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Quantum Chemical Modeling of Three-Component System Cisplatin–Fullerenol–Quinine: HF-3c Quantum Chemical Modeling

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This study investigates rational approaches to the targeted delivery of chemotherapeutic drugs, with a focus on cisplatin, and explores methods to enhance their cytotoxic effects. The work presents results from computer modeling of the structural and electronic characteristics of quinine, fullerene, and cisplatin. Using quantum-chemical modeling with the HF-3c/MINIS/MINIS11(d)(Cl)/def2-SV(P)ECP(Pt) level of theory, and accounting for intermolecular interactions within the ORCA 5.03 software package, the electronic structure and binding energy of cisplatin, quinine, and fullerene adducts, as well as their three-component systems, were investigated. By analyzing the total energies of the systems and the calculated energy diagrams of the highest occupied and lowest unoccupied molecular orbitals for the initial components and the molecular ensembles they form, we concluded the most stable combinations. The study suggests a synergistic effect and outlines the potential use of the three-component system of cisplatin–quinine–fullerene $C_{60}(OH)_{24}$ in chemotherapy for oncology practice.

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1. Introduction

The method of quantum chemical modeling with using the level of HF-3c/MINIS/MINIS11

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theory(d)(Cl)/def2-SV(P)ECP(Pt), considering intermolecular interaction within the ORCA 5.03 software package, studied the electronic structure and binding energy of cisplatin, quinine and fullerenol adducts and their three-component systems. By analyzing the total energies of the systems and the calculated energy diagrams of the higher occupied and lower unoccupied molecular orbitals for the initial components and the molecular ensembles formed by them, we drew conclusions about the most probable their combinations in terms of stability. The nature of synergistic effects is assumed and the prospects for using the three-component cisplatin-quinine-fullerenol $C_{60}(OH)_{24}$ system during chemotherapy in oncological practice are outlined.

Chemotherapeutic drugs such as cisplatin [cis-diamminodichloroplatinum(II)] **3** or carboplatin [cis-diamine(cyclobutane-1,1-dicarboxylate-O,O')platinum(II)], the mechanism of action of which is the formation of cross-links between adjacent guanine base pairs in deoxyribonucleic acids, allow suppression of nucleic acid biosynthesis and lead to the death of malignant tumor cells. However, these drugs have negative side effects on the entire body of patients. These substances have pronounced cytotoxic, bactericidal and mutagenic properties. In this regard, reducing the therapeutic concentrations of chemotherapeutic drugs by combining them with other substances that do not have cytotoxic activity, but can increase it in protocol cytostatics, is an urgent task of pharmacokinetic and oncological medicine.

Previously, a synergistic effect on reducing the therapeutic concentration of cisplatin **3** in the presence of components such as certain heterocyclic compounds or fullerenol '**2** (binary adducts) was reportedite [1–3]: both quantum chemical modeling and the effect of binary cisplatin adducts on cytotoxicity were described (proliferation) on cell lines of collection cell cultures.

2. Quantum chemical modeling of a three-component system cisplatin–fullerenol–quinine

A further development of these studies is quantum chemical modeling of a three-component system: a cytostatic (cisplatin **3**), a synergist (fullerenol **2**), and a sensitizer (quinine [(8S,9R)-6;-methoxycinchonan-9-ol] **1**). The use of three components will hypothetically make it possible to enhance the antitumor effect of a cytostatic while reducing its therapeutic concentration, that is, weakening the general toxic effect on the patient's body while maintaining the chemotherapeutic effect [4, 5].

The objective of this work is a theoretical study of optimal and rational approaches to targeted delivery of chemotherapy drugs using the example of cisplatin and the search for ways to enhance their cytotoxic effect. The article presents the results of computer modeling of the structural and electronic characteristics of adducts of quinine, fullerenol and the cytotoxic drug cisplatin **3**, formed on the basis of fullerenol $C_{60}(OH)_{24}$ **2** (see the diagrams in Fig. 1), and also proposes possible mechanisms for the formation of the biological activity of their conjugates. To solve this problem, quantum chemical modeling of the structures under study was carried out using the HF-3c/MINIS/MINIS11(d)(Cl)/def2-SV(P)ECP(Pt) method [6], taking into account intermolecular interaction using the ORCA 5.03 software package [7]. Calculations were carried out both for individual compounds and for their conjugates in an aqueous environment, which simulates the conditions existing in living cells. The aquatic environment was modeled in the PCM approximation [8].

