Structure and Magnetic Properties of L-α-Alanine Radicals in Radiation Dosimetry Applications: An Ab Initio Molecular Dynamics Simulation

Mehdi Janbazi¹, Yavar Taghipour Azar¹, Farhood Ziaie¹, Khashayar Ghandi², Chérif Matta³, and Muhammad Shadman Lakmehsari¹

¹Nuclear Science and Technology Research Institute
²University of Guelph
³Mount Saint Vincent University
⁴University of Zanjan

May 5, 2020

Abstract

Alanine is a transfer standard dosimeter using in gamma-ray and electron beam calibration. One of the important factor affecting its dosimetric response is amount of humidity which can deviate the dosimetry expert from the exact value of absorbed doses. Ab initio molecular dynamics calculations were performed to determine the environmental effects on the EPR parameters of L-α-Alanine radicals in acidic and alkaline solutions. Similar to the closed-shell amino acid molecule alanine, the zwitterionic form of alanine radical is the stable form in the gas phase while the non-zwitterionic neutral alanine radical is not a stable structure. Geometric and EPR parameters of radicals in both gas and solution phases are found to be dependent on hydrogen bonding of water molecules with the polar groups and by dynamic solvation. Calculations on the optimized free radicals in the gas phase revealed that for neutral radical, hydrogen bonding to water molecules drives a decrease in the magnitudes of g-tensor components gxx and gyy without affecting neither gzz component nor the HFCCs. For the transfer from the gas to solution phase of the alanine radical anion is accompanied with an increase in the spin density on the carboxylic group’s oxygen atoms. However, for the neutral radical, this transfer from gas to solution phase is accompanied with the decrease in the spin density on oxygen atoms. Calculated isotropic HFCCs and g-tensor of all radicals were in good agreement with their experimental counterparts in both acidic and alkaline solutions, which enhances the confidence in our calculated results.

Hosted file

Fig. 1. Structure, atoms numbering, $g$-tensor axes orientation and spin density isosurface (0.013 au) for $R^*$, $R^{*+}$ and $R^{*-}$. 
Fig. 2. Structure of radical and 55 water molecules is an arbitrary snapshot from *ab initio* molecular dynamics trajectory.
Fig. 3. The RDFs of the hydrogen bonds around the O₁ and O₂ oxygens with water molecules for (a), (b) and (c) radicals.
Fig. 4. Comparison of the average of g-tensor considering 200 snapshots along the trajectory and optimization the structure in the gas phase for (a) and (b) radicals.
Fig. 5. Comparison of the average of HFCC of atoms considering 200 snapshots along the trajectory and optimization the structure in the gas phase for (a) and (b) radicals.
Fig. 6. Variation of g-tensor components versus the MM of the oxygen atoms of the carboxyl groups for the cases of the (a), (b) and (c) radicals.

Fig. 7. Variation HFCC of methyl group versus the MM of the hydrogen atoms of the methyl groups for the
cases of the (a), (b) and (c) radicals.