

Path integral simulation on the hyperfine coupling constants of the muoniated and hydrogenated acetone radicals

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Synopsis The *ab initio* path integral simulations, which can account for both the nuclear quantum effect and thermal effect, were carried out to evaluate the structures and “reduced” isotropic hyperfine coupling constants (HFCCs) for muoniated and hydrogenated acetone radicals. Our HFCC values are in reasonable agreement with the corresponding experimental HFCC values.

A considerable amount of knowledge for muonium (Mu; complex of positive muon and electron) chemistry has been accumulated for over 30 years [1]. Compared with a proton, positive muon (μ^+) has a smaller mass and larger magnetic moment. Because of these unique features, Mu is used as the muon spin resonance/rotation/relaxation (μ SR), where hyperfine coupling constant (HFCC) is a good index for the magnetic interaction between electron and muon spins.

For instance, the HFCC value of muoniated acetone radical (Mu-ACE, Figure 1) is measured by Percival et al [2] as 10.27 MHz at 300 K (reduced using the proton magnetic moment). However, the reduced HFCC value for Mu-ACE is calculated as -5.8 MHz with the conventional DFT calculation [3], where the quantum effect of nuclei and thermal effect are excluded. In this study, thus, we performed *on-the-fly ab initio* path integral molecular dynamics (PIMD) simulation [4, 5], which can include these effects, to reproduce the HFCC value of Mu-ACE. We also calculated hydrogenated acetone radical (H-ACE) to compare with Mu-ACE.

Our HFCC values for Mu-ACE and H-ACE are calculated as 32.1 and 3.97 MHz, respectively, which are in reasonable agreement with the corresponding experimental values of 10.3 and 1.51 MHz. Such mass-dependence on HFCC values is due to the large quantum effect of muon. We will also show other results for other muoniated molecular species.

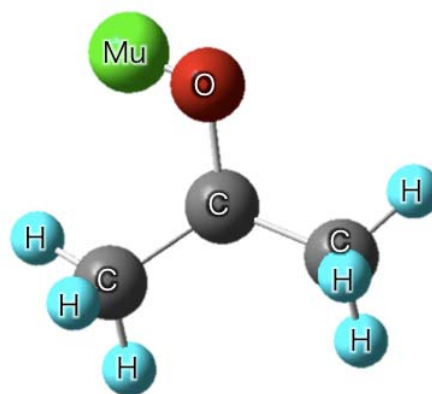


Figure 1: Structure of Mu-ACE.

References

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