Christine Beavers, Research Scientist, Beamline 12.2.2 at the Advanced Light Source.

Supervised by Quentin Williams, UC Santa Cruz

June 1st, 2013-Current (4 years, 5 months)

Responsibilities include developing/running the single-crystal diffraction experiment and facilities (70%) and providing on-site support to COMPRES users (30%). I have supported the following user groups in the last 12 months: Shim(ASU), Jackson(CIT), Mattox (LBNL), Karunadasa (Stanford), Soghomonian (VPI), Long(UCB), Ciezak-Jenkins(ARL), Alivisatos (UCB), Burtch (Sandia) and Williams (UCSC). Although some of these groups are not COMPRES, they require my expertise, either because of my chemistry background, or my assistance in collecting single crystal data on 12.2.2. I have also supported the Williams and Miyagi group, and others, when collecting data on beamline 11.3.1, which is the small molecule crystallography beamline.

Major beamline activities this year have been the development of automated DAC and diffractometer alignment scans for the Stoe Stadi-Vari diffractometer and commissioning of the diffractometer as well as the new RDI CMOS detector on the second endstation (ES2). More detail on this is given in the beamline annual report.

Cara Vennari, of the Williams group at UCSC, was awarded an ALS doctoral fellowship for her continued investigations into carbonates at high pressures. She has been using 12.2.2 independently for radial powder and axial single crystal experiments; I have provided crystallographic mentoring whenever she has required it.

I have been very active in education and outreach this year. I was again an invited speaker at the National Neutron & X-ray school, and I gave a lecture on single crystal diffraction. I was also an invited speaker at the American Crystallographic Association(ACA)’s Chemical crystallography summer school- I lectured on refinement techniques, advanced refinement topics and high pressure crystallography. I am also consulting with educators who are overhauling the Berkeley lab educational visits- the new model aims to get high school students from the community more familiar with X-ray techniques and proposing experiments. I have submitted an EOID proposal for a chemical crystallography workshop to be held at the ALS next fall. I attended two crystallographic conferences during the reporting period- the ACA meeting, and the International Union of Crystallography’s triennial congress. At both of these meetings, I advertised the capabilities of 12.2.2, shared my own work, as well as networked with others in the high-pressure diffraction community. I was also invited to the ACA to give a talk about science communication using social media. I have reviewed for a number of journals this year(JACS, Inorganic Chem, Science Advances), as well as my normal reviewing for the APS HP beamlines.

2017 & 2016 Accepted Publications:

