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**Structural Dependence of the Thermal Stability of Citrates**

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Citric acid is commonly found in the atmosphere, especially in aerosol (tiny particles suspended in the air). Citric acid commonly exist in aerosol phase as citrate salts. Detailed properties of these salts, however, are still unknown<sup>1,2</sup>. This research project investigated the thermal decomposition profiles and mechanisms of a group of ammonium citrates to determine their thermal properties. Such information will contribute to our knowledge on citrates and their transformation in the atmosphere.

Citric acid belongs to a specific class of carboxylic acids: polyacids; they are acid molecules with more than one carboxyl group on them. Since each carboxyl group can react with one ammonia molecule, polyacids can react with more than one amine. By controlling the amounts of a polyacid and ammonia is added to a reaction system, fully or partially neutralized carboxylates can be synthesized. Citric acid is a poly acid because it has three carboxyl groups. When three molecules of an ammonia react with one molecule of citric acid, the resulting citrate is considered fully neutralized and called ammonium citrate tribasic. Ammonium citrate dibasic is produced from two ammonia and one citric acid and ammonium dihydrogen citrate is from one ammonia and one citric acid.

This research determined thermal properties of three ammonium citrates: ammonium citrate tribasic (99% pure), ammonium citrate dibasic (99% pure), and ammonium dihydrogen citrate (95% pure). The compounds were purchased from Fisher Scientific and other chemical companies.

This research measured the thermal properties of the ammonium citrates, specifically investigating the thermal decay profiles using Thermal Gravimetric Analysis (TGA) method. The TGA measurements were completed using a Q-series 600 instrument. The sample sizes were about 10 mg, with an empty sample pan used as a reference. The samples were analyzed using the protocol for a fast run. The parameters for the fast run were that the respective samples were heated up by 20°C/min from 25°C to 300°C with a nitrogen flow rate of 100 mL/min. A decay profile was obtained for each citrate.

The decay profiles of the three citrates showed similar patterns. This indicated that the extra hydrogens do not have an obvious effect on the thermal decomposition of ammonium citrates. It was determined that the ammonium citrate tribasic was the most stable of the compounds studied. The percent mass loss for each of the compounds is about the same at the first derivative peak. This mass loss suggests that each of the compounds lost a water and an ammonia during the decomposition process. The data collected indicates that there is only one step of decomposition for each of the samples that were tested.

This study established a baseline of known ammonium citrates. Future research will include running slow scans to determine if a slower heating will change the information collected indicating that there is something else that can happen when these compounds are heated. The results also indicated that ammonium citrate dibasic contains water at room temperature, meaning that the sample may have to be re-analyzed after proper drying.

#### References:

1. Wyrzykowski, D., et al. "Thermal Behaviour of Citric Acid and Isomeric Aconitic Acids." *Journal of Thermal Analysis and Calorimetry*, vol. 104, no. 2, 2010, pp. 731–735.
2. Erdey, L., et al. "Thermoanalytical Properties of Analytical-Grade Reagents—IVA1 Sodium Salts." *Talanta*, vol. 11, no. 1, 1964, pp. 913–940.