International Journal of Applied and Natural Sciences (IJANS)
ISSN(P): 2319-4014; ISSN(E): 2319-4022
Vol. 4, Issue 1, Jan 2015, 1-10
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International Academy of Science, Engineering and Technology
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COMPUTATIONAL STUDY OF CONCERTED REACTION PATHWAYS FOR N-ALKYLANINE TRANSFORMATION TO ANILINE IN ACID MEDIA AND UNDER GAS PHASE

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ABSTRACT

Experimentally the transformation of N-alkylaniline to aniline is assumed to proceed by S_N2 reaction pathway. New concerted reaction pathway was proposed. These concerted reaction pathways were studied computationally and compared using different alkyl substituents (methyl and isopropyl). The computational calculation was carried out with Density Functional Theory using B3LYP (Becke-style 3-Parameter Density Functional Theory, that use Lee-Yang-Parr correlation functional) and 6-311++G (d, p) basis set. The reaction pathways were followed and verified with Intrinsic Reaction Coordinate (IRC). It was found that, in accordance with the experimental assumption, S_N2 reaction pathway was the choice of the transformation.

KEYWORDS: Aniline, Concerted Reaction Mechanism, Density Functional Theory, S_n2 Transition State, Substituents Effect