# Stability of fullerene complexes with oxazoles as biologically active compounds

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## Abstract

The ability of fullerene to form stable π → π-complexes was studied by quantum-chemical methods and the fluorescence quenching of reference dye (thiochrome). The correlation between the theoretically calculated and experimentally obtained energy of the π → π-complexes was determined. The energy of the stack interaction between fullerene and some biological active compounds, derivatives of 1,3-oxazoles, containing donor/acceptor substituents was estimated.



## Introduction

Physical and chemical, biological and pharmacological properties of fullerenes as nanoparticles have found applications in the clinical practice, in particular due to their antioxidant properties, possibility to inactivate free radicals, reduce oxidative stress, lipid peroxidation and neuronal membrane destruction (Li et al. 2008; Jain 2005; Kovtun et al. 2007). Fullerenes are potential carriers of drugs and radioactive labels: in the cavity during the synthesis process the drugs, radioactive particles can be placed (for the direct influence of diseased cells); they are used as a transporters for drugs because the "packaged" form of C60 will not cause toxic effects on the body and as a safe X-ray contrast agents in radiodiagnostics (Najam-ul-Haq et al. 2007; Movchan 2007). Studies have shown that C60 derivatives do not cause good or malignant neoplasms in animals after 2 months from the start of treatment, so fullerene is considered to have a very low level of cytotoxicity (Satoh and Takayanagi 2006). It has been experimentally proven that the human body can produce antibodies to fullerenes. The property of these specific anti-fullerene antibodies adsorbed on the surface of fullerene enable them to be used as cellular probes in immunology and to better investigate the function of the body's immune system (Ixhaky and Pecht 1998; Veetil and Ye 2007; Prato et al. 2008).