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

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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.

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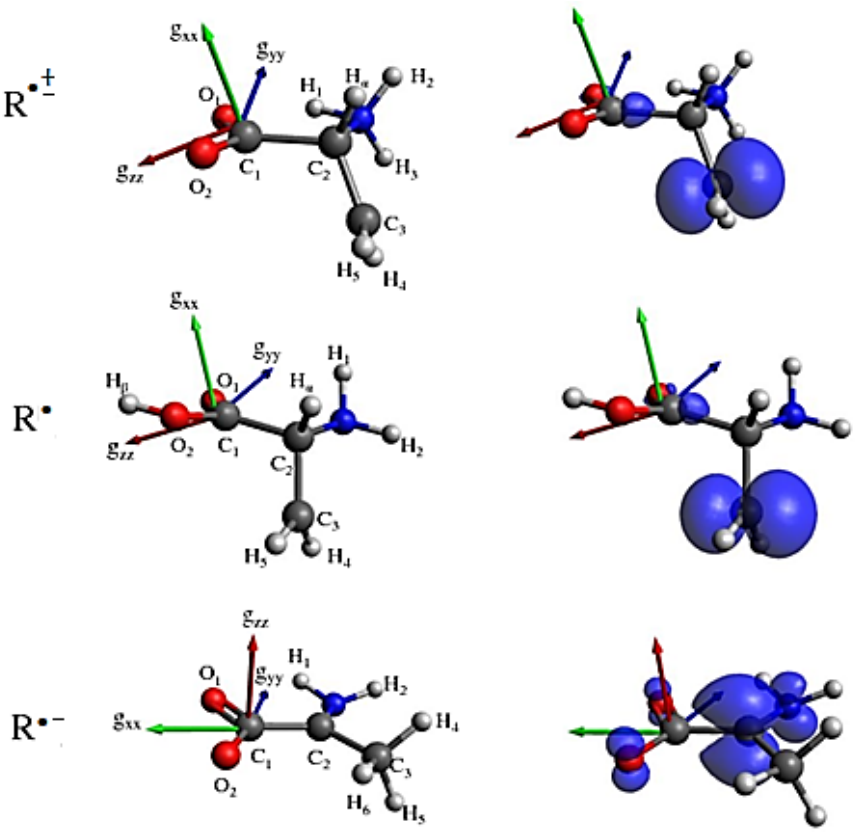

Fig. 1. Structure, atoms numbering, g-tensor axes orientation and spin density isosurface (0.013 au) for , and radicals

