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

I. McKENZIE, P. W. PERCIVAL, J.-C. BRODOVITCH, K. GHANDI, B. ADDISON-JONES, *Department of Chemistry and TRIUMF, Simon Fraser University, Burnaby B.C., Canada V5A 1S6*.

The structure and dynamics of the radical formed by muonium addition to diketene have been studied by transverse field muon spin rotation (TF-μSR) and muon level-crossing resonance (μLCR) spectroscopy. The TF-μSR spectrum showed that only one type of radical was formed and the μLCR 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.