NUCLEAR MAGNETIC RESONANCE SPECTRA OF NAPHTHYRIDINES AND RELATED HETEROCYCLES

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^{13}C Chemical shifts of naphthyridines were correlated with their electron densities obtained by SCF-MO calculations of the π-electron system. Thus, the theoretical spectra were calculated by the equation, $\Delta\delta_r = \alpha(q_r - 1)$, with the best fit α value(α= 140 ppm), where $\Delta\delta_r$ is the ^{13}C chemical shift withrespect to that of benzene and q_r is the electron density.

In order to interprete the lanthanide induced shift of bifunctional nitrogen heterocycles, such as naphthyridines and their benzo-derivatives,the induced shifts of the bifunctional compound were estimated from those of the monofunctional model compounds carrying nitrogen atoms of almost same steric environment as in the bifunctional compound. For example, the induced shifts of the ring protons of unsymmetrical naphthyridines were estimated from those of quinoline and isoquinoline. The estimated relative induced shifts agree almost quantitatively with the observed values. The relative equilibrium constants for the complexation of several nitrogen heterocycles with $Eu(fod)_3$ were obtained by means of the intermolecular competitive complexation of two heterocycles. As a consequence, we obtained the following sequence for the preference to the complex formation:

1,8-naphthyridine ≫ pyridine ≳ isoquinoline > 2-picoline ≳ quinolie > 2-methylquinoline > 1-phenanthridine ≳ 8-methylquinoline.