Quantum chemical calculations show that the formation of covalent cluster **7** from quinine **1** and fullerenol **2** with the elimination of water **14** is accompanied by an absorption of 20.72 kJ/mol. The formation of binary donor-acceptor adducts **4**–**6** was accompanied by the release of energy in the range of $\sim$ 22 − 62 kJ/mol. During the formation of three-component donor-acceptor

adducts **8**, **9**, energy was released in the range of $\sim$ 128 and $\sim$ 09 kJ/mol, respectively (see the diagram in Figs. 1 and2, Table 2).

Processes of exchange (displacement) of one ligand (NH3 **10**, pKb 4.75) in cisplatin with **3** more basic quinuclidine bases (pKb $\sim$ 3.00): **1**, **6**, **7** (see the diagram in Fig. 1) with the formation of donor-acceptor clusters **11** (binary) and three-component **12**, **13** are accompanied by the release of energy in a wide range from **13** to 150 kJ/mol. The formation of precisely these clusters (**11**–**13**), according to quantum chemical calculations, seems most likely. It should be noted that modeling of the formation of PtCl2 clusters with the elimination of two NH3 molecules (hypothetical compounds **15**–**18**) demonstrated their low probability due to high energy consumption ($\sim$ 178 – 257 kJ/mol), apparently due to steric factors. In the case of modeling the structure of **18**, due to the large volume of quinine ligands, this compound can only exist as a *trans*-isomer.

The calculation was carried out to clarify the dependence of the biological activity of the studied structures on their atomic structure and electronic structure based on an analysis of the energy position and localization of such descriptors of biological activity as frontier orbitals (FO), which are the highest occupied molecular orbital (HOMO) and the lowest vacant molecular orbital (LUMO). To visualize the results obtained, the Chemcraft software package was used [9].

The geometry of structures optimized within the framework of the HF-3c method (see the diagrams in Fig. 1)), electronic structure and localization of HOMO and LUMO are presented in Figure 2, energy characteristics in Tables 1,2

Using the quantum chemical modeling method by performing ab initio calculations at the *HF-3c* level of theory [6], a complete optimization of geometric parameters was carried out and the electronic structure of **16** compounds **1**–**18** was determined (Figure 2).

By analyzing superpositions of the total energies of systems using formula (1), similar to that used in chemical thermodynamics to calculate the thermal effects of chemical reactions (Hess's law [10]), the energy characteristics of the formation of clusters **4**–**9**, **11**–**13**, **15**–**18** from the initial ones were calculated components **1**–**3** upon elimination of **10**, **14** (ΔE_f, a.u. and ΔE_f, kJ/mol) (Tables 1 and 2):

$$\Delta E_f = \sum [E_f(\text{reaction products})] - \sum [E_f(\text{starting substantion})] \ . \quad (1)$$

By analyzing the difference between the energies of HOMO and LUMO using the method developed by K. Fukui (ΔF, eV) [11] (formula 2), the most (compounds **5, 8, 9, 12, 13, 16, 17**) and least (compounds **4**, **11**, **15**, **18**) promising compounds for their biological testing (see Table 1):

$$\Delta F = |E_{HOMO} - E_{LUMO}| \ . \quad (2)$$

The value (ΔF) shows that the smaller its value, the less energy is required for the transition of one electron from HOMO to LUMO, and, consequently, the transition of the molecule to the excited state [12]. This value correlates with the ability of compounds to exhibit biological, in particular, cytostatic activity [13].

Quantum chemical calculations showed that ΔF for all adducts of cisplatin with fullerenol, regardless of the presence of quinine **5**–**9**, **12**–**17**, is $\sim$ 3.7–4.1 eV less than for cisplatin **3** (Table 1). These data explain the experimentally observed synergistic effect of the combined action of fullerenol **2** and cisplatin **3** on cancer cells [2, 3]. The synergy of fullerenol and cisplatin manifests itself in the unexpected activation of the antitumor effect of cisplatin [2, 3]. This effect is relevant for oncology practice, since it will allow clinicians to reduce the dosage of chemotherapy drugs and, therefore, reduce the side effects of cytostatics on the patient's body while maintaining their optimal antitumor activity. Calculations of three-component molecular assemblies containing

