**Supporting Information of “Structure and spectromagnetic
properties of the superoxide radical adduct of the DMPO in
water: elucidation by theoretical investigations”**

Section “Comparison to experiment”

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FIG. 1: 3T_4 and 4T_3 conformers **min1**, **min2** and **min3** corresponding to minima of DMPO – OOH in vacuo.

TABLE I: Difference in energy ΔE (in kcal mol⁻¹) between the ³T₄ and ⁴T₃ conformers of DMPO – OOH in vacuo shown in Figure , computed from quantum approaches. E : total quantum energy in Hartree. All the structures were optimized at the B3LYP/6-311+G(d,p) level of theory.

Level of theory	$E(^3T_4)$	$E(^4T_3)$	ΔE
min1			
B3LYP/6-311+G(d,p)	-516.28373	-516.28475	0.6
B3LYP/6-311+G(2df,2p)	-516.31295	-516.31383	0.5
MP2/6-311+G(d,p)	-514.86325	-514.86439	0.7
MP2/6-311+G(2df,2p)	-515.14065	-515.14151	0.5
min2			
B3LYP/6-311+G(d,p)	-516.28154	-516.28217	0.4
B3LYP/6-311+G(2df,2p)	-516.31031	-516.31099	0.4
MP2/6-311+G(d,p)	-514.86034	-514.86206	1.1
MP2/6-311+G(2df,2p)	-515.13684	-515.13886	1.3
min3			
B3LYP/6-311+G(d,p)	-516.27990	-516.27656	2.1
B3LYP/6-311+G(2df,2p)	-516.30862	-516.30533	2.1
MP2/6-311+G(d,p)	-514.85803	-514.85402	2.5
MP2/6-311+G(2df,2p)	-515.13442	-515.13016	2.7

FIG. 2: Comparison of quantum and force field energy results for DMPO – OOH conformers in vacuo. The plots correspond to the root square deviation $\text{RMSD}(E)$ defined below. The force field parameter sets denoted by **1** to **8** are those used to generate the solvated trajectories **T1**(**T1'**) to **T8**(**T8'**), whereas those denoted by **7'** and **7''** are intermediate between the parameter sets **7** and **8**. The root mean square deviations $\text{RMSD}(E)$ are computed according to $\text{RMSD}(E) = \sqrt{\frac{1}{n} \sum (\Delta E_{\text{quantum}} - \Delta E_{\text{force field}})^2}$, based on quantum and force field ΔE values, as well as on the values ΔE corresponding to differences in energy between the conformers **min1** and **min2** at the different levels of theory (n is the number of compared values)