

Exploring the structural features of Glucose and Fructose with simulated ^1H NMR using JSPEC View (Jmol)

Abstract

The 3D structure of glucose and fructose were created in Jmol interface. The various properties of both the molecules such as bond length, bond angle, electrode potential surface, vanderwaals surface were explored. Glucose and fructose molecules are structural isomers; they possess the same structural features but with a different functional group. The glucose molecule possesses an aldehydic functional group and the fructose molecule possess a ketonic functional group. The similarity in their structure and dissimilarity in their functional group were examined with simulated ^1H NMR using JSPEC view (Jmol). In addition, few reactions of glucose and fructose were explored to examine the nature of the products formed. The simulated ^1H NMR using JSPEC View (Jmol) for the products were obtained to explore the structural differences and similarities between glucose and fructose.

Keywords:

Glucose, fructose, 3D structure, ^1H NMR, JSpecview, Jmol