ELECTRONIC STRUCTURE CALCULATIONS OF INTER-RING TORSIONAL POTENTIALS OF REGIOREGULAR POLY (3-METHYL THIOPHENE) OLIGOMERS

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The inter-ring torsional potentials of poly (3-methyl thiophene) (P3MT) oligomers are investigated by means of electronic structure calculations. Single layer and ONIOM calculations were performed at B3LYP level with 6-31++G(d,p) basis on the partially optimized geometries of dimer, tetramer and hexamer of P3MT oligomers. Potential energy surfaces are computed as a function of the multiple inter-ring torsional angles involved. The following conclusions are reached: (i) A mixture of cis and trans geometries can be expected in a disordered polymer. (ii) The cis-trans barrier is low enough to allow cis-trans conversion at room temperature. (iii) In the dimer, the potential energy minima are about 30^0 from the cis and trans planar geometries, but planar geometries are stabilized as the chain length increases. (iv) The extended conjugation causes the torsional potential about one inter-ring bond to be coupled to other torsions along the oligomer chain.