International Journal of New Chemistry, 2017, 4 (1), 12-16. Published online 2017 in <u>http://www.ijnc.ir/.</u> Original Article



Initial studies of the effects of halogenated dispersions on the amount of NICS compound ring 1- (4-fluorophenyl) -2,3-dihydro-1 H-naphtho [1 and 2-e] [1 and 3] oxazin-3-one

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Received 1 December 2016; Accepted 2 January 2017; Published 30 January 2017

Abstract

In the 1- (4-fluorophenyl) -2,3-dihydro-1 H-naphto- [1 and 2-e] [1 and 3] oxazine-3-n, there are 4 rings, respectively, rings from the side attached to the halogen They are named C, B, A, and D. Calculations and studies show that the amount of aromatics in the halogen-ring A in all cases has the highest number. In the B loop, the predicted aromatism level is zero, and in the ring C and D, relative to the A loop, the aromaticity increase is as follows: A > D > C In the next stage of the study, with the replacement of the halogen ring A from F to I, the following process was observed.In ring A, when halogens were changed, the increase in aromaticity in halogenated compounds was as follows: F > Cl > Br > I

Keywords: Aromatism, 1- (4-fluorophenyl) -2,3-dihydro-1 H-naphto- [1 and 2-e] [1 and 3] oxazine-3-n,

1. Introduction

In the naphthalene-compressed molecule, 1 and 3-oxazine is not flat with the C8H12FNO2 closed formulation, and has a boat configuration that has a two-edged angle between flat naphthalene, 6/4

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