Supporting Information

B3LYP/6-31G(d)-calculated frequencies below 260 cm^{-1} for PCDDs, polychlorinated benzenes, and other reference compounds used in this work, and the difference between the thermal corrections calculated taking the low frequencies as free rotors and as harmonic oscillators.

Compound	Low frequencies, in cm^{-1}	Difference, in kcal mol^{-1}
DD	36.3; 125.7; 232.3; 241.3	-0.45
1-CDD	33.5; 87.9; 152.1; 189.0; 244.1	-0.65
2-CDD	28.6; 101.8; 164.4; 165.9; 239.4	-0.65
2,3-DCDD	29.4; 72.9; 154.4; 159.8; 174.5; 195.1	-0.83
2,3,7,8-TCDD	20.7; 49.9; 113.0; 114.0; 138.9; 172.8; 184.6; 199.9; 222.5; 229.9; 257.8	-1.26
1,2,3,7,8-PCDD	19.2; 46.1; 81.7; 103.9; 124.6; 148.3; 176.1; 180.9; 203.5; 213.7; 224.6; 247.4	-1.47
1,2,3,4,7,8-HCDD	18.3; 44.2; 74.2; 83.6; 96.4; 141.7; 150.6; 175.9; 185.5; 205.7; 208.5; 221.8; 226.0	-1.68
1,2,3,6,7,8-HCDD	17.2; 40.9; 78.5; 86.7; 98.0; 128.1; 169.4; 174.1; 174.8; 204.0; 209.6; 217.8; 221.7	-1.69
1,2,3,7,8,9-HCDD	18.8; 39.4; 79.9; 82.8; 95.2; 145.1; 149.0; 177.1; 188.3; 200.3; 209.8; 217.2; 221.9	-1.68
1,2,3,4,6,7,8-HpCDD	16.8; 37.2; 72.0; 82.1; 86.6; 91.0; 147.2; 166.3; 175.6; 188.3; 195.0; 213.4; 216.1; 221.0; 226.4	-1.91
OCDD	15.8; 33.5; 66.3; 81.6; 83.3; 85.8; 87.6; 159.5; 169.5; 182.9; 185.4;	-2.14

	189.0; 214.1; 218.5; 219.7; 226.0; 226.2	
Chlorobenzene	190.1	-0.07
1,2-Dichlorobenzene	137.8; 201.5; 236.0	-0.22
1,3-Dichlorobenzene	168.7; 197.3; 205.3	-0.22
1,4-Dichlorobenzene	103.3; 221.0	-0.21
1,2,3-Trichlorobenzene	85.0; 204.8; 208.9; 215.4; 250.6	-0.37
1,2,4-Trichlorobenzene	97.0; 173.1; 195.5; 210.0	-0.39
1,3,5-Trichlorobenzene	136.1; 188.7; 189.0; 206.7; 206.8	-0.39
1,2,3,4-Tetrachlorobenzene	81.3; 97.3; 209.8; 213.5; 226.1; 246.0	-0.53
1,2,3,5-Tetrachlorobenzene	75.4; 139.8; 190.3; 204.4; 206.3; 218.2	-0.56
1,2,4,5-Tetrachlorobenzene	70.0; 133.1; 189.9; 206.7; 209.4; 220.2	-0.57
Pentachlorobenzene	68.7; 81.8; 145.5; 199.8; 213.8; 220.4; 231.5	-0.90
Hexachlorobenzene	66.5; 66.6; 92.6; 168.6; 220.2; 220.6; 226.9; 226.9; 243.5	-1.13
1,4-Dioxane	257.0	-0.01