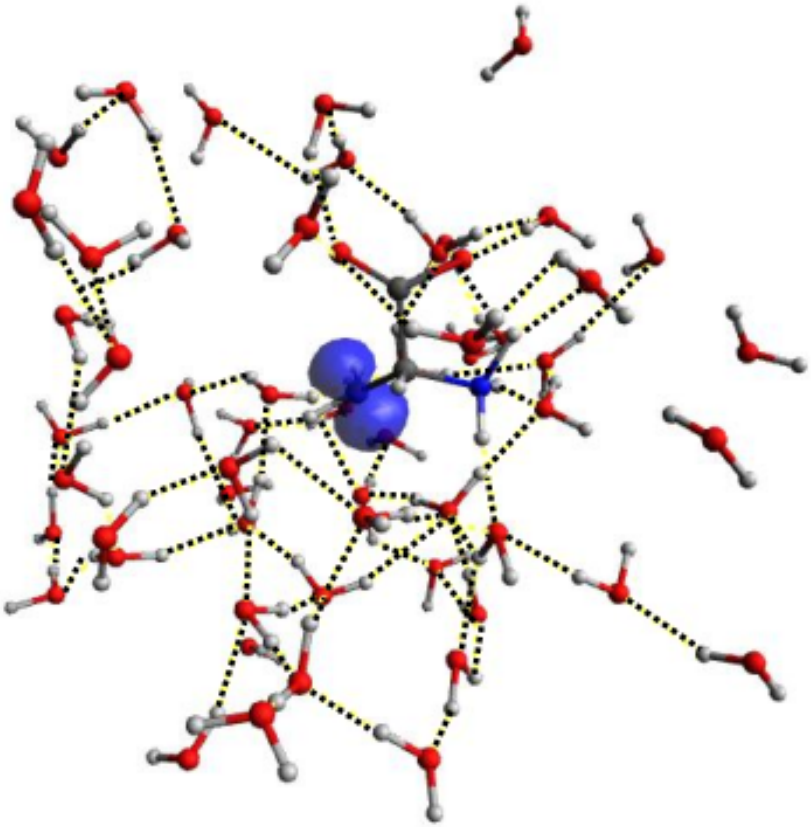

Fig. 2. Structure of radical and 55 water molecules is an arbitrary snapshot form *ab initio* molecular dynamics trajectory

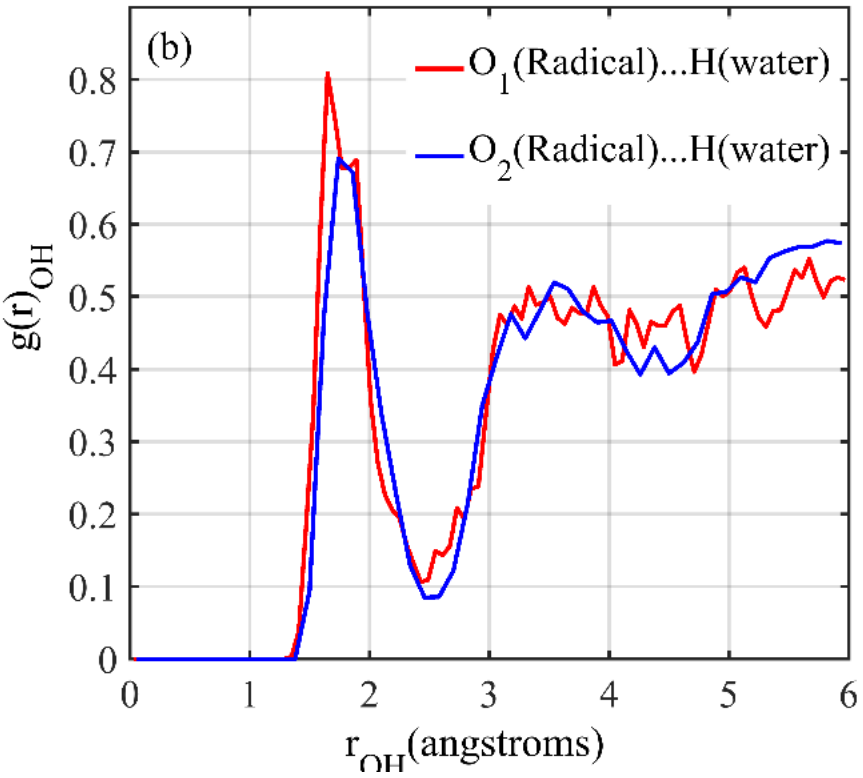

Fig. 3. The RDFs of the hydrogen bonds around the O_1 and O_2 oxygens with water molecules for (a), (b) and (c) radicals

