

Supporting Information
For
Decomposition of Selected Chlorinated Volatile Organic Compounds on
CeO₂

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TS1

<u>-269.34000000</u>	255.54000000	227.13000000
31.04000000	258.65000000	231.78000000
32.45000000	259.43000000	235.77000000
34.76000000	260.74000000	239.93000000
36.13000000	265.85000000	242.75000000
37.53000000	267.51000000	247.73000000
39.42000000	269.05000000	248.89000000
40.91000000	273.45000000	250.43000000
48.49000000	275.51000000	252.90000000
48.85000000	275.65000000	253.36000000
52.63000000	277.94000000	253.81000000
55.77000000	279.84000000	255.01000000
60.30000000	281.95000000	290.21000000
61.51000000	283.91000000	292.13000000
62.60000000	285.69000000	381.52000000
62.79000000	287.21000000	383.72000000
62.88000000	287.89000000	393.97000000
63.79000000	289.01000000	397.10000000
67.44000000	296.11000000	397.53000000
70.75000000	299.19000000	403.03000000
73.85000000	302.87000000	404.32000000
294.44000000	303.58000000	654.35000000
74.63000000	307.80000000	680.84000000
77.18000000	308.64000000	829.08000000
80.52000000	330.91000000	972.75000000
81.04000000	331.45000000	214.59000000
81.71000000	333.26000000	215.88000000
82.60000000	333.67000000	216.93000000
82.91000000	335.69000000	220.79000000
84.00000000	336.48000000	222.18000000
88.05000000	337.92000000	127.48000000
88.39000000	338.22000000	127.78000000
95.59000000	351.66000000	132.57000000
96.38000000	355.15000000	136.68000000
98.02000000	357.43000000	138.22000000
104.18000000	358.54000000	148.33000000
113.14000000	364.25000000	151.58000000
113.56000000	365.07000000	161.16000000
120.24000000	367.18000000	163.01000000
120.85000000	367.28000000	166.34000000
125.85000000	370.97000000	167.56000000
125.94000000	226.46000000	200.29000000
224.16000000	210.13000000	212.26000000

TS2

<u>-828.59000000</u>	126.67000000	288.53000000
16.87000000	127.08000000	289.25000000
28.87000000	128.51000000	295.94000000
30.51000000	131.30000000	296.59000000
32.63000000	137.26000000	298.53000000
33.65000000	148.20000000	300.31000000
33.96000000	153.86000000	302.72000000
34.90000000	155.37000000	303.79000000
38.83000000	159.09000000	309.08000000
43.05000000	165.82000000	311.15000000
44.44000000	166.30000000	312.42000000
46.67000000	168.26000000	318.84000000
52.84000000	204.55000000	320.25000000
62.93000000	207.22000000	323.60000000
63.61000000	211.06000000	325.44000000
63.68000000	212.34000000	328.73000000
65.15000000	215.08000000	342.27000000
66.27000000	215.75000000	343.93000000
67.87000000	216.50000000	345.30000000
73.85000000	218.74000000	346.73000000
74.90000000	222.13000000	348.47000000
81.43000000	224.70000000	352.42000000
83.38000000	228.66000000	358.23000000
84.05000000	233.11000000	360.29000000
85.06000000	233.84000000	361.27000000
85.66000000	234.42000000	362.72000000
86.24000000	238.39000000	364.05000000
87.60000000	248.81000000	366.19000000
88.29000000	252.06000000	366.57000000
90.33000000	266.54000000	368.18000000
92.14000000	270.14000000	375.98000000
97.08000000	273.17000000	377.78000000
97.29000000	273.60000000	378.89000000
98.86000000	275.77000000	379.70000000
100.34000000	276.43000000	382.05000000
100.78000000	279.84000000	382.85000000
104.11000000	282.70000000	383.75000000
105.79000000	283.15000000	385.83000000
108.88000000	286.67000000	386.67000000
111.16000000	287.41000000	389.67000000
114.09000000	424.21000000	397.36000000
114.26000000	425.62000000	409.67000000
423.65000000	428.93000000	413.54000000