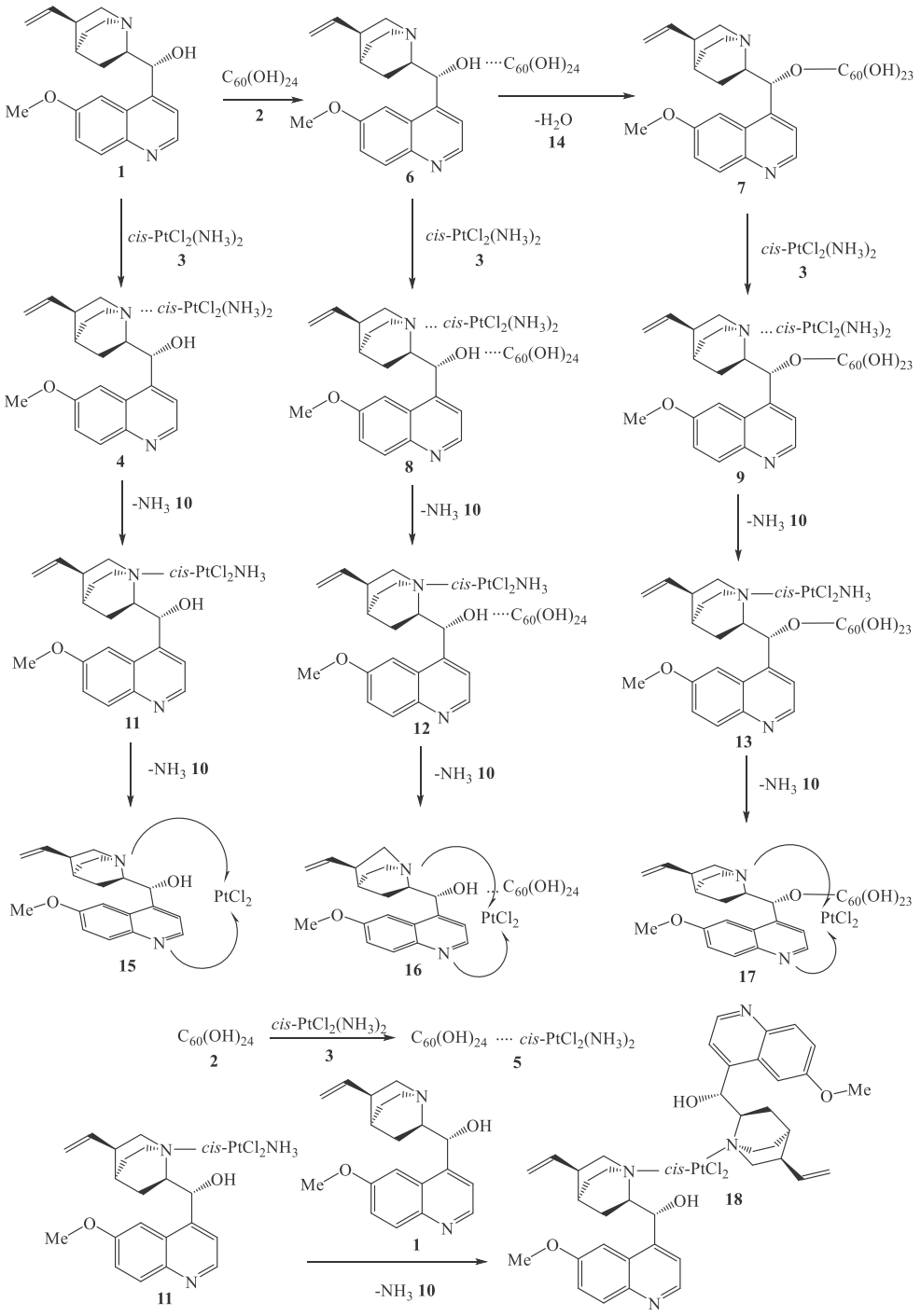

FIG. 1: The diagrams of three-component systems.

fragments of the alkaloid quinine **1**, fullerenol **2**, and cisplatin **3** (compounds **8**, **9**, **12**, **13**, **16**, **17**) showed that the presence of the quinine component leads to a slight change in the value of ΔF. At the same time, the ΔF value of adduct **8** turned out to be even $\sim$ 0.03 eV less than that of **9**, which suggests achieving a synergistic effect when using three-component

Table 1. Total energies of the system [E_f, Hartree atomic units (a.u.)], energies of the highest occupied molecular orbitals (HOMO, eV) and lowest unoccupied molecular orbitals (LUMO, eV), energy differences between HOMO and LUMO (ΔF, eV), dipole moments (D, D) of compounds **1**–**18**.

