STRUCTURAL ANALYSIS OF THE THIOUREA DERIVATIVES

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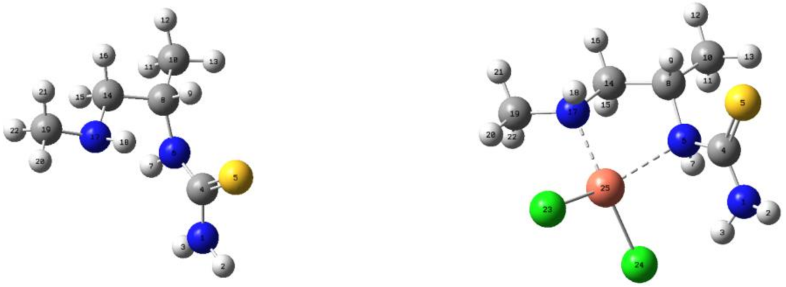
Thioureas are organic compounds that contain a sulfur atom. Thee compounds play an exceptional role in almost every field of chemistry. They have great commercial, industrial and scientific importance. Thioureas and their metal complexes are also used as antibacterial, antiviral, anti-inflammatory, antidepressants, antiallergatives, antiepileptic, anti-cancer.The biology activity of such compounds is directly related to their particular structural parameters. Therefore synthesis novel thioureas, studying their structure and properties as well as the metal complexes of thioureas is very actual. In this work, the composition and structure of the synthesized thiourea and its complex with $CuCl_2$ were investigated by XRD analysis, NMR and IR Spectroscopy. DFT/B3LYP/6-31+G(d,p) have been used to determine the structural parameters for these compounds. The quantumchemicalcalculationsare attractive methods for design of new molecules and study their structural, molecular and reactivity properties.It has been established that in complexation reactions the thiourea will be coordinated predominantly through the heterocyclic nitrogen atoms N6 and N17 with the highest localization of the negative charge. The results of the theoretical calculations were confirmed experimentally by the synthesis of complex with $CuCl_2$. Frontier molecular orbitals energies, HOMO-LUMO energy gap, ionization potential, electron affinity, global hardness, molecular softness, electronegativity, chemical potential, electrophilicity index, dipole moment, polarizability have been calculated for the reagent and complex. Mulliken charges have been determined for insight into the electronic charge distribution, molecular electrostatic potential has been visualized to identify the sites of electrophilic and nucleophilic regions of these compounds. To elucidate the electron density transfer hyper conjugative interactions NBO analysis has been carried out for these compounds.The results of the study indicate the formation a stable thiourea complex with $CuCl_2$. It was revealed that the nature of the mentioned substituent favors the formation of a stable five-membered ring via coordinate bonding N6-Cu25 and N17-Cu25 (Figure). In addition, the thiocarbonyl and methyl groups form a pseudo six-membered ring via the C10H13…S5 hydrogen bond in this complex. The mesomerism exhibited by nitrogen lone pairs and conjugated double bonds was revealed for thiourea and its complex. It is assumedthis phenomenon can increase the donor strength in metalcoordination.



(a) **(b)**

Fig. The optimized structures of the thiourea (a) and its complex with $CuCl_2$ (b)

SORPTION OF VANADIUM ION (V) BY A SORBENT BASED ON A COPOLYMER OF MALEIC ANHYDRIDE AND METHACRYLIC ACID, STUDY OF THE SORBENT AND COMPLEX BY INFRARED SPECTROSCOPY

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A modified sorbent based on a copolymer of maleic anhydride with methacrylic acid has been proposed for the sorption concentration of vanadium (V). A polymer chelating sorbent with fragments of 4-amino salicylic acid was used in the work. For sorption the optimal conditions have been determined. The dependence of the sorption capacity on the acidity of the solution has been studied. At pH 5, the degree of sorption passes through a maximum. The effect of ionic strength on vanadium sorption was studied. Studies have shown that the ionic strength up to 0.6 mol/l does not affect the sorption, after 0.6 mol/l the increase in the ionic strength at the beginning gradually, and then sharply decreases the sorption. All further experiments were carried out in solutions with an ionic strength of 0.6. It was found that with an increase in the concentration of vanadium in the solution, the amount of sorbed metal increases, and at a concentration of $8 \cdot 10^{-3}$ mol/l it becomes maximum ($pH = 5$, $C_{V^{5+}} = 8 \cdot 10^{-3}$ mol/l, $v_{total} = 20$ ml, $m_{sorb.}=0.03$ g, SC = 242,8 mg/g). Sorption equilibrium is achieved within 1 hour of contact of the solution with the sorbent. A further increase in the sorption time does not change the characteristics of the sorbent.

The development of modern industry requires operative and reliable control of the amount of toxic metals entering the environment, which have toxic properties. It is known that vanadium compounds are also highly toxic. As the valence of vanadium increases, its toxicity in both anionic and cationic forms increases.

The separation of vanadium from the waste solutions generated during the recycling of natural mineral raw materials leads to an improvement in the environment in the industry. Currently, there are a wide range of physicochemical