

Quantum-chemical investigation of acetylene reactions with aniline in a superbasic KOH/DMSO medium

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Abstract

The relevance of studying the activity of initial amines with acetylenes and the mechanisms of their mutual transformations in a superbasic medium is dictated by the interest in the synthesis of nitrogen-containing heterocyclic compounds with potential biological activity. One example is the synthesis of N-phenyl-2,5-dimethylpyrrole. Quantum chemical studies were carried out by B2PLYP/6-311+G**//B3LYP/6-31+G* approach. Using the simplest model for describing the superbasic medium, a “virtual screening” of the most probable interactions of acetylene molecules with each other and with the aniline molecule was done. Based on this, the most realistic interaction routes were selected, which were studied in more complex models, taking into account the obvious influence of alkali and solvent. This work was supported by Ministry of Education and Science of the Russian Federation. Grant Number: FZZE-2020-0025.

Speaker Publications:

1. “Self-assembly of N -phenyl-2,5-dimethylpyrrole from acetylene and aniline in the KOH/DMSO and KOBu t /DMSO superbase systems: a quantum-chemical insight”; Vol 01, 2020.
2. “Head-to-Tail Dimerization of 4-Fluoroacetophenone in the KOH/DMSO Superbase Suspension and Related SNAr Reaction”; European Journal of Organic Chemistry / Vol 23, 2020.
3. “Quantum-chemical models of KOH(KOBut)/DMSO superbasic systems and mechanisms of base-promoted acetylene reactions”; International Journal of Quantum Chemistry / Vol 120, 2020.
4. “Quantum chemical comparison of ethynylation and C-vinylation routes in superbase catalyzed reaction of acetylenes with imines”; Mendeleev Communications , Vol 29, 622-624.

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Biography:

Damir Z. graduated Bachelor’s course from the Chemical Faculty of Irkutsk State University (ISU) in 2018. He is currently a master's student and works in Laboratory of Quantum Chemistry, ISU. Damir Z. has published 2 papers in reputed journals and has been participated in several international conferences. He has won 2 personal grants and 3 personal scholarships.