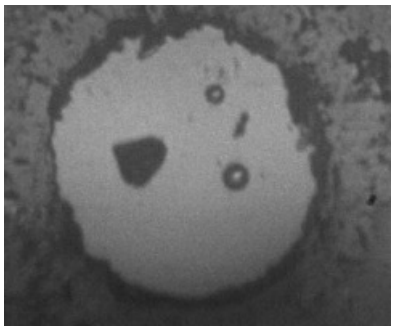
MS111.O03

A high pressure study of two polymorphs of C60·2S8

Christine M. Beavers[1], Kamran B. Ghiassi[2], Earl F. O'Bannon[3], Alan L. Balch[4], Marilyn M. Olmstead[4]
[1]*Advanced Light Source/COMPRES, Berkeley, United States,* [2]*Air Force Research Laboratory, Edwards AFB, United States,* [3]*Earth & Planetary Sciences, University of California, Santa Cruz, Santa Cruz, United States,* [4]*Department of Chemistry, University of California, Davis, Davis, United States*
E-mail: cmbeavers@lbl.gov

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.[1,2] The co-crystal C60·2S8 exists as two polymorphs at room temperature: the alpha form, in monoclinic C, and the gamma form, which adopts monoclinic P.[3] 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 α, versus ~200K for γ). 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. (2008). Acta Crystallographica Section A 64, 135-148.
[2] Hejny, C. & Minkov, V. S. (2015). IUCrJ 2, 218-229.
[3] Ghiassi, K. B., Chen, S. Y., Wescott, J., Balch, A. L. & Olmstead, M. M. (2015). Crystal Growth & Design 15, 404-410.



Keywords: high pressure, fullerenes, sulfur