No	E_f, (a.u.)	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔF (eV)	D (D)
1	−1023.32	−8.325	3.162	11.487	0.90
2	−4056.26	−7.793	1.798	9.592	16.64
3	−1144.93	−9.589	3.707	13.296	16.71
4	−2168.27	−8.345	3.117	11.463	16.29
5	−5201.21	−7.809	1.723	9.532	27.44
6	−5079.58	−7.782	1.735	9.517	27.02
7	−5004.04	−7.789	1.721	9.510	23.24
8	−6224.55	−7.797	1.734	9.531	29.77
9	−6149.02	−7.817	1.746	9.563	31.15
10	−55.81	−10.832	18.487	28.808	1.85
11	−2112.45	−8.403	3.035	11.438	16.46
12	−6168.75	−7.800	1.793	9.593	18.24
13	6093.17	−7.773	1.773	9.584	19.26
14	−75.52	−12.614	16.260	28.874	2.29
15	−2056.54	−8.323	1.417	9.741	8.21
16	−6112.82	−7.825	1.440	9.256	27.52
17	−6037.29	−7.865	1.397	9.262	20.78
18	−3079.86	−8.378	2.802	11.180	2.86

Table 2. Energy characteristics of the process of formation of clusters **4**–**9**, **11**–**13**, **15**–**18** from the initial components **1**–**3** and upon elimination of **10, 14**, calculated by formula (1).

No	ΔE_f	
	(a.u.)	(kJ/mol)
4	−0.01706	−44.78
5	−0.02360	−61.96
6	−0.00817	−21.45
7	+0.00789	+20.72
8	−0.04881	−128.15
9	−0.04137	−108.62
11	−0.00880	−23.11
12	−0.05697	−149.56
13	−0.00496	−13.03
15	+0.09391	+246.55
16	+0.06796	+178.44
17	+0.07391	+184.06
18	+0.08833	+231.90

mixtures, abandoning the process of labor-intensive synthesis and purification of covalent cluster **7**.

Possible ligand exchange [14–17] of one molecule of ammonia **10** to quinine **1** in clusters - derivatives of cisplatin **3** with the formation of clusters **12**, **13** increases the ΔF value by only ∼0.02–0.06 eV compared with this indicator in clusters **8**, **9**. The formation of compounds **15**–**18** seems unlikely and their possible reactivity has not been analyzed.

As noted above, the electronic properties of cisplatin **3**, quinine **1** and fullerenol **2** and their ternary systems are convincingly explained by the analysis of frontier molecular orbitals (FO). The highest occupied molecular orbitals act as electron donors, and the lowest, lowest unoccupied molecular orbitals act as acceptor levels capable of accepting electrons. The energy difference ΔF (formula 2) is a quantum chemical parameter that can explain charge transfer in complexes [18] and ensures the chemical stability of structures [19].

The localization of HOMO and LUMO for all optimized structures is shown in Figure 2: **1** – quinine, **2** – fullerenol, **3** – cisplatin, **4** –

