28th International Conference on
CHEMISTRY & DRUG DESIGNING
December 05-06, 2018 | Vancouver, Canada

Computational study on conducting polymer of thieno[3,4-b] pyrazines and its derivatives

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In this work, the geometrical and electronic properties of thieno[3,4-b]pyrazine (TP) based donor-acceptor conjugated oligomers were studied by density functional theory (DFT) at the B3LYP level with 6-31G (d,p) basis set. The inter-rings bonds are longer than normal double bonds but shorter than the single bonds; these indicate that the emerging of a quinoidal likes distortions as a result of oxidation. The absorption spectra of polymers were studied using the TDDFT/B3LYP/6-31G. Two main absorption peaks can be seen, the one largest in wavelength corresponding to a HOMO to LUMO transition, The result obtained from thermodynamic properties showed that all the studied compounds have almost similar properties.

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