

## Azacyclohexadienyl Radicals in Liquid Pyridine and ZSM-5 Zeolite

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It is essential to characterize transient radicals in zeolites and study their reactions in order to better understand catalytic reactions in these important materials. The reaction of the light hydrogen isotope muonium (Mu) with pyridine was studied in high silica ZSM-5 zeolite ( $\text{SiO}_2/\text{Al}_2\text{O}_3 = 900$ ) and in the neat liquid in order to determine whether the environment has any effect on either the structure or the relative yield of the resulting three azacyclohexadienyl radical isomers. The muon and ipso proton hyperfine coupling constants (hfcs), which are very sensitive to the electronic structure of a radical, were measured by avoided level crossing muon spin resonance (ALC- $\mu$ SR). The features in the ALC- $\mu$ SR spectra were assigned by calculating the hfcs of the three structures using density functional theory calculations and our assignment of the ortho and meta isomers differs from that of Rhodes et al. [1]. The hfcs of the azacyclohexadienyl radical isomers are nearly the same in ZSM-5 and pyridine but the relative yields of the three isomers change substantially with the ratio of the ortho, meta, and para isomers being 0.45:0.50:0.05 in pyridine and 0.39:0.31:0.30 in ZSM-5. Possible explanations for the greatly increased relative yield of the para isomer in ZSM-5 will be discussed.

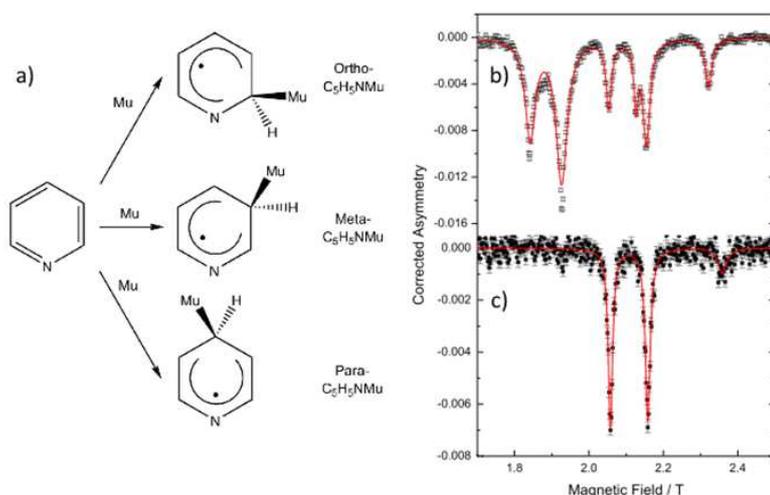


Fig. 1: Fig.1 a) Structures of the three possible Mu adducts of pyridine, b) ALC- $\mu$ SR spectrum of three azacyclohexadienyl radical isomers in ZSM-5, c) ALC- $\mu$ SR spectrum of three azacyclohexadienyl radical isomers in pyridine.

[1] C. J. Rhodes et al. Magn. Reson. Chem. 39 (2001) 438.