Inspecting the mechanism of nitration process in simple organic molecules through simulated ^{1}HNMR spectra using JSPEC View (Jmol)

Abstract

Nitration is a process of adding a nitro group to an organic compound. The process of nitration occurs via generation of an electrophile NO_2^+. The electrophile NO_2^+ was generated from the nitrating mixture (Concentrated sulphuric acid + Concentrated Nitric acid). In this project we have performed the nitration of acetanilide in the real time laboratory. The nitration product of acetanilide was p-nitro acetanilide. The 3D models of acetanilide and the product p-nitro acetanilide were created in the Jmol interface. The simulated ^{1}HNMR was obtained for both reactant and the product from JSPEC view feature in Jmol. The spectra obtained were interpreted and the structural changes in the reactant while forming the product was analysed. In addition, nitration reactions of naphthalene and benzoic acid were also examined using simulated ^{1}HNMR spectra obtained from Jmol.

Keyword

Nitration, Jmol, reactant, product, electrophile, simulated ^{1}HNMR spectrum, 3D models.