Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Structure and Dynamics of Octamethyl-POSS Nanoparticles MICHAEL CRAWFORD, KERWIN DOBBS, ROBERT SMALLEY, WILLIAM GUISE, DuPont Company, NIINA JALARVO, OLIVIER GOURDON, GEORG EHLERS, ANIBAL RAMIREZ-CUESTA, CHRISTOPH WILDGRUBER, Spallation Neutron Source, Oak Ridge National Laboratory, MADHUSUDAN TIYAGI, NIST Center for Neutron Research, SANAT KUMAR, Columbia University — Polyoligosilsesquioxanes (POSS) are a large family of Si-O cage molecules that can be viewed as 1-2 nm diameter, monodisperse silica nanoparticles. Here we report the results of a study of the crystal structure and ligand dynamics of one of the simplest POSS nanoparticles, octamethyl-POSS or $Si_8O_{12}(CH_3)_8$, where the central Si_8O_{12} cage is surrounded by eight methyl ligands. Neutron powder diffraction, inelastic neutron scattering, Raman spectroscopy, and quasielastic neutron scattering were used to characterize the structural, vibrational and dynamical properties of the polycrystalline form of this material. The structural data clearly show the presence of strongly temperature dependent methyl group torsional vibrations. The torsional vibration energy, the magnitude of the torsional energy barrier, and the activation energy for methyl rotations over the barrier were determined from the neutron measurements. These results provide a detailed picture of the structure and ligand dynamics of this POSS molecule.

Michael Crawford
DuPont Company

Date submitted: 13 Nov 2013 Electronic form version 1.4