

Abstract Submitted  
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**Characterizing the Swelling of a Crosslinked Organosilicon Polymer**<sup>1</sup> ZANE THORNBURG, None, PAUL BONVALLET, The College of Wooster — A hydrophobic crosslinked organosilicon polymer, known by the trade name Osorb, absorbs many times its own weight in liquid- and vapor-phase organic solvents. Its Si—O—Si linkage is likely flexible, analogously to physical and spectroscopic measurements in various forms of silica. Infrared spectroscopy is commonly used due to the sensitivity of certain vibrational modes to changes in geometry and environment. We hypothesized that the Si—O—Si bond angle within the Osorb matrix changes when the material swells upon exposure to organic solvents. Density functional theory calculations on a small-molecule model system qualitatively agree with the central force model of glassy solids, which relates the IR vibrational frequency of the system to the angle and force constant of this bond. Treatment of various Osorb samples with decane consistently causes a moderate increase in the frequency of the asymmetric stretching band around  $1100\text{ cm}^{-1}$ . However, the spectroscopic changes do not correlate with the swell capacity of the material. In fact, some low-swelling samples showed the same changes in frequency as high-swelling samples, thus demonstrating that the swelling of Osorb is not due to changes in the Si—O—Si bond angle.

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