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Theoretical Study on the Influence of Iron Mordant in the Optical Properties of Natural Dyes

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Abstract. Geometry optimization of free alizarin, purpurin and luteolin and coordinated Fe(II) complexes was performed at DFT/B3LYP level. TD-DFT spectra were also calculated for free and coordinated alizarin and luteolin. For the Fe(II) complexes several spin multiplicities have been calculated and quintuplet spin structures were found to be the most stable. In the luteolin-Fe(II) complex, the coordination of the chromophore with the iron leads to a decrease in the lower energy band. In the case of luteolin complex, a new band emerges due to interactions between the delocalized π electrons of the luteolin molecule with the d metal orbitals.