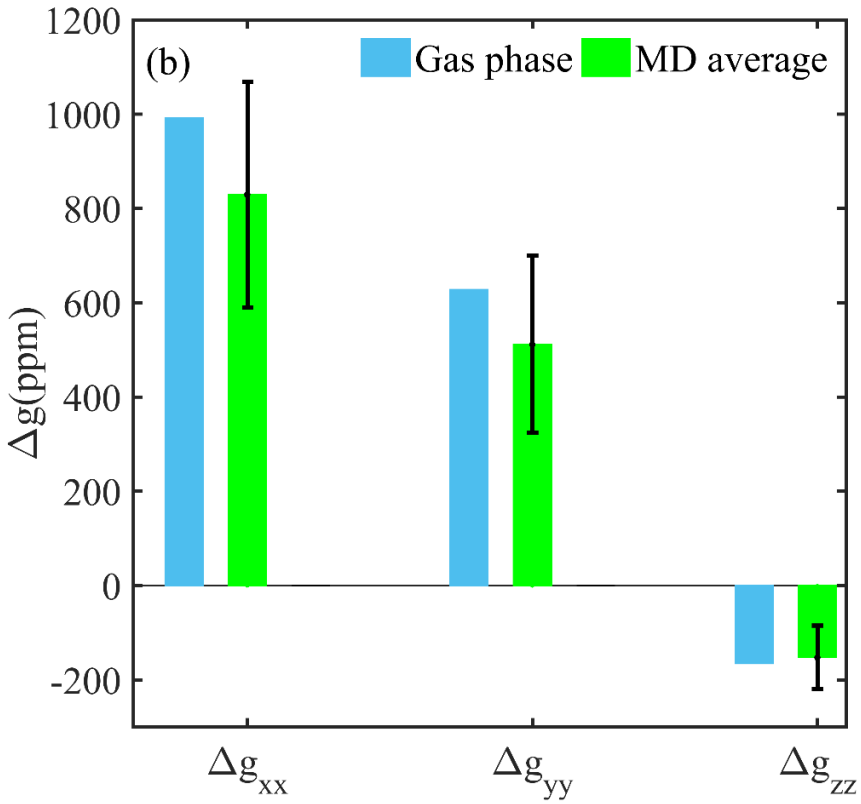

Fig. 4. Comparison of the average of g-tensor considering 200 snapshots along the trajectory and optimization the structure in the gas phase for (a) and (b) radicals

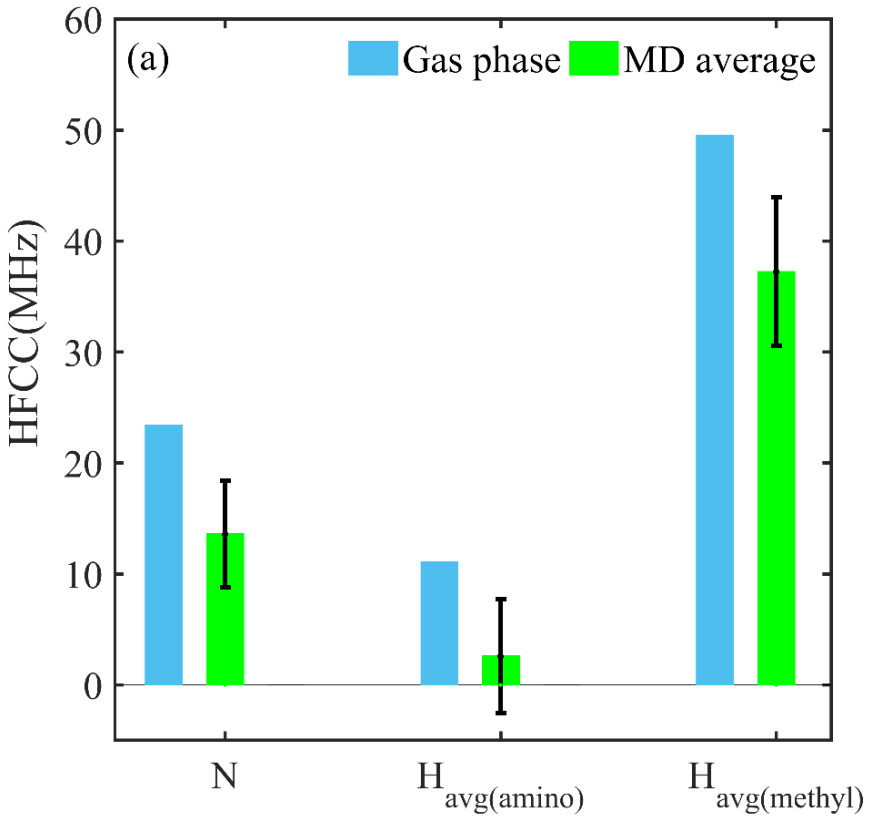

Fig. 5. Comparison of the average of HFCC of atoms considering 200 snapshots along the trajectory and optimization the structure in the gas phase for

