The Mechanism of Isomerizathion Recyclization of Pyridinium Salts

Evgenyi G. Atavin, Reva S. Sagitullin

Omsk State University
644077, Russia, Omsk, prosp. Mira 55A
e-mail: atavin@univer.omsk.su

The range of compounds capable of isomerization recyclization [1] has been broadened significantly last years. Recently we discussed the problem of mechanism this reaction used formation energy calculated by molecular mechanic method [2]. Recalculation of this data by ab initio quantum chemical methods (HF/6-31G(d) and B3LYP/6-31G(d)) have give evidence of the correctness our conclusions but show more important role of enimin forms (VII, VIII). The energy of this intermediates is low enough to be located in the reaction path way II-VII-VIII-VI:

In future the energy activation barriers for this reaction stages will be verify.

References

We are grateful to Russian for Basic Research for financial support (Grant No 04-03-32652)