

MUON SPIN SPECTROSCOPY OF THE RADICAL FORMED BY MUONIUM ADDITION TO DIKETENE

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The structure and dynamics of the radical formed by muonium addition to diketene have been studied by transverse field muon spin rotation (TF- μ SR) and muon level-crossing resonance (μ LCR) spectroscopy. The TF- μ SR spectrum showed that only one type of radical was formed and the μ LCR spectrum showed that this radical contains two sets of non-equivalent protons. The muon and proton hyperfine coupling constants (hfccs) were measured at several temperatures between 280 and 360 K. The muon hfcc falls with increasing temperature while the larger magnitude proton hfcc increases. The other proton hfcc remains constant. The magnitude and temperature dependence of the hfccs indicate that the 4-muonomethyl-oxetan-2-on-4-yl radical was formed. *Ab initio* calculations will be presented confirming the assignment of the radical and modeling the temperature dependence. The temperature dependence of the hfccs is due to a preferred conformation of the methyl group in which the C-Mu bond eclipses the orbital containing the unpaired electron.