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Theoretical IR, UV, ^{1}H and ^{13}C-NMR spectra of certain Schiff bases derived substituted-2-aminophenol and hydroxyl benzaldehyde

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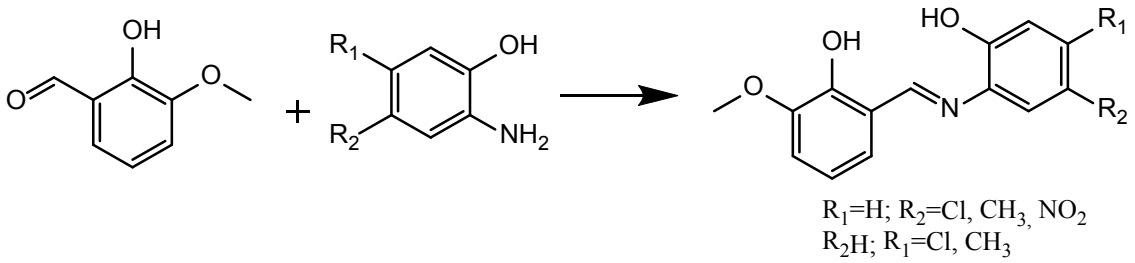
Schiff bases are compounds formed by the condensation of an active carbonyl group with primary amine or N-substituted imine containing an imino group (R-C=N-). They have been used as ligands, liquid crystals, heterogeneous catalysts, high-performance organic light emitting diodes (OLED), and to design molecular ferromagnet, in catalysis and biological applications [1]. In this study, five Schiff bases (Figure 1) have been synthesized and characterized with ^{1}H and ^{13}C-NMR. These Schiff bases' Gibbs Free Energies, Dipole moments, HOMO-LUMO values, theoretical IR, UV, ^{1}H and ^{13}C-NMR spectra have been researched by DFT method with Gaussian09 program (B3LYP/6-311++G(d,p)) [2] and compared than those with experimental values. Structure- reactivity relationship for these molecules was also searched.



R_1=H; R_2=Cl, CH_3, NO_2
R_2H; R_1=Cl, CH_3

Figure 1. The studied Schiff bases.

Biography

Dila Ercengiz has completed her Bachelor's degree in 2015 from Anadolu University. She is student of Anadolu University at Graduate School of Sciences.

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