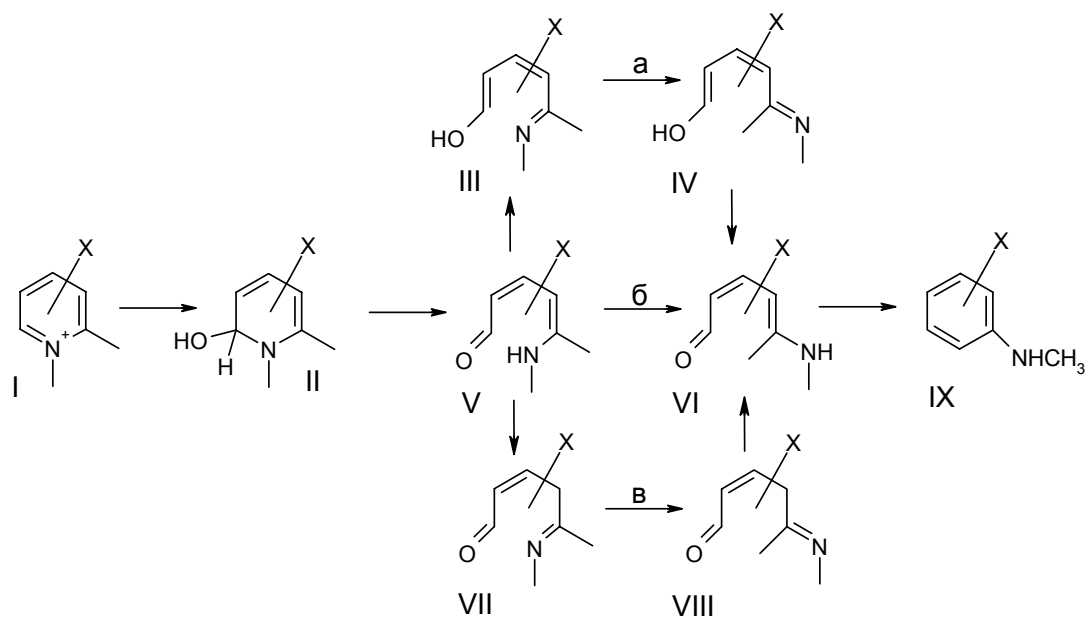


The Mechanism of Izomerizathion Recyclization of Pyridinium Salts

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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-V-VII-VIII-VI:



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

References

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