National Research Tomsk State University

THEORETICAL STUDY OF VIBRONIC SPECTRA OF THIAZINE DYES

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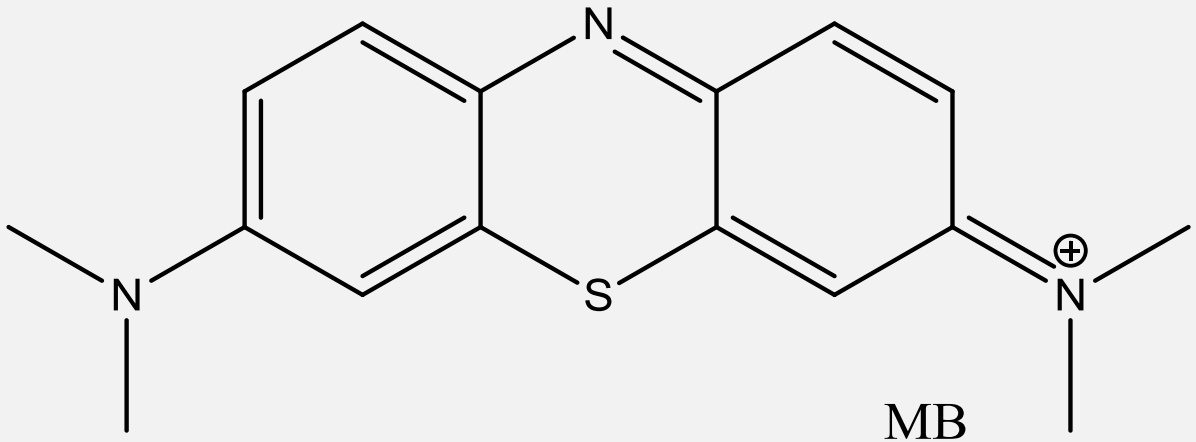
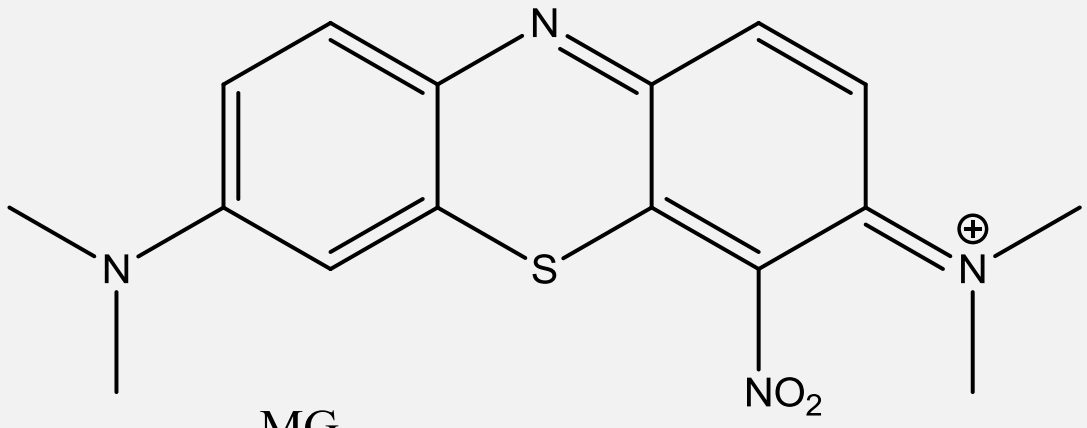
PURPOSE AND TASKS

This work is aimed for prediction of the vibronic absorption and fluorescent spectra of two thiazine dyes – methylene blue (MB) and methylene green (MG) and give some explanation of the role of the NO_2-group as a substituent in photophysical processes



