THE REACTIONS AND OPTICAL RESOLUTIONS OF 1-ARYL-4,6-DIMETHYL-2(1H)-PYRIMIDINONES

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We have investigated the chemistry of 1-aryl-4,6-dimethyl-2(1H)-pyrimidinones as the model compounds of nucleosides.
In the previous paper we reported that methyl protons of C-6 position were shifted to high field in nmr spectrum by the anisotropic effect of aryl group at N-1 position. From the calculation of modified Force Field method on the restricted rotation barrier about C-N single bond, we obtained the interesting results as follows.
(1) The rotation barriers of 1-phenyl-, 1-(m-tolyl)- and 1-(m-anisyl)-2(1H)-pyrimidinone were ca. 13-14 Kcal/mole.
(2) The rotation barriers of 1-(o-tolyl)-, 1-(o-anisyl)-, 1-(o-ethylphenyl)- and 1-(o-ethoxyphenyl)-4,6-dimethyl-2(1H)-pyrimidinone were 31.6 Kcal/mole, 25.6 Kcal/mole, 36.4 Kcal/mole, 28.1 Kcal/mole, respectively. These results were in good agreement with the experimental data, which were obtained by the optical resolutions and kinetics of 1-aryl-4,6-dimethyl-2(1H)-pyrimidinones.

Furthermore, we carried out the photochemical reactions of 1-aryl-4,6-dimethyl-2(1H)-pyrimidinones to give diazabicyclo[2.1.1]cyclohexenone derivatives in good yield.