Journal of Basrah Researches (Sciences) **50**(1), 203 (2024)
DOI: https://doi.org/10.56714/bjrs.50.1.17

Synthesis, thermodynamic and spectroscopic study of violurate salt

Huda Nouri Abdulzahra, Sadiq M.H Ismael, Faeza Abdulkareem Almashal*

Department of Chemistry, College of Education for pure sciences, University of Basrah, Basrah, Iraq.

ARTICLE INFO

Received 08 April 2024
Accepted 09 June 2024
Published 30 June 2024

Keywords:

DFT, hyperpolarizability, polarizability , violurate salt

Citation: H. N. Abdulzahra et al., J. Basrah Res. (Sci.) **50**(1), 203 (2024). DOI:https://doi.org/10.56714/bjrs.50.1.17

ABSTRACT

The organic salts are a broad class of ionic chemicals with a variety of properties. Scientists have an interest in violurate salts because of their bright color and crystal structure. In this study, 4-chloroanilinium violurate salt was synthesized and identification using infrared spectroscopy, 13C NMR spectroscopy and Electrospray ionization (ESI). Density functional theory (DFT) calculations have been performed using B3LYP/6-31++G**, and CAM-B3LYP/6-31++G** levels of theory. Practically, chloroanilinium ion $(M+H)^+$ has a relative abundance of 100% in ESI+, indicating its excellent stability. The protonation formula for violuric acid $(VA+H)^+$ shows instability, despite the observation of a low abundance of the $(VA+3H)^{3+}$ ion. DFT calculations demonstrate the exothermic nature of the salt formation reaction. The calculated enthalpy change is -26.861kJ in the B3LYP/6-31++G** level of theory and -31.82kJ in the CAM-B3LYP/6-31++G** level of theory.

1. Introduction

The organic salts are a wide range of ionic compounds possessing a wide range of characteristics, such as surfactants [1], reagents utilized for the synthesis of other organic compounds [2], lubricants [3], dyes [4], anti-inflammatory [5]. Violuric acid has astounding capacity to form salts with ions of metals and organic amines results in a wide range of colors [6]. A series of brightly colored alkali metal 1,3-dimethylviolurates have been synthesized by Edelmann and coworkers. X-ray crystal structure determination indicates that the compounds exist in the solid state as one- (Li, Na), two- (K, Cs), or three-dimensional (Rb) coordination polymers [7]. A variety of beautifully colored alkali metal 1,3-dimethylviolurates were synthesized by Lorenz and coworkers. The dimensions of synthesized compounds vary, ranging from polymeric networks to monomeric, neutral complex molecules and hydrogen-bonded ions [8]. Koleva and coworkers utilized quantum chemical calculations (MP2/6-31++G** level of theory) to discover the cinchoninium violurate monohydrate's physical characteristics. The absorption peak at about 3,400cm^{-1} in the infrared spectrum generated by quantum chemical calculations has been attributed to the stretching vibration of the hydroxyl group [9]. In the next study, Koleva and coworkers synthesized Ephedrinum violurate dihydrate salt. To determine the physical properties of salt, they used quantum chemical computations MP2 and B3LYP/6-31++G** level of theory. In the solid-state infrared spectrum, they observed that the low-frequency shifting of the υNH stretching vibration by ephedrine in type N–H…O intermolecular interactions is 87 cm-1, which is different from the theoretical value [10].

*Corresponding author email : faeza.nasser@uobasrah.edu.iq

ISSN: 1817-2695 (Print); 2411-524X (Online)
Online at: https://jou.jobrs.edu.iq