J. Chem. Lett. 1 (2020) 63-68

Research Article

Journal of Chemistry Letters
journal homepage: www.jchemlett.com
ISSN (online):2717-1892

Fullerene (C_{20}) as a potential sensor for thermal and electrochemical detection of amitriptyline: A DFT study

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ARTICLE INFO

Article history:
Received 17 March 2020
Received in revised form 30 May 2020
Accepted 15 June 2020
Available online 1 July 2020

Keywords:
Amitriptyline
Tricyclic antidepressants
Fullerene (C_{20})
Adsorption
Density functional theory

ABSTRACT

In this research, amitriptyline adsorption on the surface of fullerene C_{20} was studied by density functional theory computations. The calculated adsorption energies showed amitriptyline interaction with C_{20} is experimentally possible. The negative values of Gibbs free energy changes and great values of the thermodynamic constants indicated the adsorption process is spontaneous. The negative values of adsorption enthalpy changes and the increase of specific heat capacity in the adsorption process revealed the interaction of amitriptyline with fullerene is exothermic and this nanostructure is an admissible sensing material for thermal detection of amitriptyline. The density of states (DOS) plots showed the bandgap of fullerene reduced from -32.13% from 7.145 (eV) to 4.849 (eV) when amitriptyline adsorbed on its surface. Therefore, C_{20} can be used as a sensor for electrochemical detection of amitriptyline. The influence of the temperature on the amitriptyline interaction with fullerene was also investigated and the results showed the adsorption process is more favorable in lower temperatures.

1. Introduction

Amitriptyline (AMP, Figure 1a), is a tricyclic antidepressant medicine that is prescribed for the treatment of depression, eating disorders, neuropathic pains, migraine prevention, nocturnal enuresis, fibromyalgia, insomnia, irritable bowel syndrome, anxiety disorders, and attention deficit hyperactivity disorder [1-3]. AMP is one of the best-selling antidepressants that induces its therapeutic effects by inhibiting the uptake of norepinephrine and serotonin [4-6]. However, in high doses, AMP can be highly toxic and its adverse effects are agitation, drowsiness, coma, seizures, and tachycardia. In this respect, AMP determination is very important. To date, various analytical techniques such as high-performance liquid chromatography (HPLC), gas chromatography (GC), fluorimetry, capillary electrophoresis, and UV-Visible spectrophotometry have been reported for the quantitation of AMP [7-9].

However, these methods are too expensive, time-consuming, and tedious. Besides, large amounts of organic solvents are used in the mentioned methods. But, electrochemical and thermal sensors are prominent alternatives for the refereed analytical techniques because these types of sensors are rapid, simple, economical, portable, selective, and sensitive devices that can determine the amount of the analyte with excellent accuracy and repeatability [10-14]. However, the first step in the development of a new electrochemical and thermal sensor is to find a recognition element that interacts with the analyte selectively and this interaction should lead to a considerable change in the electrochemical and thermal conductivity of the utilized recognition element which is used as a signal for determination of the analyte concentration [15-17].

On the other hand, fullerene (C_{20}, Figure 1b) is the smallest nanomaterial with a dodecahedral cage structure

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