Supporting Information

Thiolysis and alcoholysis of phosphate tri and monoesters with alkyl and aryl leaving groups. An *ab initio* study in the gas-phase

Guilherme Menegon Arantes* and Hernan Chaimovich

Table 13S: Hartree-Fock and second order electronic correlation relative energies for the reaction C with respect to the basis set[a]

		E_{HF}		$E^{(2)}$	
Basis[b]	function[c]	I^d	II^e	I^d	II^e
d	179	-0.018	-0.028	-0.010	-0.003
d,p	218	-0.002	-0.018	-0.016	-0.008
2d,2p	300	0.000	-0.016	-0.016	-0.007
2d,2pd	386	0.003	-0.014	-0.017	-0.008
TZVP	403	-0.001	-0.017	-0.018	-0.009
2df,2p	456	0.003	-0.015	-0.019	-0.010
2df,2pd	516	0.003	-0.015	-0.019	-0.010
3df,3pd	602	0.002	-0.015	-0.018	-0.009
TZVPP	752	0.002	-0.015	-0.020	-0.010

[a] energy values in atomic unities. [b] type and quantity of the polarisation functions added to the 6-311+G set, excluding the TZVPP and TZVP sets.[45] [c] total number of basis functions for each species (C:IMC1, C:TS1 and C:I). [d] E(C:I)-E(C:IMC1) and [e] E(C:I)-E(C:TS1), where E is energy.

Table 14S: Hartree-Fock and second order electronic correlation relative energies for the reaction E (A_n+D_n) with respect to the basis set[a]

		E_{HF}		$E^{(2)}$	
Basis[b]	functions[c]	I^d	II^e	I^d	II^e
d	176	0.063	0.004	-0.018	-0.004
d,p	240	0.061	0.003	-0.017	-0.003
2d,2p	304	0.061	0.004	-0.020	-0.004
2d,2pd	344	0.061	0.004	-0.020	-0.004
2df,2p	360	0.063	0.004	-0.024	-0.004
2df,2pd	400	0.063	0.004	-0.024	-0.004
3df,3pd	464	0.065	0.005	-0.023	-0.004
TZVPP	572	0.062	0.005	-0.024	-0.005

[a] energy values in atomic unities. [b] type and quantity of the polarisation functions added to the 6-311+G set, excluding the TZVPP set.[45] [c] total number of basis functions for each species (E:IMC1a, E:TS1a e E:Ia). [d] E(E:Ia)-E(E:IMC1a) and [e] E(E:Ia)-E(E:TS1a), where E is energy.

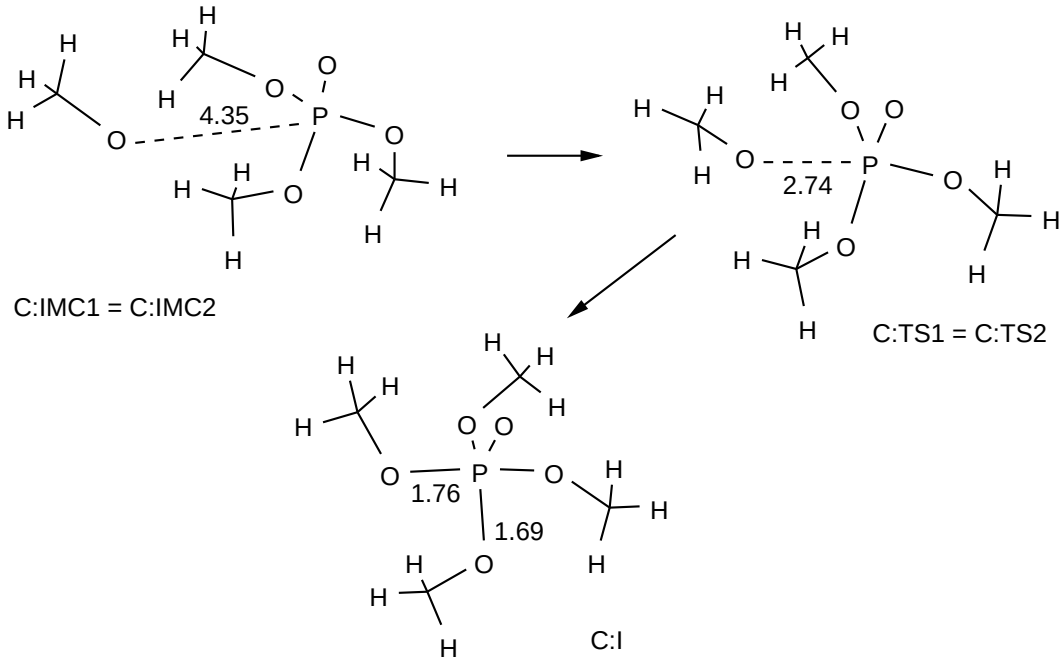

Figure 8S: MP2/6-31+G(d) optimised structures for the reaction C. Selected distances are shown in Å.

