International Journal of New Chemistry, 2015, 2 (4), 73-78
Published online January 2015 in http://www.ijnc.ir/.
Original Article

Online ISSN 2383-188X
Open Access

Computational Survey on the Effect of Changes in Halogenated Compounds on the structural properties in Chlorpromazine

Saeed Karimi *

Department of Chemistry, Ilam University, Ilam, Iran .

*Corresponding Author e-mail Address: Saeedkarimi@yahoo.com

Received 1 November 2015; Accepted 28 December 2015; Published 30 January 2016

Abstract

In this study, on the combination of chlorpromazine with two aromatic rings, halogens are attached to the rings, and changes in the angles and lengths of the ipsos are calculated. Calculations show that by changing the halogen based on the amount of electronegativity, the magnitude and variation of the angular lengths The lengths of the links also change in the following order. The angles of the IPSO mode: RF <R-Cl <R-Br. In addition, the length of the bonds in C5-C4: R-F <R-Br <R-Cl and the length of the C5-C6: R-F <R-Cl <R-Br. Similarly, bipolar moments changes in states where the halide is connected to two loops and into a loop. Calculations show that by varying the halogen based on the electronegativity and the factor occupancy, the bipolar momentum changes as follows.

Pro + 2F> Pro + 2Cl> Pro + 2Br> Pro + F> Pro + Cl> Pro + Br>

chlorpromazine

Keywords: Chlorpromazine, Chemical potential, Bipolar Moment

1. Introduction

Allergies or allergies often appear to be skin or respiratory illnesses, and various factors, such as pollen, of plants or some of the foods affect it. The root of the French scientist was the first to recapture the