Supporting Information for

A Quantum Mechanical Study on the Formation of PCDD/Fs from 2-Chlorophenol as Precursor

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Six pages

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Table S1. Imaginary frequencies (cm^{-1}) for the transition states involved in the formation of PCDD/Fs from 2-CP as precursor.

Figure S1. MPWB1K/6-31+G(d,p) optimized geometries for the transition states involved in the formation of PCDD/Fs from 2-CP as precursor. Distances are in angstroms.

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Table S1. Imaginary frequencies (cm^{-1}) for the transition states involved in the formation of PCDD/Fs from 2-CP as precursor.

Transition States	Frequencies	Transition States	Frequencies
TS1	906i	TS15	2509i
TS2	514i	TS16	2257i
TS3	371i	TS17	685i
TS4	494i	TS18	526i
TS5	427i	TS19	1546i
TS6	983i	TS20	2222i
TS7	1138i	TS21	284i
TS8	344i	TS22	901i
TS9	468i	TS23	617i
TS10	410i	TS24	412i
TS11	991i	TS25	2258i
TS12	184i	TS26	634i
TS13	1247i	TS27	503i
TS14	478i		

Figure S1. MPWB1K/6-31+G(d,p) optimized geometries for the transition states involved in the formation of PCDD/Fs from 2-CP as precursor. Distances are in angstroms.

Figure S1 (Continued).

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