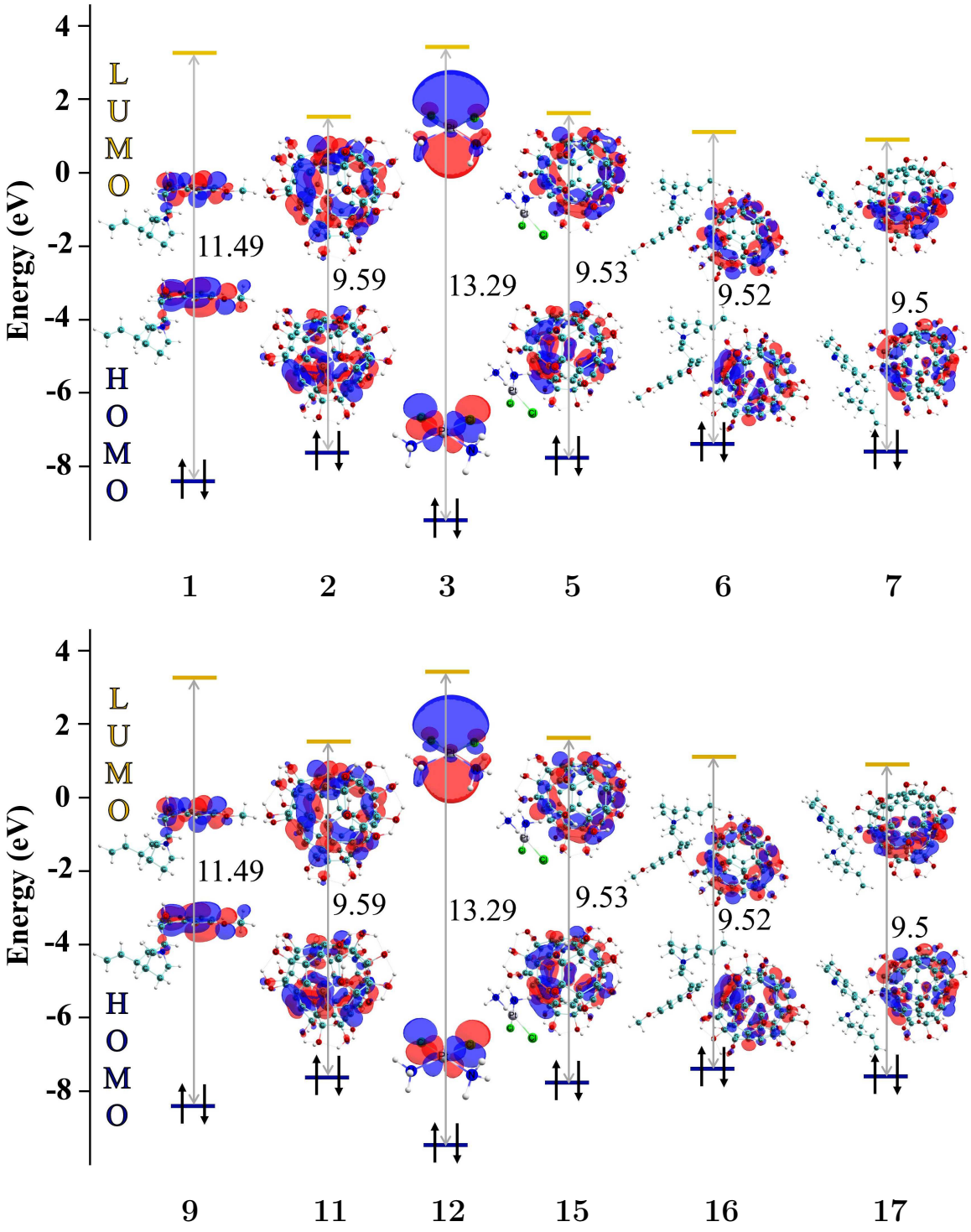

FIG. 2. (Color online) Electronic structure and localization of HOMO and LUMO for the optimized structures **1**–**3**, **5**–**7**, **9**, **11**, **12**, **5**–**7** (explanations in the text).

non-covalent adduct of quinine and cisplatin, **5** – noncovalent adduct of fullerenol and cisplatin, **6**

– noncovalent adduct of fullerenol and quinine, **7** – covalent adduct of fullerenoloquinine, **8** – molecular ensemble of noncovalently bound three-component systems, **9** – molecular ensemble of the covalent adduct of fullerenoloquinine and cisplatin, **11** – amino(quinino)dichloroplatinum, **12** – molecular non-covalent ensemble of amino(quinine)dichloroplatinum and fullerenol, **13** – molecular covalent ensemble of amino(fullerenoloquinine)dichloroplatinum, **15** – quinine dichloroplatinum, **16** – molecular ensemble of a non-covalently bound system of quinine dichloroplatinum and fullerenol, **17** – molecular ensemble of covalently bound fullerenoloquinindichloroplatinum systems, **18** – molecular an ensemble of covalently bound bis(quinine)dichloroplatinum system.

