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A Computational Study of Homolytic Bond Dissociation Process Involved in the Initiation Process of Atom Transfer Radical Polymerization

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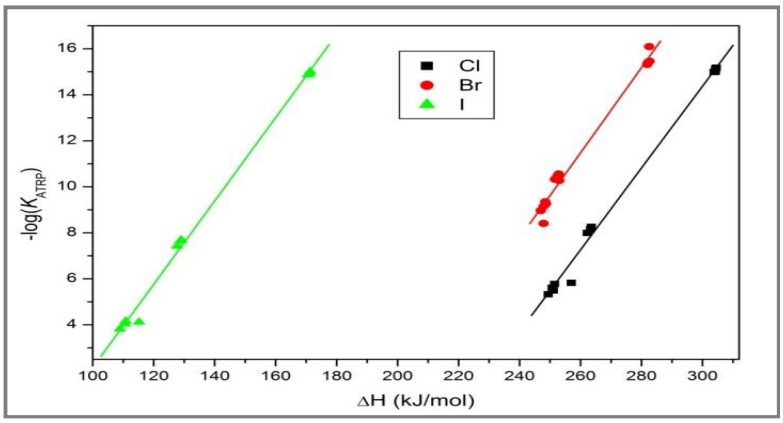
ABSTRACT

This paper presents a computational study on homolytic bond dissociation of a number of alkyl halides R–X (R = succinimide, ethyl-isobutyrate, X = Cl, Br, I) which can be potential initiators for the atom transfer radical polymerization (ATRP). The density functional theory with B3LYP functional and 6-31+G(d)/LanL2DZ basis sets is used in the prediction of geometries and energetics associated with the dissociation of R-X bond. The relative equilibrium constant for the ATRP activation/deactivation process is calculated from the free energy values, and its variation with system parameters (such as solvent, temperature and substituent) is investigated. Comparison with the known initiators for the ATRP shows that some of the studied compounds have potential to initiate the ATRP process.

Graphical Abstract



Correlation plot of relative K_{ATRP} values with R–X bond enthalpies of studied alkyl halides.

Keywords: Density functional theory (DFT), Bond dissociation energy, Homolysis, ATRP.