# Examining the structural changes in the organic molecules during hydrolysis with simulated $^{1}$HNMR using JSPEC View (Jmol)


## Abstract

Hydrolysis is a process which involves the reaction of any compound with water. This work was aimed at exploring the structural changes in the molecules during hydrolysis process. The hydrolysis of benzamide with sodium hydroxide was performed in the real time laboratory. The benzoic acid was obtained as the hydrolysis product. The (-$NH_2$) amide group in the benzamide was replaced with (–COOH) acid group to form benzoic acid. The 3D structure of the reactant benzamide and the product benzoic acid was drawn in Jmol interface. The simulated $^{1}$HNMR of both the reactant and the product were obtained through JSPEC view feature in Jmol. From the obtained simulated $^{1}$HNMR spectra, the structural analysis of the reactant and product were compared and analysed. The interpretation of the simulated $^{1}$HNMR spectra was done for these compounds. In addition, we have also explored the hydrolysis reactions of methyl acetate. The simulated $^{1}$HNMR from JSPEC view feature of Jmol was obtained for all the above mentioned reactants and their hydrolysed products. The structural changes in the reactants after subjecting to hydrolysis reaction were analysed using simulated $^{1}$HNMR spectra.



## Keywords

Hydrolysis, $^{1}$HNMR, benzamide, methyl acetate, JSpecview, Jmol