Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Venturing into the kinetics and mechanism of nanoconfined solid-state reactions: Trimerization of sodium dicyanamide in nanopores[1] BENJAMIN YANCEY, UAB, SERGEY VYAZOVKIN, University of Alabama at Birmingham — This study represents the first attempt to determine the effect of nanoconfinement on the kinetics and mechanism of solid-state reactions. FTIR, NMR, and DSC were employed to analyze the thermally initiated trimerization of sodium dicyanamide (NaC_2N_3) to sodium tricyanomelaminate ($Na_3C_6N_9$) in bulk and organically modified nanopores. The trimerization occurred at a decelerated rate as evidenced by an increase in reaction temperature as measured by DSC. Nanoconfinement did not cause apparent changes in the reaction mechanism as the products of the reaction were the same in bulk and in nanopores. Kinetic analysis linked the deceleration to a dramatic decrease (several orders of magnitude) in the pre-exponential factor. This effect is especially significant in view of previous studies on nanoconfined liquid state reactions in which the effect is opposite: considerable acceleration due to an increase in the pre-exponential factor. We propose that the difference arises respectively from disordering of the solid and ordering of the liquid reaction media.

[1]Funding provided by the NSF under grant CHE 1052828. Ultrapure silica gel was provided by Silicycle Inc (Quebec City, Canada)

Benjamin Yancey
University of Alabama at Birmingham

Date submitted: 14 Nov 2013 Electronic form version 1.4