TS3

<u>-1056.910</u>	119.30000000	264.42000000
254.76000000	122.46000000	268.64000000
134.09000000	125.22000000	270.29000000
68.76000000	125.63000000	270.69000000
13.23000000	127.06000000	274.81000000
16.13000000	127.37000000	275.65000000
19.53000000	132.11000000	277.02000000
34.05000000	136.25000000	277.04000000
35.11000000	137.90000000	277.68000000
36.47000000	147.50000000	278.66000000
38.01000000	151.12000000	281.70000000
41.31000000	161.70000000	283.62000000
48.29000000	165.34000000	285.42000000
48.71000000	167.09000000	286.83000000
52.61000000	181.38000000	287.67000000
55.56000000	201.72000000	288.71000000
60.02000000	208.45000000	292.16000000
61.52000000	213.41000000	295.35000000
62.47000000	215.42000000	296.90000000
62.55000000	217.88000000	299.09000000
62.72000000	218.51000000	299.95000000
64.23000000	220.00000000	301.40000000
73.25000000	223.29000000	307.54000000
74.19000000	224.22000000	311.24000000
76.23000000	225.63000000	330.65000000
79.78000000	226.67000000	331.99000000
80.63000000	230.20000000	333.11000000
81.59000000	232.05000000	334.02000000
82.30000000	239.13000000	335.13000000
82.51000000	244.86000000	335.57000000
83.11000000	249.11000000	337.52000000
87.72000000	250.20000000	338.03000000
88.62000000	251.21000000	349.44000000
94.96000000	255.92000000	354.15000000
96.34000000	256.87000000	354.99000000
97.54000000	257.63000000	356.71000000
101.76000000	257.75000000	360.94000000
106.47000000	260.04000000	361.70000000
112.35000000	262.10000000	363.14000000
112.97000000	262.62000000	364.55000000
374.64000000	398.38000000	366.89000000
381.88000000	401.44000000	371.76000000
391.17000000	511.19000000	613.31000000

393.32000000	571.47000000	3.100560e+003
395.75000000	1.540560e+003	3.166090e+003

TS5

-440.6	167.6	337.1
36.9	214.8	338.6
37.4	217.7	342.8
46.4	219.9	343.3
50.4	221.8	344.2
51.1	222.4	347.5
61.5	224.0	348.4
62.2	227.3	349.2
62.8	230.0	351.2
64.1	233.0	352.4
64.5	235.0	353.0
66.7	236.3	354.3
67.0	239.4	356.7
68.9	241.6	357.8
71.0	244.4	360.8
71.2	249.2	362.8
72.1	251.9	367.4
77.5	253.7	373.2
77.9	260.1	384.9
79.4	261.2	385.2
80.4	263.2	391.8
81.5	263.4	392.9
84.4	264.2	394.0
85.0	266.7	491.4
85.9	267.7	701.4
86.0	269.4	847.5
88.4	270.1	1019.7
88.6	271.1	1090.0
103.2	271.6	1245.6
104.6	273.0	1277.7
105.7	273.7	1309.9
107.4	276.3	1336.9
112.0	278.9	2781.7
112.1	280.5	2867.0
122.0	282.7	3042.4
123.9	284.1	3156.5
125.1	285.7	3316.8
125.8	286.9	308.3
128.8	287.2	309.2
129.3	289.1	312.3
135.1	290.4	329.9

137.8	291.9	164.6
138.2	293.5	167.0
153.6	301.7	
154.0	303.1	
305.2		
306.9		

TS6

	215.6	338.6
-716.4	220.1	339.3
0.9	222.1	341.7
20.4	222.6	343.5
35.4	223.2	344.3
37.9	224.9	344.7
49.6	229.5	346.0
51.2	233.9	348.3
53.8	234.5	349.0
60.2	236.4	350.5
61.9	236.6	351.6
62.9	239.5	352.5
64.0	241.5	353.1
65.2	245.0	355.0
66.4	247.9	356.9
66.8	248.9	360.3
68.8	251.0	361.1
71.3	253.5	366.1
71.4	260.6	367.5
76.7	261.4	369.9
77.0	263.2	382.5
79.2	265.0	385.7
79.6	267.4	392.1
81.2	267.9	392.6
84.1	268.0	393.3
84.8	269.9	662.8
85.3	271.3	736.1
86.9	273.1	778.8
87.9	273.7	823.8
89.1	274.8	1089.5
103.4	275.2	1220.3
105.1	282.3	1321.9
105.5	284.3	1438.6
106.8	285.4	2814.0
110.0	286.3	2880.0
111.3	287.3	2981.4
119.5	288.2	3115.1
123.7	292.7	306.6

124.7	293.2	310.8
125.7	295.6	311.5
127.9	298.3	316.4
129.1	302.6	317.5
134.9	302.8	329.6
135.7	303.4	153.8
137.3		164.6
137.8		166.5
153.0		167.0

