УДК 547.022, 544.183

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DFT-РАСЧЕТЫ КОМПЛЕКСНЫХ СОЕДИНЕНИЙ ТИТАНА (IV) С КВЕРЦЕТИНОМ

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DFT-CALCULATIONS OF TITANIUM (IV) COMPLEX COMPOUNDS WITH QUERCETIN

Аннотация. Проведен квантово-химический расчет структур кверцетина (Qu) и его комплексов с Ti (IV) в газовой фазе и представлены наиболее вероятные структуры комплексов.

Ключевые слова: кверцетин, металл, комплекс, DFT-расчеты.

Abstract. A quantum-chemical calculation of the structures of quercetin (Qu) and its complexes with Ti (IV) in the gas phase was carried out and the most probable structures of the complexes were presented.

Keywords: quercetin, metal, complex, DFT-calculations.

Quercetin (Qu) is the aglycone form of several other flavonoid glycosides such as rutin and quercitrin that are found in citrus fruits, buckwheat, and onions. It is a polyphenolic compound that exists as glucosides in vegetables or fruits [1]. Quercetin has various properties that have a positive effect on the human body [2]. Another advantage of this polyphenolic compound is its ability to form complex compounds with various metals [3], such as: Cr(III) [4], Cu(II) [5], Al(III) [6]. In the literature contains works that describe quercetin complexes with metals from the standpoint of quantum chemistry [6-7]. There is practically no information about the formation of a complex compound of quercetin with one of the representatives of the d-elements, or more precisely with titanium. In one of the studies an attempt was made to obtain a complex compound of Ti (IV) with Qu using a spectrophotometric method and optimal conditions for its formation were found [8]. The aim of this work is to study this complex compound from the point of view of quantum chemistry.

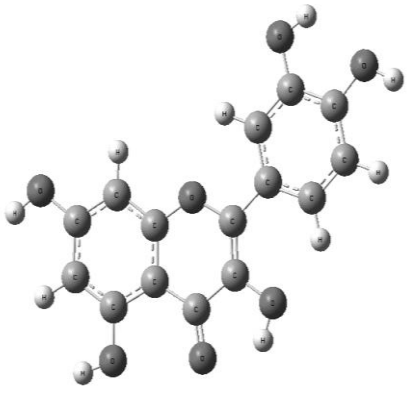
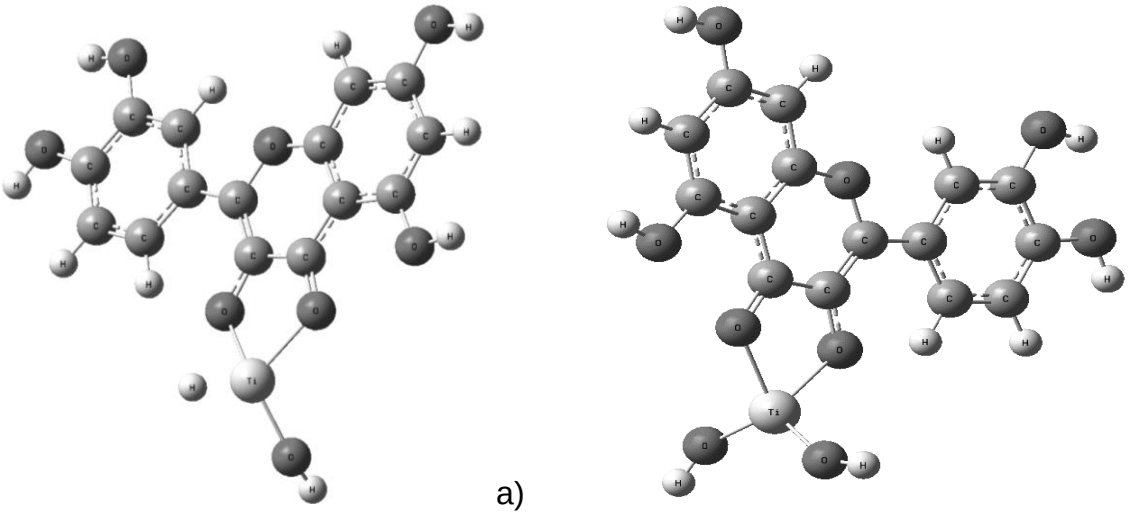


Figure 1 – Optimized structures of Qu E(h) = -1104,2407

Energetically optimized structures of Qu (Figure 1) and its titanium complexes (Figure 2, a, b, c, d) were obtained using density functional theory (DFT) calculations with the B3LYP 6-31++G(d,p) basis set level using ORCA software, with Avogadro as the visualizer.



a) b)

Figure 2 – Optimized structures of complexes of Qu with Ti (IV):
a) E(h) = -2029,6026; b) E(h) = -2104,9155

Of the large number of calculated Qu complexes with Ti (IV), the most stable of them are shown in Figure 2. In the future, we plan to make calculations taking into account the influence of the environment.

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