Supporting Information

Participation of phosphorylated analogues of nitroethene in Diels-Alder reactions with anthracene: A Molecular Electron Density Theory study and mechanistic aspect

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Table S1. The relative enthalpies, Gibbs free energy (ΔH and ΔG, in kcal·mol^{-1}) and entropies (ΔS, in cal·mol^{-1}·K^{-1}), computed in benzene, for the stationary points involved in the reactions of the bis(2-chloroethyl) 2-nitro **1a** and bis(2-chloroethyl) 2-bromo-2-nitroethenylphosphonates **1b** with anthracene **2**.

Basic set	Transition	ΔH_{353}	ΔG_{353}	ΔS_{353}
6-31+G(d)	**1+2→MC1**	-0.5	7.9	-28.1
	1+2→TS1	23.3	38.5	-51.0
	1+2→3a	-11.0	4.7	-52.4
	1+2→MC2	-4.3	3.5	-26.4
	1+2→TS2	16.4	30.3	-46.6
	1+2→3b	-16.3	-1.3	-50.6
6-31+G(d,p)	**1+2→MC1**	-0.5	8.0	-28.4
	1+2→TS1	23.4	38.8	-51.7
	1+2→3a	-10.4	5.3	-52.9
	1+2→MC2	-4.4	3.5	-26.5
	1+2→TS2	16.5	31.2	-49.1
	1+2→3b	-16.4	-1.1	-53.4

Table S2. B3LYP(PCM) total electronic energies (E, in a.u.) in benzene, of the stationary points involved in the DA reactions between bis(2-chloroethyl) 2-nitro-ethenylphosphonate **1a** and bis(2-chloroethyl) 2-bromo-2-nitroethenylphosphonates **1b** with anthracene **2**.

	6-31G(d)	**6-31+G(d)**	**6-31+G(d,p)**
1a	-1927.023739	-1927.057700	-1927.071936
1b	-4498.124762	-4498.178295	-4498.191004
2	-539.328383	-539.347094	-539.363041
MC1	-24.66.354600	-2466.404628	-2466,434805
TS1	-2466.316385	-2466.366804	-2466,396721
3a	-2466.372879	-2466.421330	-2466,450676
MC2	-5037.457886	-5037.531359	-5037.560152
TS2	-5037.422442	-5037.498303	-5037.526738
3b	-5037.476099	-5037.550494	-5037.580856

Table S3. B3LYP(PCM) enthalpies (H, in a.u.), Gibbs free energies (G, in a.u.) and entropies (S, in cal·mol-1·K-1) in benzene, of the stationary points involved in the DA reactions between bis(2-chloroethyl) 2-nitro-ethenylphosphonate **1a** and bis(2-chloroethyl) 2-bromo-2-nitroethenylphosphonates **1b** with anthracene **2**.

		H	G	S
6-31G(d)	**1a**	-1927.022795	-1927.092438	146.577
	1b	-4498.123817	-4498.198636	157.469
	2	-539.327439	-539.372564	94.975
	MC1	-2466.353655	-2466.452411	207.849
	TS1	-2466.315441	-2466.406281	191.190
	3a	-2466.371934	-2466.462610	190.844
	MC2	-5037.456942	-5037.563570	224.417
	TS2	-5037.421498	-5037.515167	197.142
	3b	-5037.475155	-5037.565167	189.445
6-31+G(d)	**1a**	-1927.056756	-1927.126411	146.601
	1b	-4498.177351	-4498.249726	152.327
	2	-539.346150	-539.391313	95.053
	MC1	-2466.403684	-2466.505135	213.521
	TS1	-2466.365860	-2466.456447	190.657
	3a	-2466.420386	-2466.510287	189.213
	MC2	-5037.530414	-5037.635391	220.942
	TS2	-5037.497359	-5037.592738	200.741
	3b	-5037.549550	-5037.643069	196.828

6-31+G(d,p)	**1a**	1927.070992	-1927.140854	147.036
	1b	-4498,190060	-4498,262504	152,471
	2	-539.362097	-539.407284	95.103
	MC1	-2466.433861	-2466.535403	213.714
	TS1	-2466.395777	-2466.486278	190.476
	3a	-2466.449732	-2466.539669	189.287
	MC2	-5037.559207	-5037.664226	221.031
	TS2	-5037.525794	-5037.620097	198.478
	3b	-5037.578250	-5037.671569	194.128