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Data Article

Thermal decomposition and kinetic analyses of sulfonamide Schiff's bases in oxygen atmosphere - A comparative study



Jaganathan Venkatesan^a, Mahalingam Sekar^{a,*},
Venugopal Thanikachalam^b, Govindasamy Manikandan^b

^a PG & Research Department of Chemistry, Government Arts College, C. Mutlur, Chidambaram-608 102, India

^b Department of Chemistry, Annamalai University, Annamalai Nagar 608 002, India

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ABSTRACT

Two sulfonamide Schiff's bases namely, 4-(benzylideneamino) benzenesulfonamide (BABS) and 4-((4-methylbenzylidene)amino) benzenesulfonamide (4-MBABS) have been synthesized from benzaldehyde or 4-methylbenzaldehyde and 4-aminobenzenesulfonamide by condensation method and characterized by micro analysis, Fourier Transform Infrared and NMR (¹H and ¹³C) techniques. The thermal decomposition of these compounds was studied by thermogravimetry/derivative thermogravimetry analysis (TG/DTG) under dynamic oxygen atmosphere at different heating rates of 10, 15 and 20 K min⁻¹. The decomposition process of BABS is single step, whereas 4-MBABS followed two steps as evidenced from the data. The kinetic parameters were estimated using model-free (Friedman, Kissinger-Akahira-Sunose (KAS) and Flynn-Wall-Ozawa (FWO)) and model-fitting methods (Coats-Redfern (CR)). Invariant kinetic parameters are consistent with the average values obtained by Friedman and KAS isoconversional methods of these compounds. Each step decomposed in different kinetic models. The calculated thermodynamic parameters values show that the decomposition process is endothermic and non-spontaneous nature.

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* Corresponding author.

E-mail address: drmschemgac@gmail.com (M. Sekar).

Specifications table

Subject area	Thermal analysis
Compounds	4-(benzylideneamino)benzenesulfonamide (BABS) and 4-((4-methylbenzylidene)amino)benzenesulfonamide (4-MBABS)
Data category	Synthesis, chemical analysis, spectral data, thermal decomposition
Data acquisition format	Elemental analysis, IR, NMR and TG/DTG
Data type	Analyzed data
Procedure	Structure, thermal characterization and reaction model determination
Data accessibility	Data are with the article

1. Rationale

Sulfonamides and their different derivatives are used as antimicrobial agents [1–3], antioxidant activity [4], cytotoxic property [5], antibacterial and antifungal activities [6,7], inhibitor activity [8,9], pharmaceutical activities [10]. Sulfonamides are analogous to PABA (p-amino benzoic acid) and suppress the synthesis of folic acid and DNA [11]. Infectious diseases which increase dramatically by resistant and multidrug-resistant microbes [12,13] are nowadays the second major cause of death worldwide and the third leading cause of death in developed countries [14,15]. Sulfonamide derivatives widely used in pharmacological agents with a wide variety of biological actions, were designed from the simple sulfanilamide lead molecule [16]. Sulfonamide Schiff's bases also used as anticancer and antiviral agents [17], and its metal complexes have been widely studied because they have industrial, anticancer herbicidal applications [18], antitubercular activities [19] and chelating abilities which give it attracted remarkable attention [20].

A series of water-soluble carbonic anhydrase inhibitors were obtained by reaction of aromatic/heterocyclic sulfonamides containing a $-NH_2$ (free amino) and $-SO_2NH_2$ (the amides of sulfonic acids), in the search of more effective topically acting antiglaucoma drugs [21]. Literature survey reveals that no work has been reported on thermal decomposition of sulfonamide Schiff's base under non-isothermal decomposition in the presence of dynamic oxygen atmosphere. This prompted us to carry out the synthesis, spectral characterization and thermal studies of sulfonamide Schiff's bases.

2. Procedure

2.1. Materials

4-Aminobenzenesulfonamide, benzaldehyde and 4-methylbenzaldehyde were purchased from Aldrich chemicals; glacial acetic acid and other reagents procured from S.d. Fine Chemicals and were used as received.

2.2. Instruments

Analytical Thin Layer Chromatography (ethyl acetate-hexane mixture) was performed on pre-coated plastic sheets of silica gel G/UV-254 of 0.2 mm thickness. Melting points of the synthesized compounds were determined in open glass capillaries on a Mettler FP51 apparatus and recorded in °C without correction. Elemental analyses were performed in EURO VECTOR EA 3000 at Central Leather Research Institute (CLRI), Chennai, India. An IR measurement was done as KBr pellets for solids using SHIMADZU-2010 Fourier Transform Infrared (FT-IR) spectrophotometer. The 1H and ^{13}C NMR spectra were recorded in DMSO- d_6 using TMS as internal standard with Bruker 400 MHz and 100 MHz high-resolution NMR spectrometers. The simultaneous TG and DTG curves were obtained with the thermal analysis system model Perkin Elmer TGA 4000 V1.04. TGA/DTG was recorded at National Institute of Technology, Triuchirapalli, India. The TG analysis of BABS and 4-MBABS were carried out under dynamic oxygen atmosphere ($100 mL \text{ min}^{-1}$) in a $180 \mu l$ ceramic pan with a sample at the heating rates of 10, 15 and $20 K \text{ min}^{-1}$ from 308 to 973 K. The sample temperature controlled by thermocouple, did not exhibit any systematic deviation from the preset linear temperature programme. The kinetic parameters E_a and A were calculated using Microsoft Excel Software®.

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