Nucleotides are organic molecules that have a wide range of functions in living organisms. They participate in cell signaling, serve as cofactors of enzymatic reactions, play a central role in cellular metabolism, and are the basic monomeric units of nucleic acid polymers. Nucleotides consist of three subunit molecules – nitrogen nucleobase, a five-carbon sugar (ribose or 2′-deoxyribose), and a phosphate group containing one to three phosphates. The subject of this master thesis is the study of various nucleotides and their self-assemblies in water by means of vibrational spectroscopy – Raman scattering and its chirally sensitive variant Raman optical activity (ROA). ROA has the potential to provide new information about the structural arrangement, dynamics, and interactions of nucleotides, as it supposes to be much more sensitive to vibrations of its sugar part containing three to four chiral carbons, compared to Raman scattering. We study spectral manifestations associated with chemical modifications (difference between ribo- and deoxyribonucleotides, the influence of different phosphate positions) and the change of physical conditions (various charge states according to the set pH, effect of concentration, influence of ions). A substantial amount of work is devoted to studying the self-association of purine nucleotides – adenosine-5′-monophosphate, which stacks at higher concentrations, and guanosine-5′-monophosphate and 2′-dexoyguanosine-5′-monophosphate, which form guanine quartets and their assemblies at higher concentrations in the presence of sodium or potassium ions. Guanine quartets represent the basis of guanine quadruplexes playing an important role in various biological processes (e.g., in gene expression).