Supplementary Information

Unveiling the reactions of triethylphosphite and its diethylamino substituted derivatives to carbon tetrachloride with a molecular electron density theory perspective

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Table S1 — B3LYP/6-311G(d,p) calculated ELF basin populations at the reagents **1- 4**

	1	**3**	**4**	**2**
V(O1)	4.77			
V(O2)	2.38	2.36		
V'O2)	2.47	2.49		
V(O3)	2.19	2.31	2.47	
V'(O3)	2.69	2.59	2.41	
V(P,O1)	1.57			
V(P,O2)	1.46	1.45		
V(P,O3)	1.41	1.39	1.38	
V(N1)		1.69	1.74	
V(N2)			1.01	
V'(N2)			1.63	
V(N3)				
V(P,N1)		2.63	2.62	
V(P,N2)			1.7	
V(P,N3)				
V(P)	2.23	2.23	2.19	
V(Cl1)				2.17
V'(Cl1)				2.13
V''(Cl1)				2.09
V(Cl2)				2.13
V'(Cl2)				2.17
V''(Cl2)				2.09
V(Cl3)				2.09
V'(Cl3)				2.17
V''(Cl3)				2.13
V(Cl4)				2.09
V'(Cl4)				2.13
V''(Cl4)				2.17
V(C,Cl1)				1.55
V(C,Cl2)				1.51
V(C,Cl3)				1.53
V(C,Cl4)				1.48

Table S2 — B3LYP/6-311G(d,p) calculated total energies, enthalpies, entropies and Gibbs freeenergies, computed in au of the stationary points involved in the reactions of **1, 3** and **4** with **2**.				
	E	H	S	G
1	-804.897505	-804.669764	121.53	-804.727506
2	-1878.977053	-1878.961267	74.127	-1878.996487
3	-863.653825	-863.354744	137.351	-863.420004
4	-922.404373	-922.034934	141.799	-922.102307
TS1C	-2683.788096	-2683.543208	164.755	-2683.621488
P1C	-2683.91232	-2683.667663	196.573	-2683.761061
TS1Cl	-2683.812938	-2683.568445	175.92	-2683.65203
P1Cl	-2683.94679	-2683.701455	196.916	-2683.795016
TS2C	-2742.546197	-2742.229788	172.771	-2742.311877
P2C	-2742.673044	-2742.356724	209.057	-2742.456053
TS2Cl	-2742.576436	-2742.260457	183.745	-2742.34776
P2Cl	-2742.71107	-2742.39401	209.354	-2742.493481
TS3C	-2801.305607	-2800.917513	184.417	-2801.005136
P3C	-2801.420309	-2801.03231	217.69	-2801.135741
TS3Cl	-2801.337874	-2800.95041	195.42	-2801.04326
P3Cl	-2801.464515	-2801.075877	220.998	-2801.18088

Table S3 — B3LYP/6-311G(d,p) calculated most significant ELF basin populations at **TS1C** and **TS1Cl**

	TS1C		**TS1Cl**
V(Cl27)	0.13	V(Cl29)	2.50
V(Cl27)	2.49	V(Cl19)	1.22
V(Cl27)	0.11	V(Cl19)	4.56
V(Cl28)	1.22	V(Cl29)	1.50
V(Cl28)	1.52	V(Cl29)	2.43
V(Cl28)	2.44	V(Cl19)	2.44
V(Cl28)	2.04	V(Cl28)	2.45
V(Cl29)	0.08	V(Cl28)	1.91
V(Cl29)	2.41	V(Cl28)	2.47
V(Cl29)	0.08	V(Cl30)	2.16
V(Cl29)	0.19	V(Cl30)	2.47
V(Cl30)	1.99	V(Cl30)	1.35
V(Cl30)	0.51	V(Cl30)	1.36
V(Cl30)	0.64		
V(Cl30)	1.51		
V(Cl30)	2.33		
V(Cl30)	0.50		
V(Cl30)	1.50		
v(C26,Cl29)	0.43	V(C27,Cl30)	2.00
V(C26, Cl28)	1.72	V(C27,Cl28)	1.52
V(C26, Cl27)	1.72	V(C27,Cl29)	1.37
V(O2)	2.46	V(O2)	2.39
V(O2)	2.35	V(O2)	2.42
V(O3)	2.45	V(O3)	2.39
V(O3)	2.10	V(O3)	2.41
V(O4)	2.08	V(O4)	2.47
V(O4)	2.37	V(O4)	2.35
V(O4)	2.45		
V(P)	1.90	V(P1)	1.51
V(C26)	1.53	V(C27)	1.73
V(P1,O4)	2.12	V(P1,O4)	1.52
V(P1,O3)	1.73	V(P1,O3)	1.53
V(P1,O2)	1.52	V(P1,O2)	1.67