(a) and (b) radicals

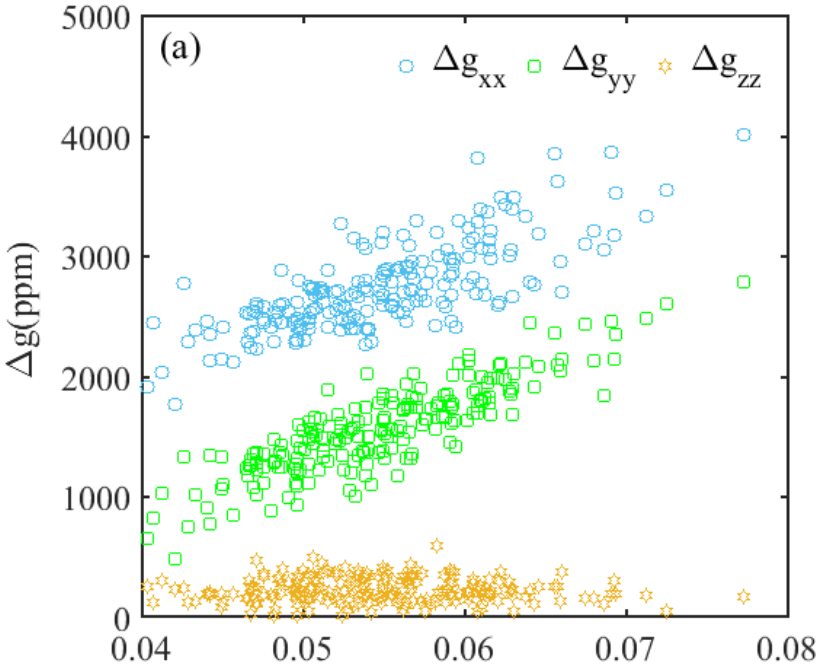

Fig. 6. Variation of g-tensor components versus the MM of the oxygen atoms of the carboxyl groups for the cases of the (a) , (b) and (c) radicals

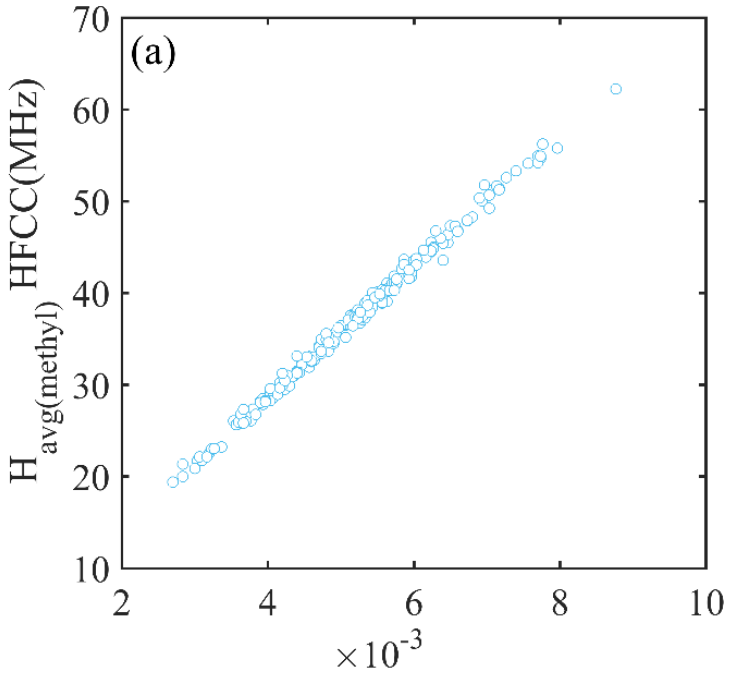

Fig. 7. Variation HFCC of methyl group versus the MM of the hydrogen atoms of the methyl groups for the

cases of the (a), (b) and (c)radicals.