ORIGINAL ARTICLE

NMR spectra of Azobenzene-bridged calix [8] arene complexes by ab initio hartree-fock calculations as nanostructure compound

Masoumeh Sayadian¹; Hamidreza Sadegh^{2, *}; Gomaa Abdelgawad Mohammed Ali^{3, 4}

 ¹Department of Chemistry, Islamshahr Branch, Islamic Azad University, Islamshahr, Iran
²West Pomeranian University of Technology, Szczecin, Faculty of Chemical Technology and Engineering, Division of Functional Materials and Biomaterials, Al. Piastow 45, Szczecin, Poland
³Chemistry Department, Faculty of Science, Al-Azhar University, Assiut, 71524, Egypt
⁴Faculty of Industrial Sciences and Technology, University Malaysia Pahang, Gambang, 26300 Kuantan, Malaysia

Received 07 January 2018; revised 13 March 2018; accepted 28 April 2018; available online 02 May 2018

Abstract

Calix[8]arenes of conformational rigid were isolated. The NMR parameters of the structure of calix[8]arenes have been compared. The study of organic structures to form nanoporous materials is well-known in chemistry phenomena to find the crystal form of calix[8]arene as supramolecule. Investigated and compared hydrogen bonding, oxygen and nitrogen atoms effect on calix[8]arene and its complexes were reported at Hartree-Fock (HF) theory by Gaussian 2003 of program package. In this work, the complexing properties of azobenzene-bridged calix[8]arene with alkali earth metal cations has studied. The complexation properties of calix[8]arene were studied by HF method. The complex of the calixarenes showed different properties for the different cations, depending on the cations and the position of the substituent grafted on the ligand.

Keywords: Calix [8] Arene; Chemical Shift; Density Functional Theory; Hartree-Fock; Hydrogen Bonding; Nanostructure

How to cite this article

Sayadian M, Sadegh H, Abdelgawad Mohammed Ali G. NMR spectra of Azobenzene-bridged calyx [8] arene complexes by ab initio hartree-fock calculations as nanostructure compound. Int. J. Nano Dimens. 2018; 9 (3): 228-237.

INTRODUCTION

In the recent years, the calixarenes are of particular interest as metal ion receptors [1-4]. The use of calix[n]arenes in analytical chemistry and separation chemical technology has been discussed [5]. It was founded that the cavity size, the position and kind of donor groups and the molecular flexibility have a pronounced impact on the complexation properties as well as the extraction power and selectivity [6, 7]. Calix[n] arenes have generated considerable interest due to their basket-shaped structure and as useful building blocks to synthesize selective receptors for the guest species, notably alkali, alkaline earth and transition metal cations [8, 9]. Supermolecular interaction is the vital initial process triggering biological and chemical events. Studies on binding between converging sites of synthetic hosts with

diverging sites of guest molecules, atoms or ions have progressively provided valuable information towards an understanding of the supermolecular interaction of complicated natural elements [10-12]. Much attention has recently been paid to achieve the binding selectivity between the host and the guest atoms by controlling the size and shape of the binding cleft of the host molecule [13]. A host molecule that can controllably switch its binding selectivity as desired is rare [14] but extremely desirable for various applications including imitating biological events. Owing to its pre-organized structure, calix[8]arene is one of the most established molecular platforms for constructing three-dimensional hosts for atoms or ions [15]. The structure of calix[8]arene consists of eight phenol rings linked together with four methylene units in a circular manner producing

* Corresponding Author Email: *Hamid-sadegh@zut.edu.pl*

This work is licensed under the Creative Commons Attribution 4.0 International License. To view a copy of this license, visit http://creativecommons.org/licenses/by/4.0/.