	3650.8107	1,4,5,10	125	3650.8034	2,3,9,10
12	3650.8149	1,2,4,8	69	3650.8074	1,4,5,11	126	3650.8005	2,4,5,6
13	3650.8257	1,2,4,9	70	3650.8189	1,4,6,7	127	3650.8150	2,4,5,7
14	3650.8091	1,2,4,10	71	3650.8224	1,4,6,8	128	3650.8188	2,4,5,8
15	3650.8042	1,2,4,11	72	3650.8324	1,4,6,9	129	3650.8178	2,4,5,9
16	3650.8038	1,2,5,6	73	3650.8254	1,4,6,10	130	3650.8177	2,4,5,10
17	3650.8178	1,2,5,7	74	3650.8301	1,4,6,11	131	3650.8125	2,4,6,7
18	3650.8217	1,2,5,8	75	3650.8178	1,4,7,8	132	3650.8201	2,4,6,8
19	3650.8223	1,2,5,9	76	3650.8285	1,4,7,9	133	3650.8272	2,4,6,9
20	3650.8246	1,2,5,10	77	3650.8277	1,4,7,10	134	3650.8130	2,4,6,10
21	3650.8069	1,2,5,11	78	3650.8248	1,4,7,11	135	3650.8186	2,4,7,8
22	3650.8039	1,2,6,7	79	3650.8226	1,4,8,9	136	3560.8135	2,4,7,9
23	3650.8135	1,2,6,8	80	3650.8208	1,4,8,10	137	3650.8175	2,4,7,10
24	3650.8211	1,2,6,9	81	3650.8256	1,4,8,11	138	3650.8180	2,4,8,9
25	3650.8224	1,2,6,10	82	3650.8173	1,4,9,10	139	3650.8146	2,4,8,10
26	3650.8087	1,2,6,11	83	3650.8060	1,5,6,7	140	3650.8091	2,5,6,7
27	3650.8047	1,2,7,8	84	3650.8158	1,5,6,8	141	3650.8188	2,5,6,8
28	3650.8126	1,2,7,9	85	3650.8224	1,5,6,9	142	3650.8181	2,5,6,9
29	3650.8113	1,2,7,10	86	3650.8057	1,5,6,10	143	3650.8088	2,5,6,10
30	3650.8089	1,2,7,11	87	3650.8075	1,5,6,11	144	3650.8226	2,5,7,8
31	3650.8147	1,2,8,9	88	3650.8158	1,5,7,8	145	3650.8255	2,5,7,9
32	3650.8114	1,2,8,10	89	3650.8260	1,5,7,9	146	3650.8235	2,5,7,10
33	3650.8067	1,2,8,11	90	3650.8204	1,5,7,10	147	3650.8260	2,5,8,9

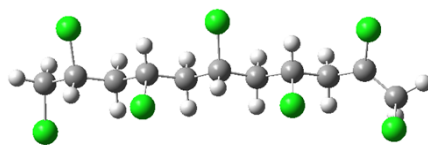
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35	3650.8132	1,2,9,11	92	3650.8232	1,5,8,9	149	3650.8248	2,6,7,9
36	3650.7873	1,2,10,11	93	3650.8200	1,5,8,10	150	3650.8175	2,6,8,9
37	3650.8027	1,3,4,5	94	3650.8142	1,5,9,10	151	3650.8209	2,7,8,9
38	3650.8204	1,3,4,6	95	3650.8065	1,6,7,8	152	3650.8036	3,4,5,6
39	3650.8181	1,3,4,7	96	3650.8191	1,6,7,9	153	3650.8178	3,4,5,7
40	3650.8153	1,3,4,8	97	3650.8108	1,6,7,10	154	3650.8218	3,4,5,8
41	3650.8277	1,3,4,9	98	3650.8198	1,6,8,9	155	3650.8209	3,4,5,9
42	3650.8138	1,3,4,10	99	3650.8147	1,6,8,10	156	3650.8153	2,4,6,7
43	3650.8032	1,3,4,11	100	3650.8268	1,6,9,10	157	3650.8241	3,4,6,8
44	3650.8092	1,3,5,6	101	3650.8053	1,7,8,9	158	3650.8323	3,4,6,9
45	3650.8149	1,3,5,7	102	3650.8019	1,7,8,10	159	3650.8192	3,4,7,8
46	3650.8206	1,3,5,8	103	3650.8192	1,7,9,10	160	3650.8322	3,4,7,9
47	3650.8211	1,3,5,9	104	3650.8007	1,8,9,10	161	3650.8185	3,4,8,9
48	3650.8236	1,3,5,10	105	3650.7982	2,3,4,5	162	3650.8171	3,5,6,7
49	3650.8153	1,3,5,11	106	3650.8170	2,3,4,6	163	3650.8268	3,5,6,8
50	3650.8187	1,3,6,7	107	3650.8154	2,3,4,7	164	3650.8335	3,5,6,9
51	3650.8270	1,3,6,8	108	3650.8123	2,3,4,8	165	3650.8244	3,5,7,8
52	3650.8338	1,3,6,9	109	3650.8073	2,3,4,9	<b>166</b>	<b>3650.8339</b>	<b>3,5,7,9</b>
53	3650.8192	1,3,6,10	110	3650.8107	2,3,4,10	167	3650.8065	3,6,7,8
54	3650.8204	1,3,6,11	111	3650.8064	2,3,5,6	168	3650.8044	4,5,6,7
55	3650.8152	1,3,7,8	112	3650.8194	2,3,5,7	169	3650.8143	4,5,6,8
56	3650.8269	1,3,7,9	113	3650.8245	2,3,5,8	170	3650.8126	4,5,7,8
57	3650.8259	1,3,7,10	114	3650.8248	2,3,5,9			

