Abstract:

Density functional theory is used to study the electronic properties of aurone derivatives that can be affected by ligand substitution procedures. After ligand substitution, the changes in the properties can be analyzed through density functional theory. Electronic properties include electronegativity, chemical hardness, and softness. While the values of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) and their energy difference are also calculated through DFT. From the geometry optimization structures values of RMSD (root mean square deviation) have been calculated. For this process, two molecules must have the same optimized geometries. Basis and functionals have been used to optimize the desired structures of aurone derivatives. Basis has two sets smaller basis set (def2-SVP) and a larger basis set (def2-tzvp) with different functionals B3LYP and TPSS. Through these bases and functionals, the values of HOMO LUMO and their energy gap are calculated. From the data, it has been examined that E aurones are more stable than the Z ones as their energies are lower. Aurones are used as plant dyes and as a defense against various infections.