ABSTRACT

Interaction of magnesium ions, the divalent ions with the highest concentration inside living cells, with the key biomolecules of nucleic acids was studied with aim to find out structural details of the interaction mechanism and effect of the magnesium ions presence on the nucleic-acid structure and structural transitions. Raman spectroscopy was chosen as the main experimental method, some complementary measurements of UV absorption spectra were also performed. Basic analyses of the spectral series obtained as a function of temperature and/or for various concentrations of Mg^{2+} ions were done by means of factor analysis. Where possible the factor analysis outputs were used for fits of appropriate thermodynamic equations.

For the studies, various nucleic-acid molecular models were employed, in particular complementary RNA homopolynucleotides polyA and polyU, DNA homopolynucleotides polydA and polydT and RNA 14-mer oligonucleotide representing the apical hairpin of the TAR segment of HIV-1 genomic RNA.

We have confirmed via Raman spectroscopy that magnesium ions added to a solution of polyA-polyU duplexes force some of them to dissociate and to form triplex structures, and obtained Raman signature of the specific binding site, being in the major-major groove between the adenyl and the Hoogsteen uridyl chain.

The thesis also presents the first study of magnesium ions effect on subtle premelting transitions. It was demonstrated on two model systems, poly(dA)-poly(dT) duplex and apical TAR hairpin, that magnesium ions influence them measurably, but in quite different ways. In the case of poly(dA)-poly(dT) duplex, magnesium effect is much stronger and concerns mainly the stabilization of the low temperature conformation. In the case of the apical TAR hairpin, the main effect of magnesium ions is the support of the structural changes in favor of the arrangement of the nucleobases in the hairpin loop reached at the temperature above the premelting.