5th National Conference on New Researches in Chemistry and Chemical Engineering
Tehran-2019

NMR and natural bond orbital (NBO) calculation of (1S,8aR)-4,7-dimethyi-1-(propan-2-yl)- 1,2,3,5,6,8a-hexahydronaphthalene and 17-Bis(4-hydroxy-3-methoxyphenyl)-(1E6E)16-heptadiene-35-dione : Nano physical parameter investigation

Shamsa Sharifi
Department of chemistry, Robat Karim Branch, Islamic Azad University, Robat Karim, Iran.
Email address: d_sharifi60@yahoo.com

ABSTRACT

In this article, theoretical methods have been used for calculation of physical parameters in (1S,8aR)-4,7-dimethyi-1-(propan-2-yl)- 1,2,3,5,6,8a-hexahydronaphthalene and 17-Bis(4-hydroxy-3-methoxyphenyl)-(1E6E)16-heptadiene-35-dione compounds. We calculated physical parameters like atomic charge, energy, chemical shift anisotropy, asymmetry parameter, chemical shift anisotropy , dipole moment, isotropic, anisotropic, NMR determinant and distance matrix determinant. In this work we used Gaussian 98 at NMR and natural bond orbital calculation by using density functional theory (DFT) and 6-31G basis set and B3LYP methods has been applied to analyze the substituent effect on the electronic structural parameters and thermodynamic properties. In addition, thermochemical parameters including thermal energy, entropy, Gibbs free energy and entropy of (1S,8aR)-4,7-dimethyi-1-(propan-2-yl)- 1,2,3,5,6,8a-hexahydronaphthalene and 17-Bis(4-hydroxy-3-methoxyphenyl)-(1E6E)16-heptadiene-35-dione compounds have been computed.*

Keywords: atomic charge, anisotropy, entropy

1. INTRODUCTION

Turmeric is a spice which is obtained from rhizomes of plant Curcuma longa. A member of the family Zingaberaceae. Components of turmeric are named curcuminoids, which include mainly curcumin(diferuloyl methane), demethoxycurcumin and bisdemethoxycurcumin (Figure1).

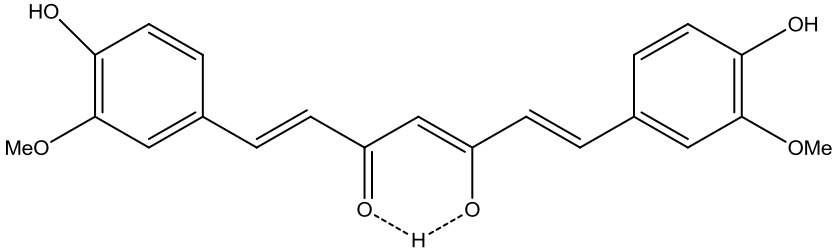

***Fig.1**. 17- Bis (4-hydroxy-3-methoxyphenyl)-(1E6E)16-heptadiene-35-dione(Curcumin)*