

## $\alpha$ and $\gamma$ C<sub>60</sub>·2S<sub>8</sub> Under Pressure: A High Pressure Study of Two Polymorphs.

Christine M. Beavers<sup>1,2</sup>, Kamran B. Ghiassi<sup>3</sup>, Earl F. O'Bannon III<sup>2</sup>, Alan L. Balch<sup>4</sup> and Marilyn M. Olmstead<sup>4</sup>

<sup>1</sup>Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley CA 94720

<sup>2</sup>Earth & Planetary Sciences, University of California, Santa Cruz, Santa Cruz, CA 95064

<sup>3</sup>Air Force Research Laboratory, Aerospace Systems Directorate, Edwards AFB, California 93524, United States

<sup>4</sup>Department of Chemistry, University of California, Davis, Davis, CA 95616

High pressure diffraction, although known as the technique of choice among geologists and mineral physicists, is becoming more common among chemists and materials scientists. Pressure can be used to probe polymorphism, phase changes and intra and intermolecular contacts.<sup>1,2</sup> The co-crystal C<sub>60</sub>·2S<sub>8</sub> exists as two polymorphs at room temperature: the  $\alpha$  form, in monoclinic C, and the  $\gamma$  form, which adopts monoclinic P.<sup>3</sup> Both polymorphs exhibit dramatic whole molecule disorder at room temperature, and both also undergo phase transitions at low temperatures to produce ordered structures. Despite having similar structures, at both 90K and room temperature, the phase transition temperatures of the two polymorphs are quite different (~250K for  $\alpha$ , versus ~200K for  $\gamma$ ). To further explore the phase behavior, intermolecular interactions and their relative strengths, these samples have now been subjected to pressure. This presentation will explore the structural similarities and differences detected from the high pressure single crystal diffraction data, as well as discussing the synergy between the structural data and high pressure FTIR.

1. Katrusiak, A. High-pressure crystallography. *Acta Crystallographica Section A* 2008, 64, 135.
2. Hejny, C.; Minkov, V. S. High-pressure crystallography of periodic and aperiodic crystals. *IUCrJ* 2015, 2, 218.
3. Ghiassi, K. B.; Chen, S. Y.; Wescott, J.; Balch, A. L.; Olmstead, M. M. New Insights into the Structural Complexity of C<sub>60</sub>·2S<sub>8</sub>: Two Crystal Morphologies, Two Phase Changes, Four Polymorphs. *Crystal Growth & Design* 2015, 15, 404.