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| 1 | 2017 | Thomas, K. E.; Beavers, C. M.; Gagnon, K. J.; Ghosh, A., beta-Octabromo- and beta-Octakis(trifluoromethyl)isocorroles: New Sterically Constrained Macrocyclic Ligands. *Chemistryopen* **2017,** *6* (3), 402-409. |
| 2 |  | O'Bannon, E.; Beavers, C. M.; Kunz, M.; Williams, Q., The high-pressure phase of lawsonite: A single crystal study of a key mantle hydrous phase. *Journal of Geophysical Research-Solid Earth* **2017,** *122* (8), 6294-6305. |
| 3 |  | Mattox, T. M.; Groome, C.; Doran, A.; Beavers, C. M.; Urban, J. J., Anion-mediated negative thermal expansion in lanthanum hexaboride. *Solid State Communications* **2017,** *265*, 47-51. |
| 4 |  | Doran, A.; Schlicker, L.; Beavers, C. M.; Bhat, S.; Bekheet, M. F.; Gurlo, A., Compact low power infrared tube furnace for in situ X-ray powder diffraction. *Review of Scientific Instruments* **2017,** *88* (1). |
| 5 |  | Bryant, M. J.; Skelton, J. M.; Hatcher, L. E.; Stubbs, C.; Madrid, E.; Pallipurath, A. R.; Thomas, L. H.; Woodall, C. H.; Christensen, J.; Fuertes, S.; Robinson, T. P.; Beavers, C. M.; Teat, S. J.; Warren, M. R.; Pradaux-Caggiano, F.; Walsh, A.; Marken, F.; Carbery, D. R.; Parker, S. C.; McKeown, N. B.; Malpass-Evans, R.; Carta, M.; Raithby, P. R., A rapidly-reversible absorptive and emissive vapochromic Pt(II) pincer-based chemical sensor. *Nature Communications* **2017,** *8* (1), 1800. |
| 1 | 2016 | Kou, F.; Yang, S.; Qian, H.; Zhang, L.; Beavers, C. M.; Teat, S. J.; Tian, G., A fluorescence study on the complexation of Sm(III), Eu(III) and Tb(III) with tetraalkyldiglycolamides (TRDGA) in aqueous solution, in solid state, and in solvent extraction. *Dalton Transactions* **2016,** *45* (46), 18484-18493. |
| 2 |  | Woodall, C. H.; Christensen, J.; Skelton, J. M.; Hatcher, L. E.; Parlett, A.; Raithby, P. R.; Walsh, A.; Parker, S. C.; Beavers, C. M.; Teat, S. J.; Intissar, M.; Reber, C.; Allan, D. R. Observation of a re-entrant phase transition in the molecular complex tris(μ2-3,5-diisopropyl-1,2,4-triazolato-κ2 N1:N2)trigold(I) under high pressure. *IUCrJ* **2016**, *3*, 367. |
| 3 |  | Norheim, H. K.; Capar, J.; Einrem, R. F.; Gagnon, K. J.; Beavers, C. M.; Vazquez-Lima, H.; Ghosh, A. Ligand noninnocence in FeNO corroles: insights from beta-octabromocorrole complexes. *Dalton Transactions* **2016**, *45*, 681. |
| 4 |  | Jaffe, A.; Lin, Y.; Beavers, C. M.; Voss, J.; Mao, W. L.; Karunadasa, H. I. High-Pressure Single-Crystal Structures of 3D Lead-Halide Hybrid Perovskites and Pressure Effects on their Electronic and Optical Properties. *ACS Central Science* **2016**, *2*, 201. |
| 5 |  | Alexandropoulos, D. I.; Moushi, E. E.; Papatriantafyllopoulou, C.; Beavers, C. M.; Teat, S. J.; Tasiopoulos, A. J.; Christou, G.; Stamatatos, T. C. Cyanate groups in higher oxidation state metal cluster chemistry: Mixed-valence (II/III) Mn-16 and Mn-18 clusters. *Polyhedron* **2016**, *108*, 131. |
| 6 |  | Aromi, G.; Beavers, C. M.; Sanchez Costa, J.; Craig, G. A.; Minguez Espallargas, G.; Orerad, A.; Roubeau, O. Snapshots of a solid-state transformation: coexistence of three phases trapped in one crystal. *Chemical Science* **2016**, *7*, 2907. |
| 7 |  | Su, N. C.; Sun, D. T.; Beavers, C. M.; Britt, D. K.; Queen, W. L.; Urban, J. J. Enhanced permeation arising from dual transport pathways in hybrid polymer-MOF membranes. *Energy & Environmental Science* **2016**, *9*, 922. |
| 8 |  | Xian, L.; Tian, G.; Beavers, C. M.; Teat, S. J.; Shuh, D. K. Glutarimidedioxime: A Complexing and Reducing Reagent for Plutonium Recovery from Spent Nuclear Fuel Reprocessing. *Angewandte Chemie-International Edition* **2016**, *55*, 4671. |

Submitted Publications:

McCormick, L.J.; Giordano, N.; Teat, S.J.; Beavers, C.M.; “Chemical Crystallography at the Advanced Light Source,” *Crystals* (accepted after minor revisions)

Stan, C.V.; Beavers C.M.; Kunz, M.; Tamura,N. “X-ray diffraction under extreme conditions at the Advanced Light Source,” *Quantum Beam Science*