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Quantum-chemical modeling of the metal chelate cycles of methylphloroglucine phenylazo derivatives

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Abstract

We performed quantum-chemical modeling of five- and sixmembered metalchelate cycles of the complex Ni^{2+} with 2-phenyl-4-nitro-2,4,6-trihydroxytoluene H_4L.

Based on the relevant changes of the experimental and calculated electronic absorption spectra upon complexation we determine the most preferable type of coordination.