Jordan University of Science and Technology

Theoretical derivation for reaction rate constants of H abstraction from thiophenol by the H/O radical pool

Authors: Marwan Batiha, Mohammednoor Altarawneh, Mohammad Al-Harahsheh, Ibrahem Altarawneh, Saleh Rawadieh

Abstract: Reaction and activation energy barriers are calculated for the H abstraction reactions (C6H5SH + X?C6H5S + XH, X = H, OH and HO2) at the BB1K/GTLarge level of theory. The corresponding reactions with H2S and CH3SH are also investigated using the G3B3 and CBS-QB3 methods in order to demonstrate the accuracy of BB1K functional in finding activation barriers for hydrogen atom transfer reactions. Arrhenius parameters for the title reactions are fitted in the temperature range of 300 K? 2000 K. The calculated reaction enthalpies are in good agreement with their corresponding experimental reaction enthalpies. It is found that H abstraction by OH radicals from the thiophenol molecule proceed in a much slower rate in reference to the analogous phenol molecule. DfHo 298 of thiophenoxy radical is calculated to be 63.3 kcal/mol. Kinetic parameters presented herein should be useful in describing the decomposition rate of thiophenol; i.e., one of the major aromatic sulfur carriers, at high temperatures.