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Final Report. IUT No. B560420 with UC Berkeley. Organic Chemistry at High Pressures &Temperatures

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Organic Chemistry at High Pressures &Temperatures

We have successfully completed the research outlined in our proposal: Organic Chemistry at High Pressures and Temperatures. We have experimentally determined a phase diagram (Figure 1) which documents the phases and reaction regimes of cyanuric acid , $H_3C_3N_3O_3$ (1,3,5-triazine-2,4,6-trione), from 300 - 750 K and 0 – 8.1 GPa. We utilized a comparatively new technique to study thin samples of cyanuric acid in the diamond anvil cell in order to collect ambient temperature, high pressure FTIR and Raman data as well as the high-pressure, high-temperature data used in the phase diagram. These experiments made use of the CMLS High-pressure lab's diamond anvil facilities as well as the FTIR and Raman systems.

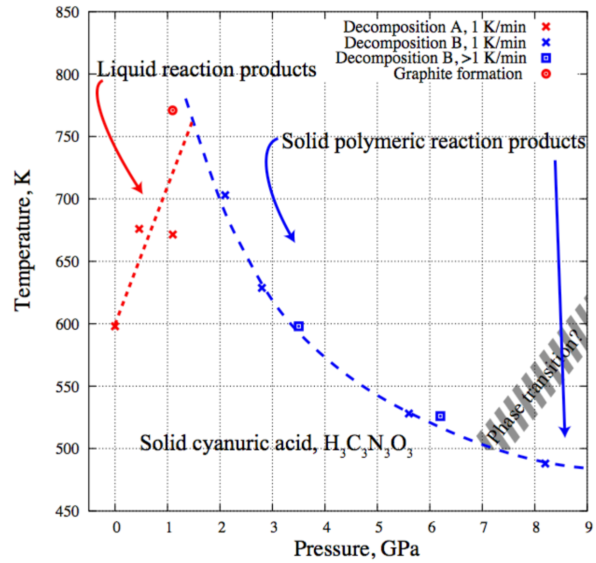

Figure 1: Experimentally determined phase and reaction diagram of cyanuric acid, dashed lines indicate reactions observed. The blue dashed line indicates at least one reaction in which solid pure cyanuric acid is converted to a solid reaction product containing substituted aromatic materials as identified by FTIR spectroscopy.

Cyanuric acid is a heterocyclic molecule of relatively high symmetry and low molecular weight compared with most other heterocycles. It contains all of the elements thought to be necessary for ``life"–H,C,N,O–and has been recovered from meteorites. [1] The effects of pressure are of interest both because primordial planetary material undergoes high pressures and because prebiotic materials formed within a young planet would be protected from destructive forces such as collision and ionizing radiation. Knowledge of the pressure and temperatures at which cyanuric acid remains stable provides a guide to both the conditions undergone by meteorites before impact and the conditions under which more complex molecules may be formed from cyanuric acid. The phase diagram of cyanuric acid therefore has important implications for both the origin and survival of life on early Earth. Our analysis of the FTIR data at non-ambient pressures and temperatures show that for certain regions in pressure-temperature space (~2-6 GPa and ~525-700 K), chemical reactions lead to the formation of purines and pyrimidines, which are biologically significant; nucleobases, fundamental to RNA and DNA, are a subset of pyrimidines and purines. The abiotic formation of such biologically significant materials under pressures associated with young planets suggests a new pathway for the formation of life.

A paper documenting the phase/reaction diagram research is in preparation now and will be submitted for publication by mid-May 2007. The ambient temperature data is under discussion with LLNL modeling experts.

The results just described will also be compared to CHEETAH thermochemical code predictions. Comparison of the experimental with the calculated melting curve, other phase boundaries and reaction products will offer a sensitive test of the code and will help to validate and improve it.

[1] R. Hayatsu, M. H. Studier, A. Oda, K. Fuse, and E. Anders. Origin of organic matter in early solar system–II. Nitrogen compounds. *Geochim. Cosmochim. Acta*, 32:175–90, 1968.