TS8

-227.2	210.7	338.7
17.1	211.2	339.7
27.1	214.7	341.4
31.4	216.2	345.5
32.4	220.8	347.7
34.0	222.9	353.1
36.7	224.8	355.1
40.2	227.5	357.7
46.4	231.3	370.5
48.1	231.8	374.7
49.8	235.9	378.3
55.4	238.2	381.0
57.7	241.9	386.6
61.4	245.4	389.0
62.5	247.2	391.1
63.0	249.0	393.9
64.1	253.5	409.5
65.3	256.0	413.6
73.6	258.3	592.8
74.8	259.5	684.5
75.9	260.1	690.5
76.5	261.7	937.1
79.1	263.9	1255.2
80.8	264.6	1453.5
81.4	266.2	2994.0
83.2	269.1	3060.4
84.7	270.2	3083.4
87.0	273.1	331.7
87.4	275.1	333.8
93.8	276.3	334.6
94.7	277.8	
96.7	280.2	
103.5	283.5	
111.5	284.6	

112.0	286.7
115.1	288.1
123.2	289.9
125.3	291.2
126.6	292.5
127.6	294.3
130.1	297.6
133.6	301.8
137.7	303.8
138.6	305.3
149.3	311.2
149.9	320.4
163.5	323.4
163.9	323.5
166.4	
188.7	

TS16

-370.5	114.4	370.0
11.9	122.0	374.4
27.8	123.6	382.3
37.4	124.6	385.9
37.5	125.0	387.4
50.7	129.1	393.2
50.9	129.7	393.7
61.4	135.6	395.4
62.0	138.0	500.4
62.4	138.9	532.7
64.2	153.6	571.0
64.8	154.0	594.7
66.5	165.1	671.8
66.7	167.1	683.6
68.9	167.5	763.1
70.6	200.3	874.5
71.1	213.1	949.3
77.1	217.0	978.0
78.7	220.5	1017.5
79.0	222.5	1086.7
79.6	223.6	1181.2
81.0	226.0	1278.0
84.3	227.9	1306.0
84.5	232.6	1355.9
85.9	234.3	1404.5
85.9	235.4	1433.0

88.1	238.6	2977.0
88.4	241.1	2990.3
102.4	244.7	2994.5
103.9	247.3	3001.2
105.2	248.2	301.4
105.8	255.7	303.4
110.3	256.3	304.7
111.7	261.1	305.9
271.9	262.6	306.7
273.5	264.9	308.6
274.3	265.3	313.0
277.0	266.2	329.6
278.6	267.1	335.6
280.2	269.1	336.8
281.9	269.6	343.6
283.1	270.7	344.9
285.0	271.5	345.4
285.3	347.6	356.0
286.0	348.4	357.1
287.4	350.2	357.4
289.0	353.2	362.3
290.7	354.0	364.5
292.4	354.5	299.0

TS21

	327.6	217.2
-678.4	335.5	223.0
35.3	338.5	223.8
39.2	339.2	224.7
47.5	340.9	225.5
49.7	341.4	226.4
52.8	343.4	231.8
59.9	346.7	234.3
60.2	347.6	235.0
62.6	348.2	237.4
63.5	353.3	237.8
64.4	356.5	241.0
65.2	357.4	243.3
66.6	360.0	248.8
68.4	364.4	250.2
70.3	369.2	254.6
70.9	373.2	255.4
73.4	376.3	256.9
76.3	380.7	261.3
77.2	388.5	264.8

78.8	390.1	265.9
79.7	391.8	266.5
81.8	393.1	267.3
83.7	399.7	269.4
84.9	405.8	270.4
86.7	425.1	271.0
88.7	456.5	271.9
88.9	510.9	272.8
96.0	568.3	275.3
98.7	599.3	277.2
103.0	654.8	281.3
105.2	708.2	282.4
107.3	781.1	283.5
109.5	804.3	285.0
112.8	841.8	285.7
117.0	920.6	287.3
123.5	983.9	289.3
124.7	1058.6	290.0
125.2	1117.7	291.2
128.7	1129.1	294.4
130.5	1223.4	296.7
130.7	1297.4	298.4
133.0	1335.5	302.4
137.5	1402.0	305.3
140.2	1414.6	305.6
140.5	1445.6	306.9
155.1	1472.6	318.0
156.7	1631.6	
168.4	2849.5	
169.9	2858.8	
174.8	2880.3	
180.6	2956.9	

TS19

-39.9	305.3	234.6
30.2	306.9	235.1
36.4	310.8	236.3
37.5	312.5	238.5
41.7	315.3	239.6
48.7	317.6	246.1
50.3	322.8	246.8
51.0	328.7	255.2
60.4	336.3	257.0
61.1	340.2	257.4

