

Synthesis, X-ray crystal structure and DFT study of potential ligands of (2Z)-3-[(2-hydroxyphenyl)amino]-1-phenyl"alk"-2-en-1-one type.

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The main aim of the study was the synthesis and X-ray and spectroscopic investigations of potential ligands of transition metal complexes. A new compound, (2Z)-3-[(2-hydroxyphenyl)amino]-1-phenylpent-2-en-1-one, was obtained and the detailed experimental results are reported. Theoretical investigations based on the Density Functional Theory (DFT) were also performed for the presented compound as well as for its two analogues. Conformational analysis was done to find minima on the potential energy surface (PES). Analysis of the electrostatic potential (ESP) showed regions in the molecules sensitive to external interactions. Furthermore, topological analysis of the electron density (AIM theory) was applied to confirm the existence of an intramolecular H-bond in the molecules studied. The obtained theoretical results are in good agreement with the available experimental data.

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