HETEROCYCLES, Vol. 2, No. 2, 1974

CYCLIZATION AND CYCLOADDITION REACTIONS OF 1,3-OXAZEPINE AND 1,2-DIAZEPINE DERIVATIVES

Toshio Mukai, Hiroshi Sukawa, Yoshiro Yamashita, and Takahiro Tezuka

Department of Chemistry, Faculty of Science, Tohoku University, Aobayama, Sendai

In connection with the interesting behavior of valence isomerization of heteropines such as oxepines and azepines, we studied the electrocyclic and cycloaddition reactions of 2-phenyl-1,3-oxazepine (I), which has recently been synthesized in this laboratory. On the basis of evidence obtained, it may be concluded that in the cycloheptatriene $\rightleftarrows$norcaradiene type equilibrium, 1,3-oxazepine (I) is directed towards the triene side at ordinary temperatures. The reactivities of 1,2-diazepine derivatives (II) were compared with those of the 1,3-oxazepine (I) from the view point of valence isomerization.

The most intriguing finding is the fact that both compounds, I and II, add to 2,5-dimethyl-3,4-diphenylcyclopentadienone to give 1 : 1 adducts III and IV. In addition, irradiation of adducts III and IV results in the formation of novel cage compounds containing two hetero atoms such as 1,3-dimethyl-6,9,10-triphenyl-5-oxa-7-azapentacyclo[8.2.0.0^{3,9}.0^{4,12}.0^{8,11}]dodeca-6-en-2-one and 7-substituted 1,3-dimethyl-9,10-diphenyl-6,7-diazapentacyclo[8.2.0.0^{3,9}.0^{4,12}.0^{8,11}]dodeca-5-en-2-one.