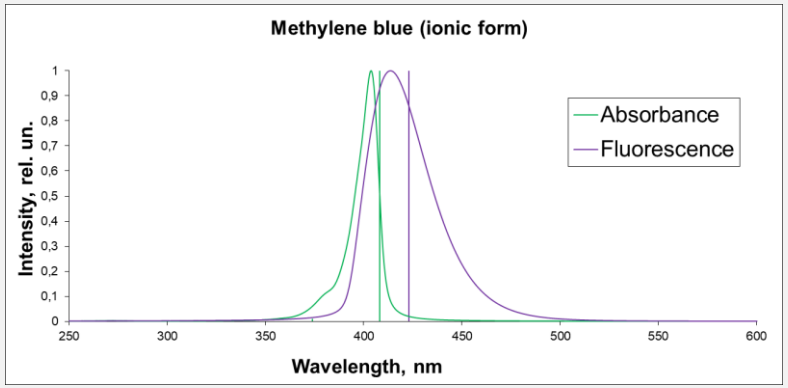
MB

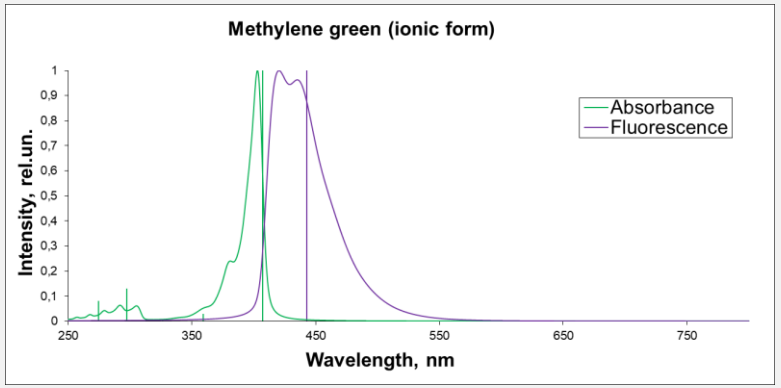


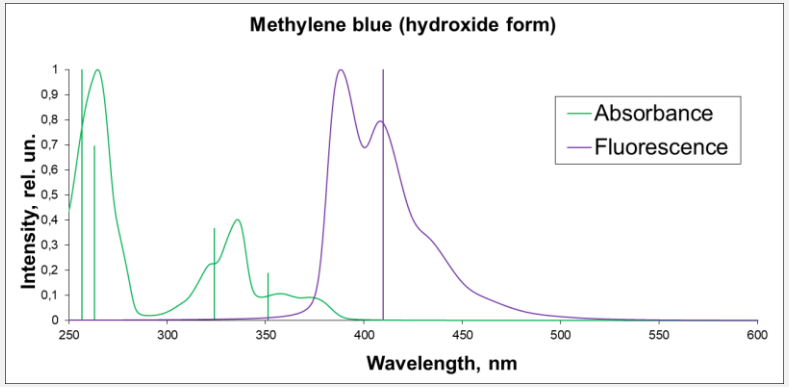
MG

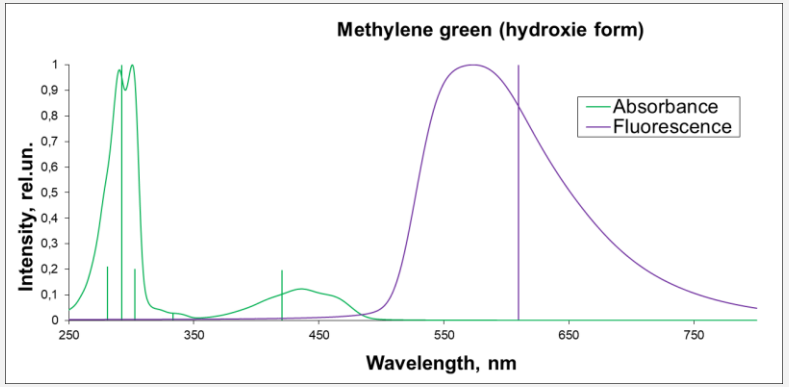
SIMULATED SPECTRA

All calculations were carried out in the quantum-chemical software package Orca 4.2.1 with using of stationary and time-dependent density functional theory (DFT and TD-DFT) and orca_asa (where ASA stands for “Advanced Spectral Analysis”) was used for simulation of the vibronic spectra. All calculations were performed at BHandHLYP / aug-cc-pvdz level of theory.









CONCLUSION

- Introduction of the NO_2-group lead to more resolved vibronic spectra in low pH conditions (ionic form) and has the opposite effect in high pH conditions (hydroxide form).

- For the second case it can be explained by intramolecular interaction between OH- and NO_2-groups, so molecule become more rigid. In the first case introduction of the NO_2-group lead to new degrees of freedom.

THANK YOU FOR YOUR ATTENTION