In the case of cisplatin **3**, it was found that the HOMO is distributed only over the chlorine and platinum atoms, while the LUMO is dispersed throughout the molecule. The lowest vacant molecular orbital of fullerenol **2** is localized predominantly on one side of the molecule, while the highest occupied molecular orbital covers almost the entire molecule. The localization of the frontier molecular orbitals for the noncovalent fullerenol–cisplatin adduct **5** and the noncovalent fullerenol–quinine adduct **6** remains on fullerenol. The HOMO of the covalent adduct of fullerenoloquinine **7** is uniformly distributed throughout fullerenol, and the HOMO, in comparison with the noncovalent adduct **6**, captures the oxygen atom connecting fullerenol and quinine.

The structural components of quinine **1** are two heterocyclic systems: quinoline and quinuclidine. In the quinine molecule, these two fragments are linked to each other through the –CH(OH)– group. For quinine, **1** HOMO and LUMO are located on quinoline. The localization of the boundary molecular orbitals for the noncovalent adduct of quinine and cisplatin **4** coincides with the localization of the FMO for the quinine molecule. The LUMO of the ensemble non-covalently bound by the three-component system of cisplatin, fullerenol and quinine **8** is located on fullerenol mainly on the side closest to cisplatin and quinine, while the HOMO is localized along the surface of fullerenol.

In the ensemble of the covalent adduct of fullerenoloquinine and cisplatin **9**, the position of the FMO is similar to the position of the LUMO and HOMO for structure **7**. The HOMO for the structure of amino(quinino)dichloroplatinum **11** is distributed on quinoline and partially captures the carbonyl group connecting the two quinine rings. HOMO is redistributed onto quinoline. It covers only the outer rings of pyridine and benzene, as well as the oxygen atom of the carbonyl group and the common nitrogen atom of cisplatin and quinuclidine. The position of the boundary molecular orbitals in the conjugate of the noncovalent ensemble of amino(quinine)dichloroplatinum and fullerenol **12** and the covalent ensemble of amino(fullerenoloquinine)dichloroplatinum **13** is determined on fullerenol in the same way as for structures **6**, **7**, **8**, **9**: LUMO is distributed on one side of fullerenol, HOMO along its surface. In quinine dichloroplatinum, the **15** HOMO is located predominantly on quinoline, partly on the platinum atom, and on one of the chlorine atoms closest to the heterocyclic system of pyridine and benzene. LUMO is completely localized on the platinum atom, the nitrogen atom covalently bonded to it and the chlorine atoms, and also partially covers quinuclidine. The transition from HOMO to LUMO suggests that electron density is transferred from quinine to dichloroplatinum. In the complex of a noncovalently bound system of quinine dichloroplatinum and fullerenol, **16** HOMO is distributed over the surface of fullerenol, and LUMO is localized exclusively in the dichloroplatinum region, capturing nitrogen atoms of this molecular ensemble with complete separation of densities. For the complex of the covalently bound fullerenoloquinindichloroplatinum system **17**, the situation is similar: the HOMO is distributed on fullerenol, the LUMO is again localized on dichloroplatinum. Thus, in the structures **16** and **17**, charge transfer occurs between

fullerenol and quinine dichloroplatinum. The HOMO of the ensemble of the covalently bound bis(quinine)dichloroplatinum system **18** is located on the quinoline of one of the quinines, and the HOMO is transferred to the quinoline of the opposite quinine molecule, also localizing on the platinum atom and carbonyl group.

3. Conclusion

An analysis of the localization of MOs obtained after calculating the electronic structure showed that if the solvent (water) is taken into account, the contribution of the orbitals of the $C_{60}(OH)_{24}$ **2** atoms to the formation of LUMO and HOMO, which determine the reactivity of two- and three-component complexes, increases. These molecular assemblies can lead to an increase in the likelihood of direct participation of fullerenol **2** atoms in reactions that determine the biological, in particular, cytostatic activity of these conjugates. Analysis of MO localization demonstrates that fullerenol **2** is not only an indifferent carrier of cisplatin **3** or quinine **1**, but is also directly involved in the processes of action on the tumor. The combination of these factors explains the possibility of enhancing the antitumor effect of cisplatin **3** and quinine **1** when they interact with fullerenol **2** [20].

These findings confirm the results of a colorimetric test for assessing the metabolic activity of cells (MTT test) based on studies conducted at the Institute of Physiology of the National Academy of Sciences of Belarus, which made it possible to establish the proliferative activity of rat *C*6 glioma cells in the presence of a combination of the drug cisplatin 3 in the presence of microquantities of fullerenol **2**. Detailed results of this experiments will be published separately.

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