Substituted phenylhydrazono derivatives of curcumin as new ligands, a theoretical study

Arrue L.

Zarate X.

Schott-Verdugo S.

Schott E.

A family of phenylhydrazono curcumin ligands was studied to see the influence of the substituents over the composition of the molecular orbitals, electronic transitions and reactivity by means of DFT and TDDFT calculations. The substituents varied between electron-donor groups (EDG) to electron-withdrawing groups (EWG). The geometrical parameters remain almost unchanged when the character of the substituent was changed. On the other hand the HOMO, LUMO and HOMO-LUMO gap (HLG) energies changed dramatically. TDDFT calculations were performed in order to propose the main absorption bands of this family of compounds. All the obtained showed a good correlation with a Hammett correlation.