

SUPPLEMENTARY MATERIAL TO  
**Photodegradation kinetics of organophosphorous with hydroxyl radicals: Experimental and theoretical study**

SEYDA AYDOGDU<sup>1</sup>, ARZU HATIPOGLU<sup>1\*</sup>, BAHAR EREN<sup>2</sup>  
and YELDA YALCIN GURKAN<sup>2</sup>

<sup>1</sup>*Yıldız Technical University, Department of Chemistry, 34220 Istanbul, Turkey and*

<sup>2</sup>*Tekirdag Namık Kemal University, Department of Chemistry, 59030 Tekirdag, Turkey*

*J. Serb. Chem. Soc.* 86 (10) (2021) 955–969

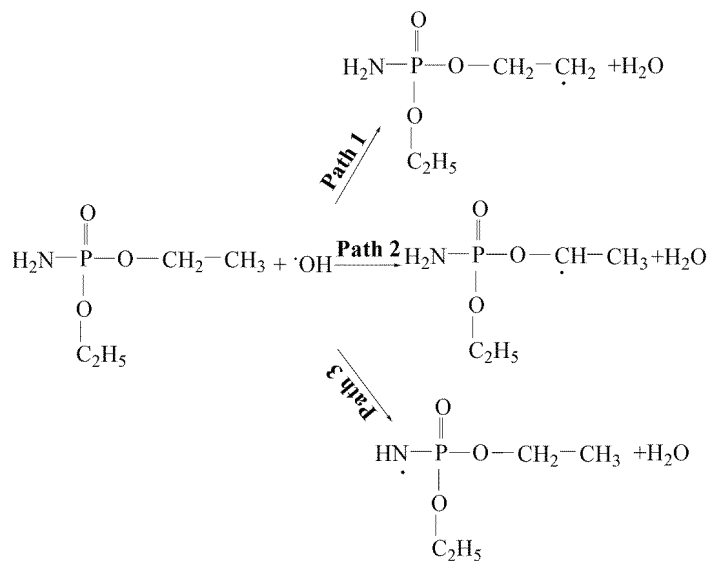


Fig. S-1. Possible reaction pathways of the DEP with  $\cdot\text{OH}$ .

\* Corresponding author. E-mail: hatiparzu@yahoo.com

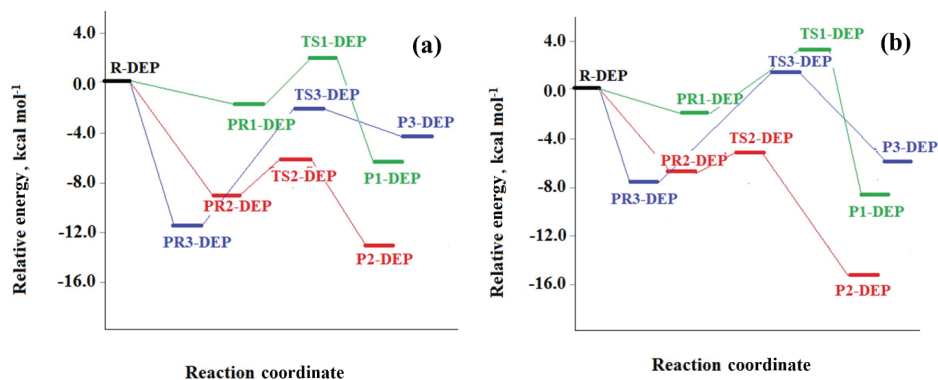


Fig. S-2. Relative energies of the reaction for DEP+•OH: a) gas phase, b) aqueous medium.

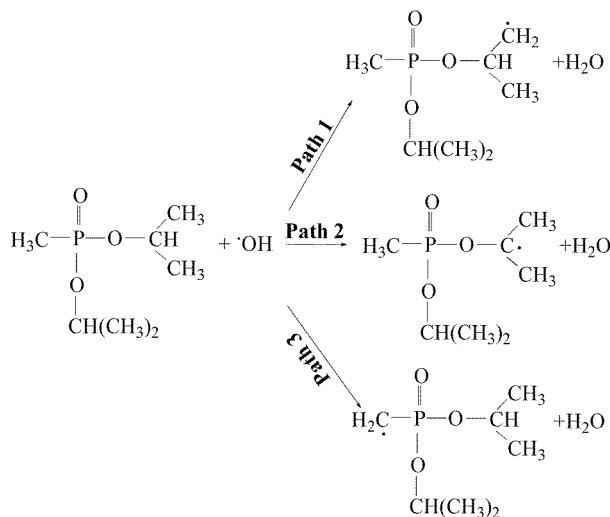


Fig. S-3. Possible reaction pathways of the ISPC with •OH.

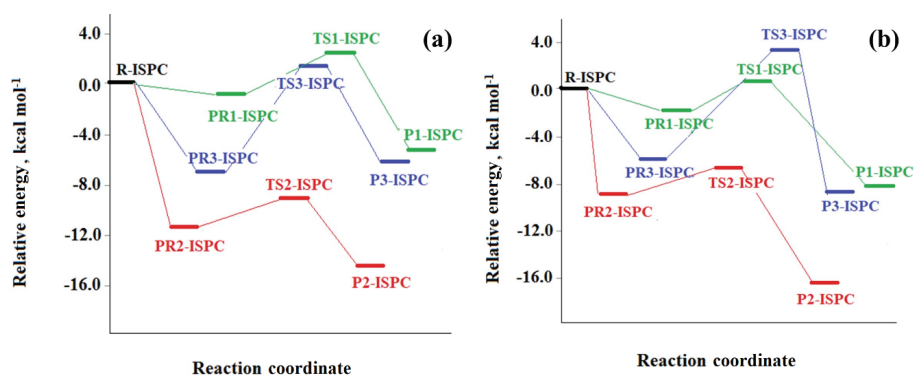


Fig. S-4. Relative energies of the reaction for ISPC+•OH: a) gas phase, b) aqueous medium.

TABLE S-I. Energies of reactants, prereactive complexes, transition states and products for DDMP + •OH reaction

Molecule	$E_h / \text{Ha}$	
	Gas	Aqueous
DDMP+•OH	-857.2071	-857.2207
TS1	-857.2156	-857.2284
TS2	-857.2125	-857.2228
PR1	-857.2177	-857.2297
PR2	-857.2256	-857.2343
P1	-857.2305	-857.2471
P2	-857.2238	-857.2340

TABLE S-II. Energies of reactants, prereactive complexes, transition states and products for DEP + •OH reaction

Molecule	$E_h / \text{Ha}$	
	Gas	Aqueous
DEP+•OH	-857.2272	-857.2455
TS1	-857.2225	-857.2404
TS2	-857.2378	-857.2533
TS3	-857.2303	-857.2431
PR1	-857.2301	-857.2479
PR2	-857.2420	-857.2565
PR3	-857.2459	-857.2581
P1	-857.2378	-857.2588
P2	-857.2493	-857.2694
P3	-857.2346	-857.2540

TABLE S-III. Energies of reactants, prereactive complexes, transition states and products for ISPC +•OH reaction

Molecule	$E_h / \text{Ha}$	
	Gas	Aqueous
ISPC+•OH	-919.8349	-919.8445
TS1	-919.8175	-919.8287
TS2	-919.8232	-919.8367
TS3	-919.8390	-919.8473
PR1	-919.8324	-919.8429
PR2	-919.8309	-919.8474
PR3	-919.8440	-919.8600
P1	-919.8321	-919.8485
P2	-919.8349	-919.8445
P3	-919.8175	-919.8287