Aromatic C-H Bond Rupture; a Density Functional, B3LYP, Study

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Unrestricted Density Functional (B3LYP) calculations with the 6-311G(d) basis were done for benzene (C_6H_6) with successive elongation of one C-H bond. Gradual increase in the total energy resulted til C-H bond length of about 3.7 Å, followed by a sudden decrease in energy on further elongation of the bond. The estimated activation energy for the reaction was 152.346 kcal/mol, much higher than the value calculated with the semiempirical PM3 method.

Key words: Benzene; C-H Rupture; Density Functional; Calculation.