Molecular Motion in Tetraphenyltin Studied by NMR

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NMR second moment and spin-lattice relaxation times in the laboratory (60 and 25 MHz) and in the rotating frame (B_1 = 2.1 mT) were studied for polycrystalline tetraphenyltin $Sn(C_6H_5)_4$ in a wide temperature range. Two kinds of motions were detected: isotropic rotation of whole molecules and reorientations/oscillations of phenyl rings. A dependence of the potential energy of the molecule in the crystal on the angle of the phenyl ring rotation about the Sn–C bond was obtained on the basis of atom-atom calculations. The amplitude of the ring-oscillations at 133 K was estimated as ± 7°. Below room temperature the magnetisation recovery is significantly non-exponential, which may be interpreted as due to the correlated motion of phenyl rings.

Key words: NMR; Relaxation; Potential Energy.