„Dimolybdenum carboxylates as auxiliary chromophores in structural studies of organic compounds transparent in UV-Vis range"

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In the course of realisation of this dissertation, I worked on application and development of dimolybdenum methodology to determine the absolute configuration of various groups of ligands transparent in the UV-Vis range. To this extent, my work has focused on finding an alternative to dimolybdenum tetraacetate carboxylate, which in electronic circular dichroism spectroscopy (ECD) can act as an auxiliary chromophore in structural studies of transparent compounds. The first task was to synthesise a series of dimolybdenum complexes and to further verify their usefulness in chiroptical studies of such ligands as 1,2-diols, 1,2-diamines, 1,2-aminoalcohols, α-amino- and α-hydroxy acids. I also made attempts to determine the structure of the chiral Mo_2-complex formed *in sit*u in the examined mixture by using other spectroscopic methods than CD and DFT calculations. In the implementation part of the dissertation, I complemented the initially planned dichroic techniques electronic CD (in particular the *in situ* methodology) with a comparison of results of vibrational circular dichroism (VCD) .

The results obtained allowed me to select, from six synthesized and tested dimolybdenum carboxylates, two the most useful for structural studies, namely dimolybdenum *tetrakis*(μ-isovalerate) and *tetrakis*(μ-pivalate). Based on the outcome I formulated the rules correlating the individual Cotton effects with the structure of the studied molecules.

The calculated ECD and UV-Vis spectra of chiral adducts of appropriate carboxylate with ligands representing all of the examined groups of compounds allowed me to assign the structures of complexes prevailing in solution based on their best agreement with the experimental spectra.

I employed two chiroptical techniques - ECD and VCD - to assign the absolute configuration of tested 1,2-diols unit with higher degree of confidence.

It was especially appropriate in cases such as, for example, *erythro* diols or molecules having other chromophores absorbing in the diagnostic range, in particular where one of the methods proved ineffective.

In the course of the present work I showed that vibrational and electronic circular dichroism are not mutually exclusive or competing techniques. They represent a partnership instrument in the work of a modern analytical chemist useful in solving structural problems due to possibility of choosing the most appropriate technique or improving the credibility of assignment made.

I demonstrated the complementarity of both techniques which increases the reliability of chiroptical methods as a stereochemical probe.