Multivariate Analysis Applied to Microwave-Driven Cyanide Polymerization: A Statistical View of a Complex System

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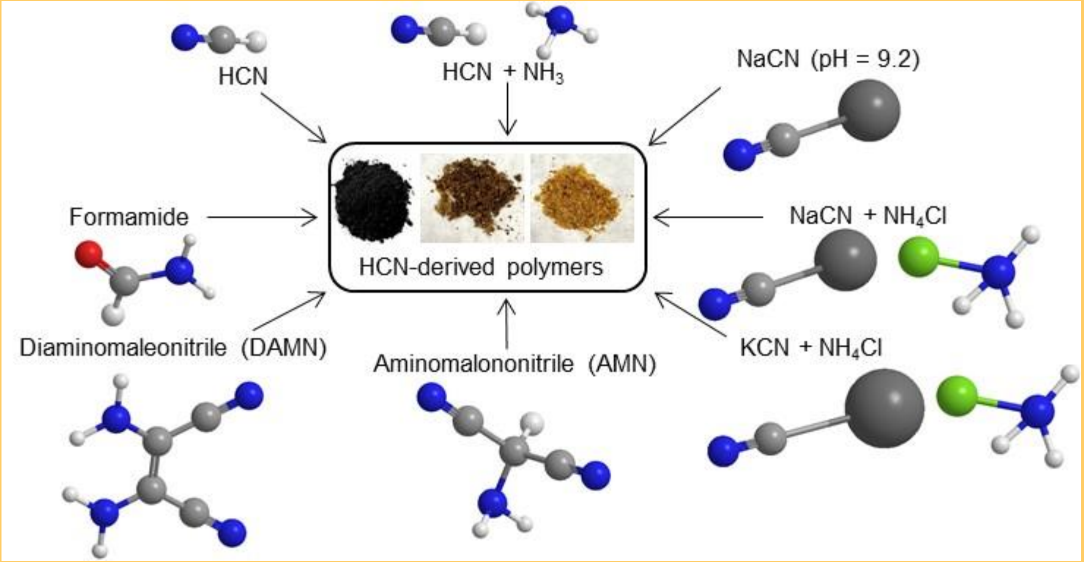
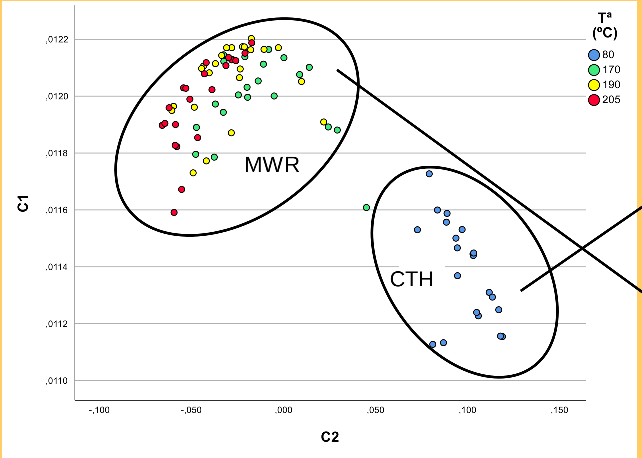
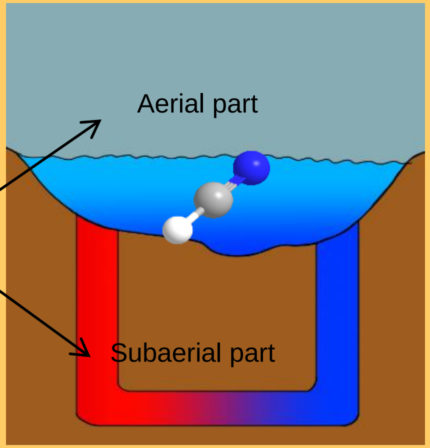




ALKALINE HYDROTHERMAL ENVIRONMENTS



For the first time, chemometrics was applied to the recently reported microwave-driven cyanide polymerization. Fast, easy, robust, low-cost, and green-solvent processes are characteristic of these types of reactions. These economic and environmental benefits, originally inspired by the constraints imposed by plausible prebiotic synthetic conditions, have taken advantage of the development of a new generation of HCN-derived multifunctional materials. HCN-derived polymers present tunable properties by temperature and reaction time. However, the apparently random behavior observed in the evolution of cyanide polymerizations, assisted by microwave radiation over time at different temperatures, leads us to study this highly complex system using multivariate analytical tools to have a proper view of the system. Two components are sufficient to explain between 84 and 98% of the total variance in the data in all principal component analyses. In addition, two components explain more than 91% of the total variance in the data in the case of principal component analysis for categorical data. These consistent statistical results indicate that microwavedriven polymerization is a more robust process than conventional thermal syntheses but also that plausible prebiotic chemistry in alkaline subaerial environments could be more complex than in the aerial part of these systems, presenting a clear example of the "messy chemistry" approach of interest in the research about the origins of life. In addition, the methodology discussed herein could be useful for the data analysis of extraterrestrial samples and for the design of soft materials, in a feedback view between prebiotic chemistry and materials science.

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