Special topic paper

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Computational investigation of thallium interactions with functionalized multi-walled carbon nanotubes for electrochemical sensing applications

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Abstract: Thallium (Tl) is a heavy toxic element which can cause several health issues. WHO and EPA have set a maximum permissible limit for thallium in drinking water above which it is hazardous, so its determination in our environment becomes crucial. Multi-walled carbon nanotubes (MWCNTs) are preferred for use in thallium sensing due to their large surface area and high conductivity, which allow them to be readily functionalized to selective groups. Previous experimental results showed that Tl selectively interacted with the MWCNTs functionalized with 3-amino-1,2,4-triazole-5-thiol (T-MWCNTs) with a limit of detection of 1.29 μg L^{-1} and linear range 10–100 μg L^{-1} by using voltammetry under optimized conditions. In actual water samples, the electrochemical sensor fabricated with the above-mentioned functionalized MWCNTs nanocomposite demonstrated high reproducibility and recovery. Molecular recognition and the outcomes of chemical and biological processes are shaped by non-covalent interactions among molecules. It is essential to investigate how these interactions impact binding preferences to enhance our understanding of these events. Here, we examine the structures of complexes of Tl and T-MWCNTs using quantum chemical calculations. Our results show that the most favourable complex of Tl-T-MWCNTs involve strong interaction of Tl with the nitrogen lone pair and additional stabilising interaction provided by the oxygen lone pair of amide linkage of T-MWCNTs. Moreover, we observed that the thiol group within T-MWCNTs readily undergoes deprotonation due to its acidic nature. Non-covalent interactions among molecules influence chemical and biological processes and molecular recognition. To improve our knowledge of these events, it is important to explore the ways in which these interactions affect binding preferences The negative value of adsorption energy (–1.53 eV) of this structure suggested that the interaction process between Tl and T-MWCNTs is spontaneous.

Keywords: density functional theory; MWCNTs; quantum chemistry; sensing; thallium; toxicity; VCCA-2023.

Introduction

Pollutants from the environment are being released as a result of the overuse of environmental resources caused by population growth. There is a continuous release of both organic and inorganic pollutants by natural and anthropogenic activities. Pollutants such as heavy metal ions, volatile organic compounds and dyes can cause serious health problems if exposed to humans for a long time [1]. Thallium is a post-transition metal, soft,

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