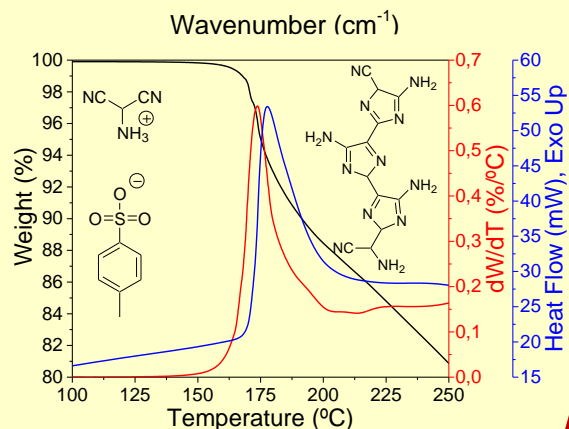
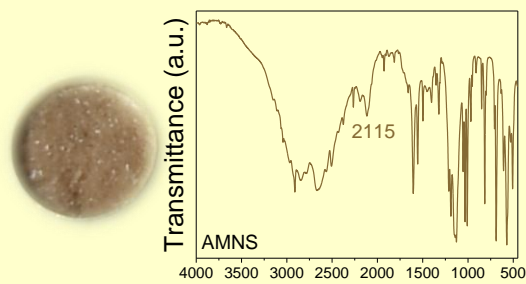
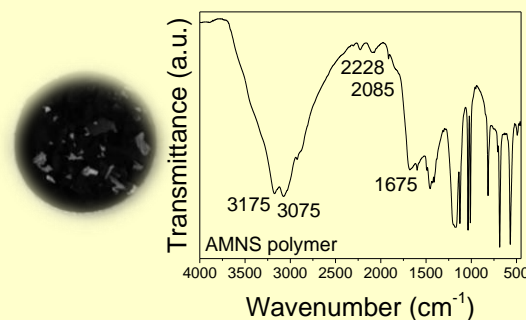


Kinetic Study of the Effective Thermal Polymerization of a Prebiotic Monomer: Aminomalononitrile



Non-isothermal heating



Aminomalononitrile (AMN), the HCN formal trimer, is a molecule of interest in prebiotic chemistry, in fine organic synthesis, and, currently, in materials science, mainly for bio-applications. Herein, differential scanning calorimetry (DSC) measurements by means of non-isothermal experiments of the stable AMN p-toluenesulfonate salt (AMNS) showed successful bulk AMN polymerization. The results indicated that this thermally stimulated polymerization is initiated at relatively low temperatures, and an autocatalytic kinetic model can be used to appropriately describe, determining the kinetic triplet, including the activation energy, the pre-exponential factor, and the mechanism function (E_a , A and $f(\alpha)$). A preliminary structural characterization, by means of Fourier transform infrared (FTIR) spectroscopy, supported the effective generation of HCN-derived polymers prepared from AMNS. This study demonstrated the autocatalytic, highly efficient, and straightforward character of AMN polymerization, and to the best of our knowledge, it describes, for the first time, a systematic and extended kinetic analysis for gaining mechanistic insights into this process. The latter was accomplished through the help of simultaneous thermogravimetry (TG)-DSC and the in situ mass spectrometry (MS) technique for investigating the gas products generated during these polymerizations. These analyses revealed that dehydrocyanation and deamination processes must be important elimination reactions involved in the complex AMN polymerization mechanism.