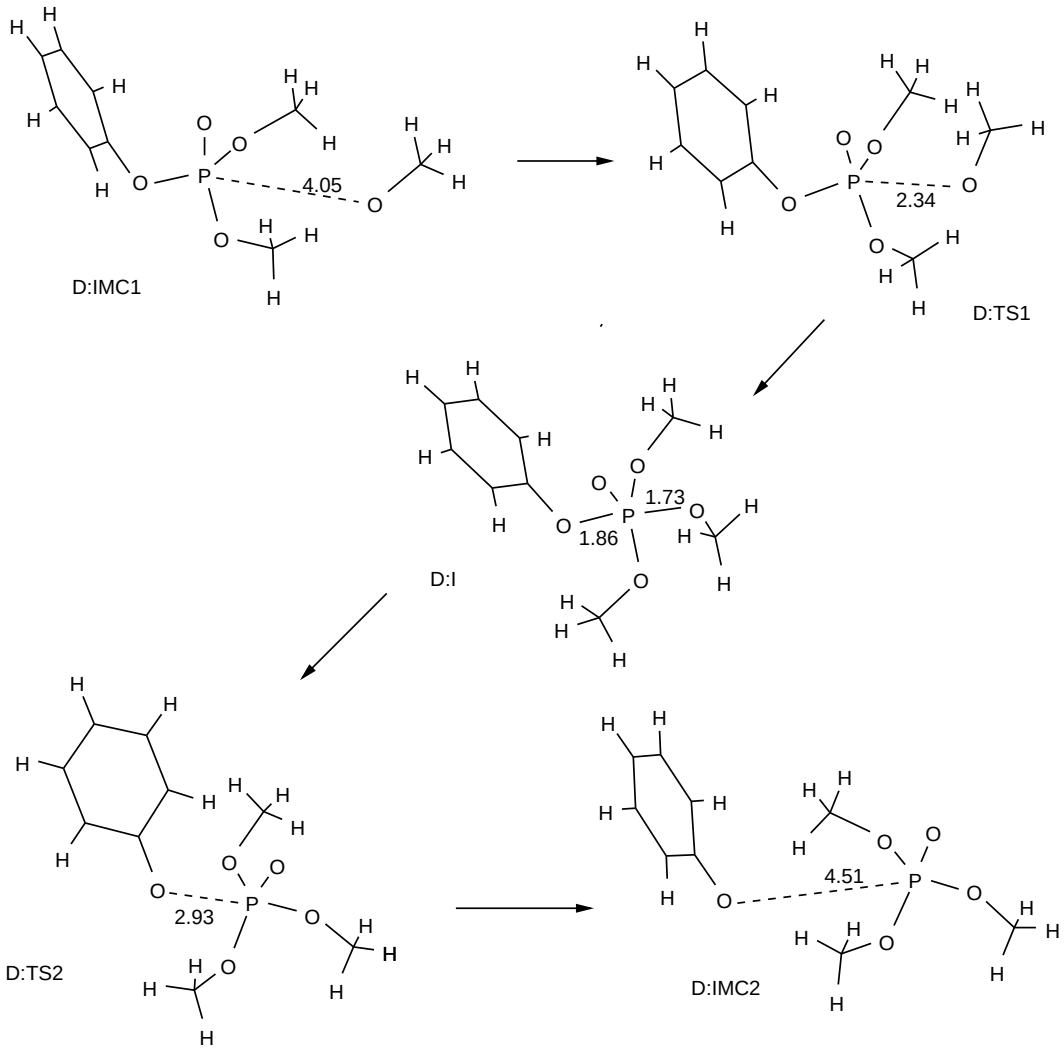

Figure 9S: MP2/6-31+G(d) optimised structures for the reaction D

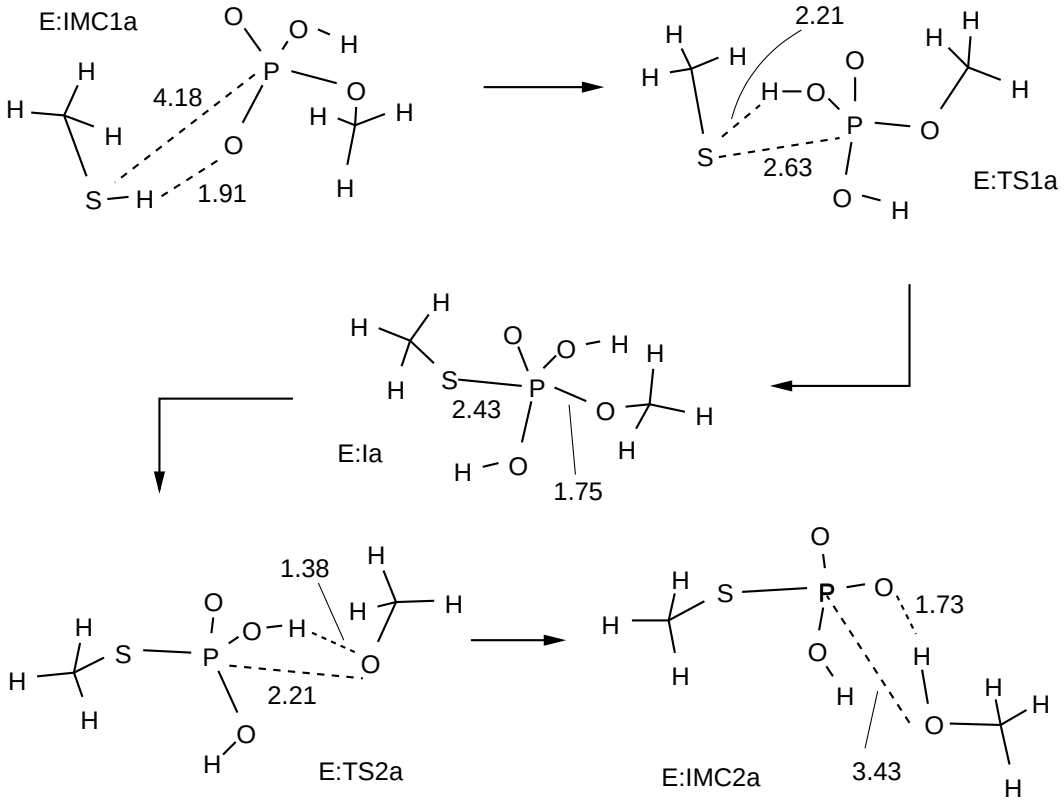

