

Abstract: L-3,4-dihydroxyphenylalanine (L-DOPA, levodopa) is a gold standard treatment of Parkinson's disease. Lately, it has been found that some of its deuterated analogues exhibit higher potency in the treatment; thus, they could replace L-DOPA. The subject of this thesis was a study of L-DOPA and its deuterated derivatives by the means of vibrational spectroscopy (Raman, ROA, IR, and VCD) and a comparison of the experimental results to a quantum mechanical simulations of the spectra. ROA and VCD are chiroptical methods, thus they are suitable for measurement of chiral molecules amongst which L-DOPA indeed belongs. Thanks to the quantum chemistry calculations, which yielded spectra with a very good agreement with the experiment, we were able to assign experimental spectral features to individual vibrational modes of the L-DOPA. The use of chiroptical techniques (mainly ROA) enabled an assignment of an absolute configuration of double deuterated derivative of L-DOPA, α,β -D₂-L-DOPA. It revealed that it occurs in a (*S*- α ,*S*- β)-enantiomeric form.