عنوان مقاله:

Theoretical Study of First Singlet Excited State of Para-Substituted Platinabenzene Complexes

محل انتشار:

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خلاصه مقاله:

The structure, electronic properties, and aromaticity of the para-substituted platinabenzenes were illustrated by applying the hybrid density functional MPW1PW91 theory. The electron donor groups (EDG) and electron withdraw groups (EWG) effects on geometry, frontier orbital energies, reactivity indices and aromaticity in the first singlet excited state of platinabenzene were investigated and compared to ground state. The contribution of the fragments of the studied complexes in the frontier orbitals were calculated both in terms of the ground state and the first singlet excited state. Linear correlations between the studied parameters with Hammett s constants (sp) were given in the .two studied states

کلمات کلیدی:

(Platinabenzene, Substituent effect, Excited state, nucleus-independent chemical shift (NICS