

CONFORMATIONAL ANALYSIS OF MESITYLOXIDE (1-PHTHALAZINYL)  
HYDRAZONE (DJ-1461) BY LANTHANIDE-INDUCED SHIFTSReimei Moroi, Keiichi Tomita, and Mitsui SanoResearch Institute, Daiichi Seiyaku Co., Ltd.Minamifunabori-cho, Edogawa-ku, Tokyo 132

The behaviour of the trivalent lanthanide chelate complexes of  $\text{Ln}(\text{dpm})_3$ ,  $\text{Ln}=\text{Pr}$ ,  $\text{Eu}$  on its pmr spectra was quantitatively studied. Upfield and downfield shifts in the proton signals were observed for  $\text{Ln}(\text{dpm})_3$ . 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  $\text{Ln}(\text{dpm})_3$  agreed well with the calculated values, on the assumption that their origin is of pseudo-contact nature. The  $\text{Eu}-\text{N}^2$  bond length was as long as 3.2A (phthalazine  $\text{N}^2$  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  $\text{C}=\text{N}$  double bond, and the two double bonds S-cis configuration.