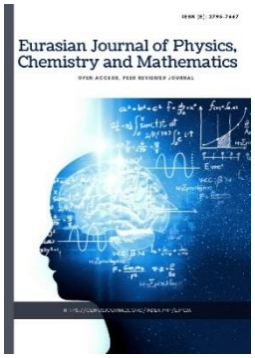

Thermogravimetric Analysis Of The Complex Compound Formed By 4-Nitrophenylacetic Acid With Ce Ion

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ABSTRACT

4-Nitrophenylacetic acid (4-NPA), belonging to the class of nitroaromatic acids, is one of the important intermediate compounds widely studied in the fields of pharmaceuticals, coordination chemistry, materials science, and biochemistry. Its molecule simultaneously contains an electron-accepting nitro group (-NO2) and an aromatic ring bonded with an acidic carboxyl group (-COOH) and a methylene group (-CH2-). This structure forms the basis for its manifestation as a compound with diverse physicochemical, complexing, and biologically active properties. This article summarizes the physicochemical, structural, and biological properties of 4-nitrophenylacetic acid based on various literary sources, providing a comprehensive analysis of their interrelationships, potential applications, and chemical reactivity.

Keywords: 4-NPA 4-nitrophenylacetic acid, Apelblat, NRTL, TGA and DTA analysis, crystallization reaction, complex compound, Ce (SO4) 2 crystal hydrate, DNA.

Introduction

By measuring the solubility of 4-NPA in 13 different solvents at different temperatures, it was determined that its solubility largely depends on the solvent's dipolarity and ability to form hydrogen bonds. They analyzed experimental data using NRTL, Apelblat, and other mathematical models, noting that the Apelblat model showed the best correlation.[1] Having studied the coordination complexes formed with alkaline earth metals (Mg, Ca, Sr) by crystallographic and spectral methods, he found that they are structured in the form of 1D coordination chains [2]. They also showed the strengthening of the ligand's binding to DNA through methoxy and bromo substituents in Cu (II) complexes and their electrochemical activity [3]. A new monoclinic crystalline form of 4-NPA was identified and compared with the previously known orthorhombic polymorph. It has been shown that molecular conformation and contacts (e.g., hydrogen bonds) differ among these forms [4].

Literature Review And Methodology

Cocrystals based on 4-NPA were synthesized, and supramolecular ribbon structures were identified through the interactions of O-H···N and C-H···O in them [5]. The crystallization of metal complexes of Mn (II), Co (II), Ni (II), Zn (II) based on 4-NPA in the

polymer structure and their thermal and magnetic properties were investigated. These complexes have a distorted octahedral {MO_6} geometry and exhibit significant thermal stability [6]. The biological activity of derivatives obtained from 4-NPA has been confirmed in several studies. Synthesized benzamide derivatives have a cytotoxic effect on lung, breast, and prostate cancer cells [7]. He created gel-forming salts based on the amino derivatives of 4-NPA and demonstrated their adsorption properties [8]. By proposing the production of 4-NPA by electrosynthesis, the ecological advantages of this method are shown. This compound serves as an intermediate product of many medicinal substances[9]. Based on 4-NPA, he was able to quickly and effectively obtain pentacyclic pyrrole-acridine skeletons. This method plays an important role in the creation of new drug molecules [10].

0.404 g (1 mmol) of the crystal hydrate Ce (SO4) 2 *4H2O were dissolved in water, respectively, and 0.3623 g (2 mmol) of 4-nitrophenylacetic acid were dissolved in water and alcohol, respectively, and solutions were prepared in a 1:2 ratio. Then, with the help of a magnetic stirrer, intensive stirring was carried out at 60°C for 2.5 hours. The precipitate was filtered, and the filtered clear solution was left at room temperature. As a result, after a few days, a white crystal of the complex compound grew at the bottom of the container. Crystals suitable for TGA analysis were isolated and examined.

Discussion

The composition and properties of the synthesized complex compound were studied using modern physicochemical analysis methods. The study of the thermal properties of substances is important for determining their stability, decomposition temperature, and thermal reactions. Thermal analysis methods, such as thermogravimetric analysis (TGA) and differential thermal analysis (DTA), allow for the determination of weight and thermal changes of substances with respect to temperature. Based on the TGA/DTA diagrams of the sample substance given in this article, its stepwise decomposition and thermal phenomena were analyzed.

Results

On the derivatogram (DTA) curve, five exothermic effects were observed at 64.34 °C, 161.46 °C, 262.95 °C, 310.50 °C, and 414.61 °C, with no endothermic effects detected. The analysis of the thermogravimetric (TGA) curve indicates that decomposition occurs in four distinct temperature intervals. The first decomposition stage occurred in the temperature range of 37.71–284.13 °C**,** with a weight loss of 3.822 mg or 25.323%**.** The second stage was observed in the range of 284.13–362.27 °C**,** where a mass loss of 6.643 mg or 44.014% was recorded. The third stage occurred between 362.27–425.29 °C, with a weight loss of 2.814 mg or 18.644%**.** The fourth stage took place in the range of 424.40–725.35 °C, with a mass loss of 0.817 mg or 5.413%**.** Over the full temperature range of 37.71–725.35 °C**,** the total weight loss was determined to be 14.096 mg, and the total analysis time was 71.77 minutes**.**

