# SEARCH FOR THE OPTIMAL ORGANIC LIGANDS FOR EXTRACTION OF HEAVY METALS

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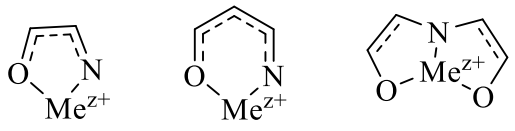
In the process of applying galvanic coatings there is a significant removal of working solutions from the baths with the surface of the workpiece (up to 10÷15 % of the bath volume). Usually the main amount of the removed solution is returned to the working process when washing parts in the capture baths. This significantly reduces the loss of working solutions that contain valuable components in the form of metal salts from which the coating is formed, and other functional additives. After the capture bath, the workpieces enter one or more washing baths, where the surface of the galvanic coated products is finally cleaned of electrolyte residues. The water from the washing baths is returned to the operating cycle to compensate for the loss of the volume of the baths or sent for cleaning from toxic components, followed by discharge to the sewer. The most common toxic components that need to be removed from the wash water are ions of heavy metals – copper, zinc, nickel, cobalt, cadmium. Their removal from wastewater requires the use of additional equipment and reagents that can reduce the ion content to an acceptable level, this causes a problem of disposal of metal compounds formed during the treatment stage. Therefore, it is more expedient to develop reagent-free methods of extraction metal ions, which allows their concentration from dilute wash water with subsequent return to the working bath. Such methods include ion exchange and extraction processes, which are widely used for the production of desalinated water, extraction of metals from their mixtures.

There are a considerable amount of empirical material has been accumulated regarding the extraction characteristics of the developed materials. However, attention should be paid to the need to systematize data and develop an effective approach that will create a material with certain extraction characteristics (degree of extraction and selectivity of extraction).

A method that provides quantum chemical calculation of complexation energies is proposed. The complexation energies of selected cations ($Zn^{2+}$, $Cu^{2+}$) with a series of model ligands – iminodiacetic acid analogs – as the difference between the total energies of complexes with the sum of cation and ligand energies was calculated by ROHF with 3-21G(d,p) basis.




1 2 3

It was established that ligands of type 3 (with three coordination centers) are more efficient complexing agents, higher selectivity can probably be provided by ligands of types 1 and 2 (with two coordination centers): the energy of complexation depends on the structural factors due to the nature of the ligand.