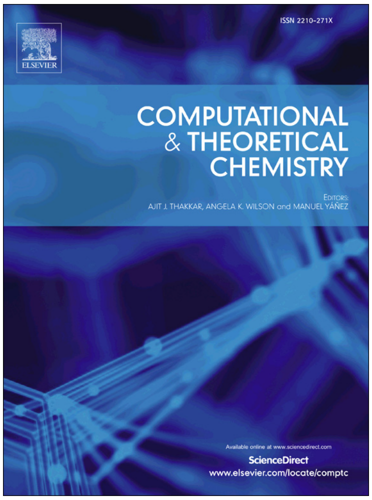

Inactivation possibility of pyrene by C_{20} fullerene *via* cycloaddition reactions: A theoretical study

Mousa Soleymani, Hossein Dashti Khavidaki

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Inactivation possibility of pyrene by C_{20} fullerene *via* cycloaddition reactions: A theoretical study

Mousa Soleymani*, Hossein Dashti Khavidaki

Department of Chemistry, Faculty of Basic Science, University of Ayatollah Alozma Borujerdi, Borujerd 69199-69411, Iran.

Abstract

In recent years, the air pollutant species has adventured the health of humans and other organisms. One of the pollutants are polycyclic aromatic compounds which are usually produced from defective combustion of fossil fuels. The removing or inactivation of these pollutants from environment is one of the research aims of scientists. In present work, the possibility of inactivation of the one of the polycyclic aromatic hydrocarbons namely pyrene with C_{20} fullerene was investigated theoretically. For this purpose, several [2+2] and [4+2] cycloaddition reactions between C_{20} and pyrene were considered and their thermodynamic and kinetic parameters were calculated. The results indicated that a) one of the [4+2] paths is more favorable relative to others, b) the most probable [4+2] Diels-Alder reaction of C_{20} and pyrene occurs with the rate constant of 5.09×10^{-6} $M^{-1}s^{-1}$ at 25 °C, and c) the reaction have relative polar character so that C_{20} fullerene and pyrene act as electron acceptor and donor, respectively. The Frontier Effective-for-Reaction Molecular Orbital (FERMO) concept was successfully applied for the description of the reactivity of the different active sites of pyrene. Finally, the synchronicity of the reactions was calculated and its correlation with activation enthalpy was elucidated.

Keywords: C_{20} Fullerene, Pyrene, DFT, Cycloaddition reaction, Global electron density transfer (GEDT), FERMO.

1. Introduction

Polycyclic aromatic hydrocarbons (PAHs) are a group of aromatic compounds containing two or more benzenoid rings in linear, angular, or cluster structure. They are a large class of

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[*] Corresponding author, Tel: (+98) 6642468320, Fax: (+98) 6642468223, E-mail: m.soleymani@abru.ac.ir, m_soleymani2007@yahoo.com