

ABSTRACT

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| Department | Department of Pharmaceutical Chemistry and Drug Control |
| Candidate | Miroslava Lásková |
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| Title of Thesis | Synthesis of azaphthalocyanines bearing one 2,6-di(<i>tert</i>-butyl)phenol substituent |

In this work, azaphthalocyanines (AzaPc) bearing one 2,6-di(*tert*-butyl)phenol substituent were synthesized. Phenolic OH in this moiety is a weak donor for intramolecular charge transfer (ICT). However, this group can be ionized in basic media and the resulting phenolate anion is very strong donor. This was expected to cause ICT and quench fluorescence of this compound.

The precursors for AzaPcs are substituted pyrazine-2,3-dicarbonitriles. They were prepared *via* one-step reaction of 5,6-dichloropyrazine-2,3-dicarbonitrile with 2-methylpropane-2-thiolate, respectively octanethiolate or *via* two-step reaction of 5,6-dichloropyrazine-2,3-dicarbonitrile with 2,6-di(*tert*-butyl)phenolate followed by nucleophilic substitution by 2-methylpropane-2-thiolate, respectively octanethiolate. Another precursor was prepared *via* reaction of glyoxylic acid with diaminomaleonitrile followed by chlorination with phosphoryl chloride and by subsequent nucleophilic substitution by 2,6-di(*tert*-butyl)phenolate. Resulting AzaPcs were prepared by cyclotetramerization of two precursors initiated by magnesium butoxide. Congeners (in metal-free form) bearing one 2,6-di(*tert*-butyl)phenol substituent were isolated in metal free form from the mixture of six congeners and converted to zinc or cobalt complexes.

The influence of properties of environment on fluorescence of zinc complex was subsequently studied – in particular the influence of polarity of solvent and presence of a base. The more polar solvents appeared to support the ICT. AzaPc was also sensitive to bases and formation of the phenolate anion quenched the fluorescence leading to decrease of fluorescence quantum yield for more than one order of magnitude. The process was found to be fully reversible.