Figure 10S: MP2/6-31+G(d) optimised structures for the reaction E

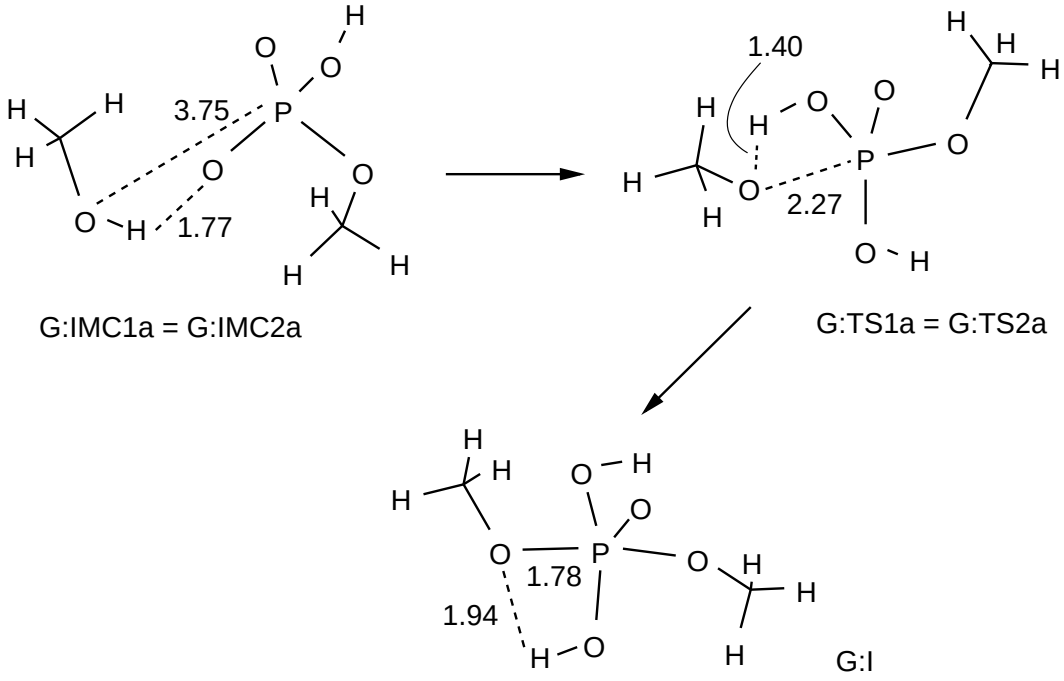

Figure 11S: MP2/6-31+G(d) optimised