62.3	341.1	259.3
63.8	344.9	261.9
64.5	346.2	265.6
64.9	348.0	266.2
66.2	349.1	267.0
68.6	351.0	267.3
70.6	351.9	268.6
71.5	353.0	270.7
73.0	353.8	271.5
77.4	354.8	271.9
78.1	355.7	273.2
79.5	357.1	273.9
80.5	361.5	276.9
82.1	363.0	278.0
83.5	364.9	281.7
85.0	365.7	284.8
85.8	369.9	285.4
88.2	384.4	286.9
89.0	387.3	288.4
95.1	392.9	290.2
103.5	393.9	291.3
104.4	394.8	293.7
105.6	502.5	294.8
106.2	514.6	298.5
111.3	531.8	300.8
113.4	564.8	303.5
120.1	584.4	234.6
123.5	604.2	235.1
124.8	642.7	236.3
126.7	713.8	238.5
128.0	763.3	239.6
129.7	790.8	246.1
132.1	933.5	246.8
134.6	962.1	255.2
138.6	979.3	257.0
140.2	1013.1	257.4
141.7	1095.3	259.3
153.7	1096.0	261.9
154.2	1230.0	265.6
165.3	1352.3	266.2
168.1	1366.6	267.0
169.5	1412.4	267.3
190.1	1449.4	268.6
209.7	1464.0	270.7
218.0	2987.3	271.5

221.4	2991.8	271.9
223.6	2998.6	273.2
224.3	3005.9	273.9
227.1	3007.3	276.9
229.9	3234.0	278.0
232.6	281.7	
290.2	284.8	
291.3	285.4	
293.7	286.9	
294.8	288.4	
298.5		
300.8		
303.5		

TS17

-187.4	306.6	167.1
9.4	309.7	173.1
15.0	310.8	218.9
28.1	317.2	221.8
33.7	321.2	223.7
37.3	324.8	227.2
44.0	326.5	228.0
47.3	330.7	229.4
49.2	333.5	231.3
51.7	337.5	233.2
59.3	338.1	233.9
61.0	340.0	236.8
61.8	343.8	240.6
63.5	344.3	244.5
64.0	346.4	247.8
64.4	347.8	251.0
66.8	354.8	253.9
68.5	355.5	254.4
69.3	360.4	256.7
70.9	361.3	261.7
74.4	363.1	264.0
75.2	369.2	267.1
76.1	373.7	268.2
77.6	377.4	268.5
79.4	386.7	270.0
81.9	393.0	271.4
83.1	393.8	273.0
84.5	398.0	276.7
85.1	403.9	278.4

87.6	521.4	279.8
88.9	525.9	281.8
92.2	541.5	285.4
97.5	602.4	286.9
98.8	652.0	289.1
102.6	709.0	290.8
105.4	783.6	295.1
108.0	813.3	295.6
109.1	864.2	297.6
111.7	929.3	301.6
112.7	975.9	302.8
118.4	991.6	305.1
123.6	1076.2	138.4
125.4	1089.6	139.4
126.7	1195.2	146.7
129.6	1302.8	150.7
130.8	1313.9	161.5
132.3	1375.8	163.2
137.7	1382.2	2890.5
2980.2	1526.6	2978.3
2989.0	2855.0	

TS22

-388.5	323.0	220.6
26.6	330.7	223.6
38.0	334.6	225.4
43.8	335.7	226.9
48.0	338.8	230.5
49.9	340.5	232.2
59.6	341.9	234.3
61.7	342.9	234.6
62.6	346.2	236.7
64.3	347.0	240.8
64.7	350.6	242.7
65.3	353.4	249.2
66.1	355.7	251.8
68.4	356.6	254.8
69.0	363.1	257.7
70.9	370.3	260.5
74.4	373.0	261.2
75.8	375.4	262.9
78.5	379.1	265.2
79.6	381.7	266.9
81.3	389.7	268.1

82.7	392.7	269.6
84.4	398.1	270.3
85.2	404.7	272.2
86.6	410.1	274.1
88.3	418.9	275.6
88.9	456.3	276.2
99.6	508.9	278.2
100.4	544.4	282.2
103.1	574.2	283.4
105.0	608.1	284.5
108.2	613.3	285.9
113.2	696.4	287.7
114.9	752.4	289.9
118.2	800.4	291.0
121.1	802.8	293.5
123.9	941.7	296.1
128.5	978.0	296.8
129.1	1027.7	299.1
131.4	1097.3	302.4
132.3	1105.9	303.6
138.6	1203.6	307.1
140.2	1244.6	310.6
143.1	1357.5	2982.4
153.3	1392.0	2992.3
156.0	1421.4	2997.3
161.6	1465.9	3004.5
166.4	1483.7	
169.0	2968.8	
169.9	185.0	
174.9	187.6	