ACADEMICIA: An International Multidisciplinary Research Journal
ISSN: 2249-7137 Vol. 11, Issue 12, December 2021 SJIF 2021 = 7.492
A peer reviewed journal

STUDY OF HYDROGEN-BONDED COMPLEXES USING *AB-INITIO* CALCULATIONS

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DOI: 10.5958/2249-7137.2021.02604.5

ABSTRACT

In this work the vibration frequencies of the formamide molecule C=O and N–H were investigated on the basis of the method of density function theory (DFT) and a set of bases B3LYP/6-311++G(2d, p) and also geometric and optical parameters of molecules were studied. Theoretical calculations have shown that that the C=O and N–H vibration bands of formamide shown shifted towards low frequencies in the formation of molecular aggregates. As the amount of water in the solution increases, the energy of aggregate formation increases. Aggregates were formed by different types of H-bonds. Calculations have shown that as the amount of water increases, H-bonds are formed not only through O-H···O, but also through O-H···N-type non-classical bonds. Density distributions and 3 D potential energy graphs for formamide and water systems were also studied. This allows us to learn more about the intermolecular interaction energies in the formamide aquatic environment.

KEYWORDS:*Formamide; Raman Spectra; H-Bond; Vibration Spectrum; Frequency; Simulation.*

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