Supplemental Material

Detection of chemical weapon agents using spectroscopic probes: A Computational Study

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S1. Surface Response

Table S1. Values for angles. energies of ground-state (GS) and excited-state (ES) and wavelength calculated for combination of angles employed for building Surface Response.

α 1	**α 2**	**E (GS)**	**E1 (ES)**	**λ (nm)**
0	0	-1900.32	3.00	385.75
180	180	-1900.17	2.59	478.47
-180	180	-1900.21	2.62	472.07
-180	-180	-1900.17	2.59	478.48
180	-180	-1900.17	2.59	478.48
0	180	-1900.30	3.10	398.72
0	-180	-1900.30	3.10	398.84
180	0	-1900.29	3.03	408.72
-180	0	-1900.29	3.04	407.05
90	90	-1900.31	3.44	360.26
-90	90	-1900.31	3.53	351.21
90	-90	-1900.30	3.45	359
-90	-90	-1900.31	3.48	355.29
0	100	-1900.31	3.19	387.91
100	0	-1900.30	3.46	357.87
50	0	-1900.31	3.28	377.02
0	50	-1900.31	3.14	393.92
-50	0	-1900.31	3.33	372.27
-40	0	-1900.31	3.28	377.32
-30	0	-1900.31	3.24	381.89
-20	0	-1900.31	3.21	385.34
-10	0	-1900.31	3.20	386.84
10	0	-1900.32	3.23	383.83
20	0	-1900.32	3.25	381.22
30	0	-1900.31	3.22	384.3
40	0	-1900.31	3.25	380.66
50	0	-1900.31	3.28	377.02

Table S2. Values for angles. energies of ground-state (GS) and excited-state (ES) and wavelength calculated for combination of angles employed for building Surface Response in water solvent.

α 1	α 2	E (GS)	E1 (ES)	λ (nm)
0	0	-1900.34	3.00	394.16
180	180	-1900.19	2.64	468.36
-180	180	-1900.24	3.04	407.09
-180	-180	-1900.19	2.64	468.36
180	-180	-1900.19	2.64	468.36
0	180	-1900.32	3.12	397.35
0	-180	-1900.32	3.11	398.17
180	0	-1900.31	3.18	389.78
-180	0	-1900.31	3.18	389.21
90	90	-1900.33	3.26	379.36
-90	90	-1900.33	3.18	389.05
90	-90	-1900.33	3.26	380.17
-90	-90	-1900.34	3.55	348.74
0	100	-1900.34	3.14	393.67
100	0	-1900.33	3.43	361.34
50	0	-1900.34	3.22	384.39
0	50	-1900.33	3.07	402.71
-50	0	-1900.33	3.28	377.71
-40	0	-1900.34	3.23	383.04
-30	0	-1900.34	3.19	387.79
-20	0	-1900.34	3.16	391.52
-10	0	-1900.34	3.14	393.78
10	0	-1900.34	3.04	407.1
20	0	-1900.34	3.07	402.93
30	0	-1900.34	3.10	398.79
40	0	-1900.34	3.14	394.54
50	0	-1900.34	3.22	384.41

Table S3. Values for geometric properties from Organophosphorus compounds and the complex with Oxime (distances in Å).

	1P – 2O	1P – 3O	1P – 4O	1P – 5X	1P – 6S	1P – 24N	1P - C	1P - O
Ciclosarin	1.46	1.58	1.59	1.60				
DCP	1.47	1.58	1.60	2.08				
DFP	1.47	1.58	1.60	1.60				
GV	1.48			1.61	2.10	1.66		
VG	1.50	1.71	1.71		1.71			
Sarin	1.46	1.59		1.60			1.58	
Soman	1.46	1.59		1.60			1.58	
Oxime-Ciclosarin	1.48	1.66	1.60					1.80
Oxime-DFP	1.50	1.70	1.71					1.70
Oxime-GV	1.48	1.67	1.82			1.67		
Oxime-VG	1.47	1.60	1.59					1.64
Oxime-Sarin	1.48	1.66	1.60				1.80	
Oxime-Soman	1.48	1.66	1.60				1.80	