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A DFT study on the interaction of alprazolam with fullerene (C_{20})

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ABSTRACT

In this paper, the detection of alprazolam by fullerene (C_{20}) was studied by infrared (IR), frontier molecular orbital (FMO) and natural bond orbital (NBO) computations. All of the computations were done by density functional theory method in the B3LYP/6-31G (d) level of theory. The calculated adsorption energies, Gibbs free energy changes and thermodynamic constants showed alprazolam adsorption is experimentally possible, spontaneous and irreversible. The calculated values of enthalpy changes and specific heat capacity demonstrated alprazolam interaction with fullerene is exothermic and C_{20} can be used as a recognition element for the construction of a new thermal sensor for detection of alprazolam. The DOS spectrums showed the bandgap of fullerene decreased from 7.190 eV to 4.460 eV (%-37.9) in the alprazolam adsorption process and this nanostructure is a good electroactive sensing material for development of novel electrochemical sensors for alprazolam determination. Some important structural parameters including chemical hardness, chemical potential, electrophilicity, maximum charge capacity and the dipole moment of alprazolam in the adsorption process was also investigated.

1. Introduction

8-Chloro-1-methyl-6-phenyl-4H [1,2,4] triazolo [4,3-a] [1,4] benzodiazepine or alprazolam (AP, Figure 1) is a benzodiazepine prescribed for insomnia, depression, bipolar disorder, panic disorder and different kinds of phobia [1]. AP is one of the bestselling medicines and it is widely abused. Compressed tablets and extended-release capsules are the more commonly available forms of AP [2]. AP reacts selectively with the interaction sites of y-aminobutyric acid (GABA) receptors in the body and induces its effects by this mechanism [3]. The toxicity of AP is observable in high doses. Bradycardia, coma, nausea, diarrhea, syncope and even death are the common adverse effects of AP in high doses [4-7]. Therefore, developing a rapid, simple and sensitive thermal and electrochemical sensor for the detection of AP is very important [8].

On the other hand, in the fullerene family, C_{20} is the smallest member with a dodecahedral cage structure (Figure 1). C_{20} composed of pentagonal rings and its structure is highly curved. This nanostructure has special features that can make it an appropriate sensing material including high conductivity and outstanding reactivity and good surface area to volume ratio [9-11]. In this regard, the performance of this fullerene as an electrochemical and thermal sensing material for the detection of AP has been investigated for the first time in this research by density functional theory calculations.