

A model potential for the internal rotation of neighbouring rings of bithiophene and bipyrrrole

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Based upon ab initio Hartree-Fock calculations we propose a model potential for simplifying the study of the internal rotation of neighbouring rings. The quality of the proposed analytic potential was numerically verified in the case of bithiophene and bipyrrrole by determining the deviations of the predicted energy values along the torsional angle with respect to 19 independent reference values. It is found that our model potential describes correctly the torsional motion the average deviations of the predicted energies along the torsional angle with respect to the ab initio reference energies are 0.20 and 0.22 kJ mol⁻¹ for bithiophene and bipyrrrole, respectively. In both molecules, when going from a coplanar to a perpendicular conformation, two stable isomers have been detected. These isomers are separated by a barrier height of about 4 kJ mol⁻¹. Full optimization of the structural parameters along the torsional angle shows that they remain almost constant along the isomerization proc