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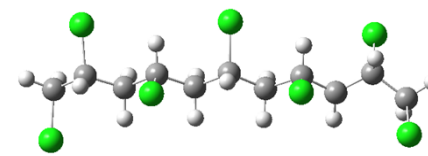
## S2 Structures of intermediates, transition states and products



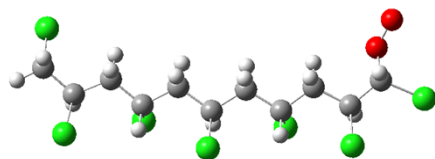
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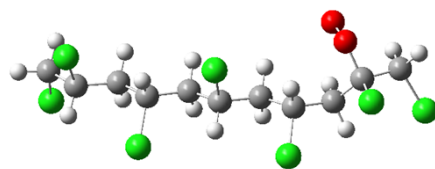
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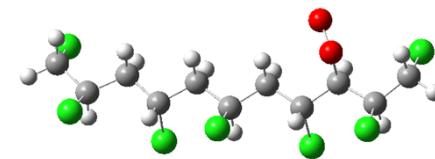
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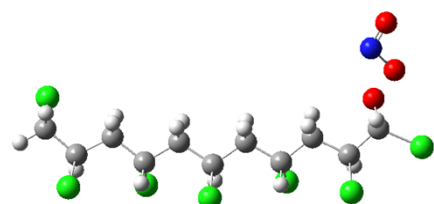
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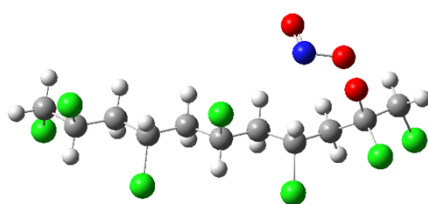
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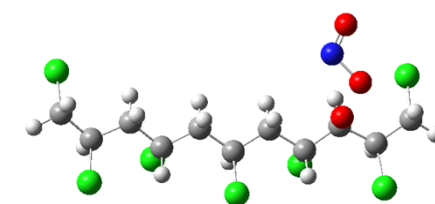
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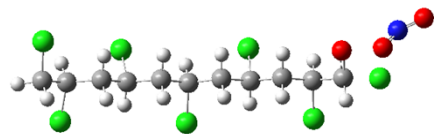
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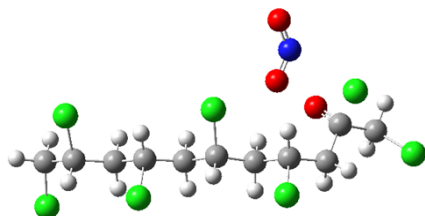
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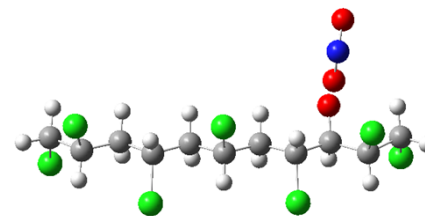
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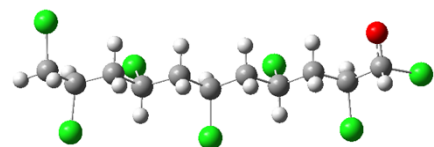
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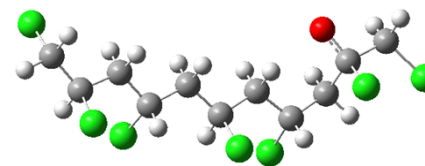
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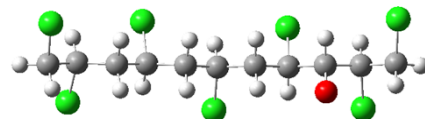
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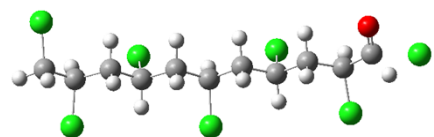
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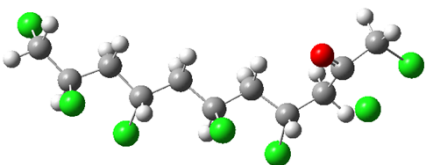
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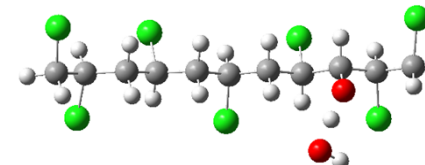
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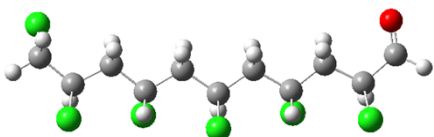
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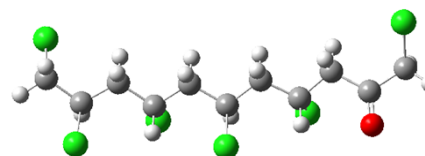
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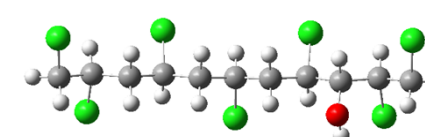
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Pb1



Pb3



Pb5