[L13] Path integral simulation for accurate HFCC values on muoniated acetone radical

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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 (μSR), where hyperfine coupling constant (HFCC) is a good index for the magnetic interaction between electron and muon spins.

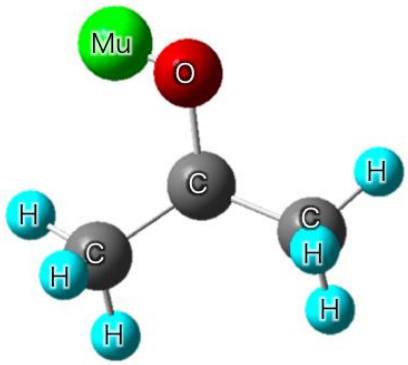

Figure 1: Structure of Mu-ACE.

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.

Bibliography:

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