CONFORMATIONAL ANALYSIS OF MESITYLOXIDE (1-PHTHALAZINYL) HYDRAZONE (DJ-1461) BY LANTHANIDE-INDUCED SHIFTS

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The behaviour of the trivalent lanthanide chelate complexes of $Ln(dpm)_3$, Ln=Pr, Eu on its pmr spectra was quantitatively studied. Upfield and downfield shifts in the proton signals were observed for $Ln(dpm)_3$. The best position of the lanthanide ion and the protons of substrate in the complex were determined using the McConnell-Robertson equation. The shifts induced by $Ln(dpm)_3$ agreed well with the calculated values, on the assumption that their origin is of pseudo-contact nature. The Eu-N^2 bond length was as long as 3.2A (phthalazine N^2 is set at the origin of the right handed polar co-ordinates). It was found that the side chain of the DJ-1461 has an anti form towards the C=N double bond, and the two double bonds S-cis configuration.