Studies of Dihydropyridines by X-Ray Diffraction and Solid State ^{13}C NMR

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Fourteen dimethyl 4-aryl-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylates (DHPs) were evaluated by means of single crystal X-ray diffraction in order to investigate the effects of the structure in the crystals on the solid state ^{13}C NMR chemical shifts. These include the analysis of three DHPs containing two molecules per asymmetric unit. The chiral rotamer unit generated by the *s-cis*/*s-trans* orientation of the carbonyl groups, as well as by rotation of the 4-phenyl ring out of the bisecting plane containing the N1, C4, C7 atoms, resulted in a significant magnetic non-equivalence for the C2-CH_3/C6-CH_3 and the $COOCH_3$ pairs of signals. The solid state ^{13}C NMR data reveal that the substitution pattern of the phenyl ring has a marked effect on the extent to which the signals of the carbonyl carbon atoms and those of C-2/C-6 peaks are split.

Key words: ^{13}C CP-MAS NMR, 1,4-Dihydropyridines, Chiral Rotamers, Crystal Structures