Benjamin Thomas Class of 2019 Chemistry & Forensic Science Investigation of Thermal Properties of Carboxylates with Various Structures Mentors: Dr. Chong Qiu & Dr. Pier Cirillo

Thermal gravimetric analysis (TGA) is the analysis of the mass of a sample as it is exposed to temperature changes. This kind of analysis looks at the mass change of a sample as a function of temperature and reveals the thermal stability of the compound being tested. TGA can also be used to look at phase transitions and kinetics of the decomposition of the tested compound. Different compounds will produce different thermograms from the TGA analysis based on the makeup of the compound.

The project looked in to finding a parameter to determine the TGA properties of carboxylate salts. I used three different carboxylate acids, an aliphatic organic acid, an aromatic organic acid, and a hybrid of the two types and synthesize their salts. The aliphatic acid used is acetic acid, benzoic acid was used as an example of aromatic acid, and salicylic acid served as the hybrid of the two.

The ammonium salts of the three chosen carboxylate acids are already commercially available and were obtained for the project. The TGA instrument was then used to obtain thermal scans of benzoic acid and salicylic acid to establish a baseline for comparison. The thermal scan of acetic acid was not performed due to the high volatility of the acid.

The ammonium benzoate was tested first followed by the ammonium salicylate and the ammonium acetate. The TGA analysis yielded the thermal properties for each salt tested. To compare these scans, excel was used to produce first derivative graphs of the mass percent versus temperature scans. The peak on these graphs is the point at which mass decrease is at its fastest, this was used as a comparison point for the salts tested. The ammonium benzoate salt peak temperature is 194.72°C with a mass loss of 88.4% There are two possible ways for the salt to lose mass: the vaporization of ammonia and the vaporization of whole salt. Based on the mass loss at the peak temperature, I determined that 86.78% of the salt was completely evaporated and the rest lost its ammonia base. The ammonium acetate salt peak is 133.8°C with a mass loss of 94.16%. The ammonium salicylate peak is 204.23°C with a mass loss of 78.08%. Using this data, a trend was discovered between the molar mass of the salt and the peak temperature of its decomposition: the heavier the salt, the more stable it is. This trend has a R squared value of 0.967. Future research can be done by synthesizing and testing more salts to solidify the trend for all salts.