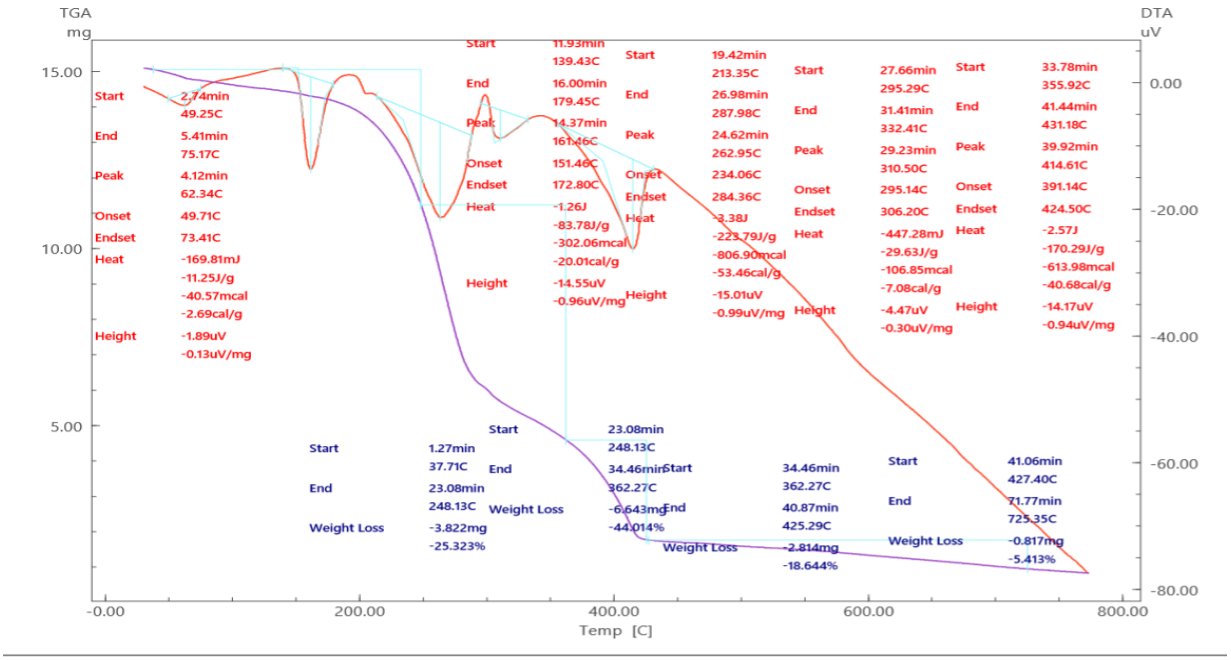

Figure 1. Thermogravimetric analysis of the complex of 4-nitrophenylacetic acid with the crystal hydrate Ce (SO4) 2*4H2O

The analysis of the thermogravimetric analysis curve and the differential thermal analysis curve is presented in Table 1 below. From the table, it can be seen that the highest mass loss occurs in the 2nd intermediate decomposition, i.e., 44.014% of the mass is lost in this intermediate.

Table 1

Analysis of the thermogravimetric (TGA) curve

Temperature (°C)	Time (minutes)	Mass (mg)	Mass loss (%)
37,71-284,13	21,81	3,822	25,323
248,13–362,27	11,38	6,643	44,014
362,27-425,29	6,41	2,814	18,644
427,40-725,35	27,71	0,817	5,413

A detailed analysis of the thermogravimetric analysis curve and the differential thermal analysis curve is presented in Table 2 below.

Table 2

Influence of temperature on the weight loss of the sample of the complex of 4-nitrophenylacetic acid with the crystal hydrate Ce (SO4) 2*4H2O

№	dw	1/T	dw/dt	M.g	Mint	T^0+K
1	14,6719	0.0026	0,0619	0,4211	6,8	373
2	14,0588	0.0021	0,0615	1,0342	16,808	473
3	6,523699	0.0017	0,3197	8,5693	26,808	573
4	3,829	0.0014	0,306	11,264	36,808	673
5	1,628099	0.0012	0,2876	13,465	46,825	773
6	1,3931	0.0011	0,2413	13,7	56,783	873
7	1,0927	0.0010	0,2097	14	66,758	973
8	0,826599	0,00093	0,186	14,266	76,692	1073

The values of the activation energy of this process are presented in Table 3.

Table 3

Results of thermal oxidation analysis of the complex of 4-nitrophenylacetic acid with the crystalline hydrate Ce (SO4) 2 *4H2O.

№	dw 15,093	Ln(W_1/W_2)	1/T *10^{-3}
1	14,6719	0,02829696	2.6
2	14,0588	0,070982526	2.1
3	6,523699	0,838789514	1.7
4	3,829	1,371627388	1.4
5	1,628099	2,226817984	1.2
6	1,3931	2,38269958	1.1
7	1,0927	2,625579363	1,10
8	0,826599	2,904666647	0,93

Thus, based on the obtained experimental data on the kinetics of processes in the temperature range from 250 to 800 K, the properties of thermo-oxidative degradation of the complex of 4-nitrophenylacetic acid formed by the crystal hydrate Ce (SO4) 2·4H2O were studied.

Conclusion

The properties of the complex compound synthesized on the basis of 4-nitrophenylacetic acid, which forms a complex as a result of the crystallization reaction, were investigated. The properties of the synthesized complex compound and its complexes with Ce (SO4) 2 *4H2O were studied using modern physicochemical analysis methods using the thermogravimetric method. The results obtained from thermogravimetry were analyzed, and the results were presented according to the table.

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