Studies of structure of azo-linked 4H-pyrans using ab-initio calculations

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Xanthane derivatives have attracted many chemists due to their various biological activities and pharmacological properties such as antiviral, antibacterial and anti-inflammatory activities. In recent years, various studies have been devoted to the synthesis of novel derivatives of these compounds and several protocols have been devised for their preparation. In this research, Density functional theory (DFT) calculations at the B3LYP level is used to optimize the geometry of the compounds. In the continuation of our study, we were interested in evaluation of homoaromaticity of the ed compounds using nucleus independent chemical shift (NICS).

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