structures for the reaction G

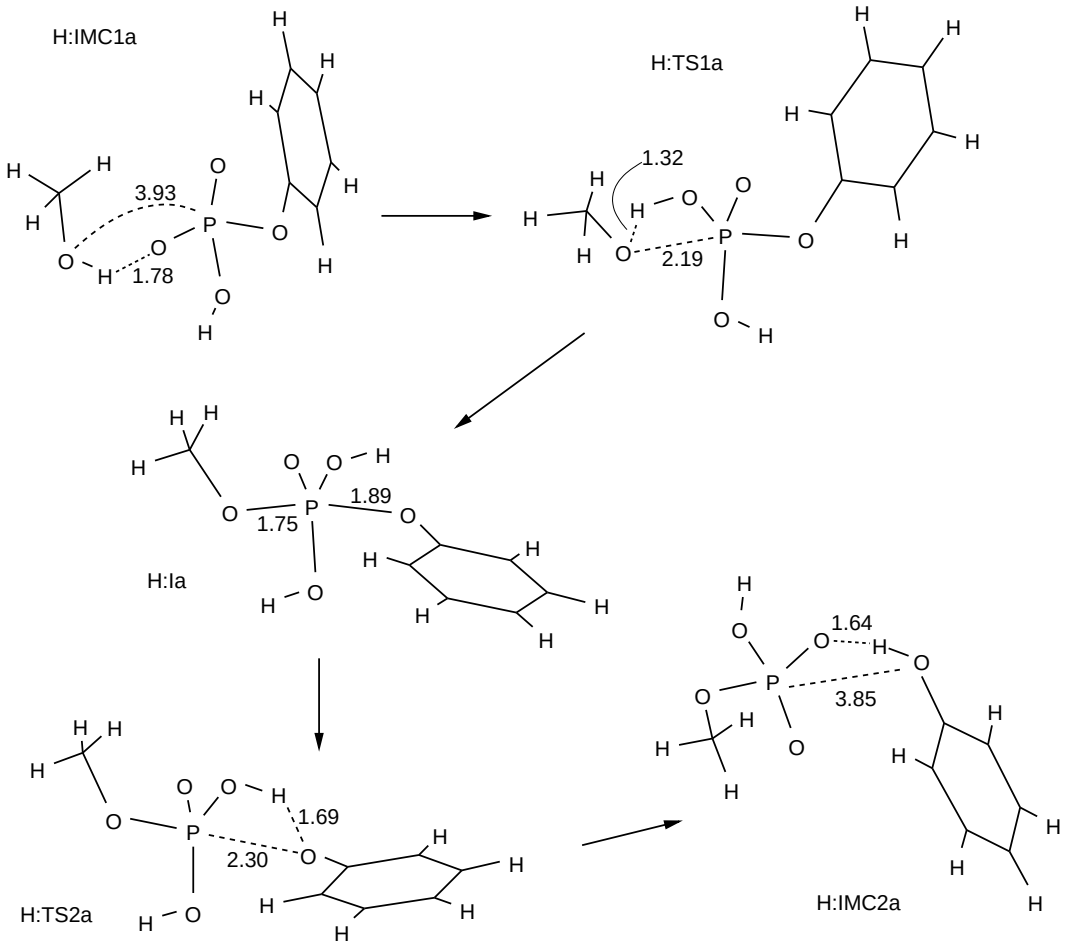

Figure 12S: MP2/6-31+G(d) optimised structures for the reaction H