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

Supervised by Quentin Williams, UC Santa Cruz

June 1st, 2013-Current (2 years, 5 months)

Responsibilities include developing/running the single-crystal diffraction experiment and facilities (80%) and providing on-site support to COMPRES users (20%). I have supported the groups of Williams(UCSC), Ross(VTech), Jackson(CIT), Karunadasa(Stanford), Olmstead(UC Davis), Clearfield(TAMU), Tolbert(UCLA) & Ciezak-Jenkins(Army). Although some of these groups are not COMPRES, they require my expertise in some facet of collecting single crystal data on 12.2.2.

Within my single-crystal work, I divide time between analyzing data and developing the resources to teach users to analyze data efficiently, as well as exploring options to further improve the single crystal experiment at beamline 12.2.2. This exploration has lead to the recent purchase, by the ALS, of a single-crystal diffractometer and detector system, worth ~$250k, that will be installed in Spring 2016. This acquisition has added project work planning to my day-to-day responsibilities.

I am involved with numerous projects concerned with single crystal HP, with groups around the country. The Williams group at UCSC is closely working with myself and other beamline staff to implement HPHT single crystal, and this development is ideally suited to match our upcoming installation. The Karunadasa group at Stanford is heavily engaged in HPSXD of materials relevant to energy. This project is expected to accelerate with the new equipment, but there are already a number of papers, in press and preparation.

The current single crystal system on 12.2.2 has been continuously improved over the last two years, thanks to user feedback. We are nearing the limitation of our current equipment, however, so optimization of this system will slow, as we invest more time on integration of the new system. Goals of the new system are identical to the current goals: data will be portable and contain necessary experimental information, to enable users to correctly process data in a timely fashion.

As far as outreach, I was invited to the National School on Neutron & X-ray scattering as a lecturer on single crystal diffraction. My lecture was well received, and numerous students were intrigued by the concept of HP diffraction. I also attended the national meeting of the American Crystallographic Association, and publicized 12.2.2 at the ALS sponsored booth. I met many scientists interested in high pressure single crystal, and some of these contacts produced proposals in the most recent call.

**Publications (2014-2015)**

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| 77 | 2015 | Capar, J.; Conradie, J.; Beavers, C. M.; Ghosh, A. Molecular Structures of Free-Base Corroles: Nonplanarity, Chirality, and Enantiomerization. *JPCA* **2015**, *119*, 3452. |
| 76 |  | Palacios, M. A.; McLellan, R.; Beavers, C. M.; Teat, S. J.; Weihe, H.; Piligkos, S.; Dalgarno, S. J.; Brechin, E. K. Facile Interchange of 3d and 4f Ions in Single-Molecule Magnets: Stepwise Assembly of Mn-4 , Mn(3)Ln and Mn(2)Ln(2) Cages within Calix 4 arene Scaffolds. *Chemistry-a European Journal* **2015**, *21*, 11212. |
| 75 |  | Capar, J.; Berg, S.; Thomas, K. E.; Beavers, C. M.; Gagnon, K. J.; Ghosh, A. Improved syntheses of -octabromo-meso-triarylcorrole derivatives. *Journal of inorganic biochemistry* **2015**. |
| 74 |  | Thomas, K. E.; Vazquez‐Lima, H.; Fang, Y.; Song, Y.; Gagnon, K. J.; Beavers, C. M.; Kadish, K. M.; Ghosh, A. Ligand Noninnocence in Coinage Metal Corroles: A Silver Knife‐Edge. *Chemistry–A European Journal* **2015**. |
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| 73 |  | Tian, G.; Shuh, D. K.; Beavers, C. M.; Teat, S. J. A structural and spectrophotometric study on the complexation of Am (iii) with TMOGA in comparison with the extracted complex of DMDOOGA. *Dalton Transactions* **2015**, *44*, 18469. |
| 72 |  | McLellan, R.; Palacios, M. A.; Beavers, C. M.; Teat, S. J.; Piligkos, S.; Brechin, E. K.; Dalgarno, S. J. Linked Supramolecular Building Blocks for Enhanced Cluster Formation. *Chemistry-a European Journal* **2015**, *21*, 2804. |
| 71 | 2014 | Fowler, D. A.; Pfeiffer, C. R.; Teat, S. J.; Beavers, C. M.; Baker, G. A.; Atwood, J. L. Illuminating host-guest cocrystallization between pyrogallol[4]arenes and the ionic liquid 1-ethyl-3-methylimidazolium ethylsulfate. *Crystengcomm* **2014**, *16*, 6010. |
| 70 |  | Woodall, C. H.; Fuertes, S.; Beavers, C. M.; Hatcher, L. E.; Parlett, A.; Shepherd, H. J.; Christensen, J.; Teat, S. J.; Intissar, M.; Rodrigue-Witchel, A.; Suffren, Y.; Reber, C.; Hendon, C. H.; Tiana, D.; Walsh, A.; Raithby, P. R. Tunable Trimers: Using Temperature and Pressure to Control Luminescent Emission in Gold(I) Pyrazolate-Based Trimers. *Chemistry-a European Journal* **2014**, *20*, 16933. |
| 69 |  | Kennedy, S.; Beavers, C. M.; Teat, S. J.; Dalgarno, S. J. Salt formation affects the conformational and assembly properties of p-carboxylatocalix 4 arenes. *Crystengcomm* **2014**, *16*, 3712. |
| 68 |  | Alemayehu, A. B.; Vazquez-Lima, H.; Beavers, C. M.; Gagnon, K. J.; Bendix, J.; Ghosh, A. Platinum corroles. *Chemical Communications* **2014**, *50*, 11093. |
| 67 |  | Hatcher, L. E.; Bigos, E. J.; Bryant, M. J.; MacCready, E. M.; Robinson, T. P.; Saunders, L. K.; Thomas, L. H.; Beavers, C. M.; Teat, S. J.; Christensen, J.; Raithby, P. R. Thermal and photochemical control of nitro-nitrito linkage isomerism in single-crystals of Ni(medpt)(NO2)(eta(2)-ONO). *Crystengcomm* **2014**, *16*, 8263. |
| 66 |  | Albrett, A. M.; Thomas, K. E.; Maslek, S.; Mlodzianowska, A.; Conradie, J.; Beavers, C. M.; Ghosh, A.; Brothers, P. J. Mono- and Diboron Corroles: Factors Controlling Stoichiometry and Hydrolytic Reactivity. *Inorganic Chemistry* **2014**, *53*, 5486. |
| 65 |  | Alberto Rodriguez-Velamazan, J.; Fabelo, O.; Beavers, C. M.; Natividad, E.; Evangelisti, M.; Roubeau, O. A Multifunctional Magnetic Material under Pressure. *Chemistry-a European Journal* **2014**, *20*, 7956. |
| 64 |  | O'Bannon, E., III; Beavers, C. M.; Williams, Q. Trona at extreme conditions: A pollutant-sequestering material at high pressures and low temperatures. *AmMin* **2014**, *99*, 1973. |
| 63 |  | Sanchez Costa, J.; Rodriguez-Jimenez, S.; Craig, G. A.; Barth, B.; Beavers, C. M.; Teat, S. J.; Aromi, G. Three-Way Crystal-to-Crystal Reversible Transformation and Controlled Spin Switching by a Nonporous Molecular Material. *Journal of the American Chemical Society* **2014**, *136*, 3869. |
| 62 |  | Zuo, T.; Dorn, H. C.; Beavers, C. M.; Olmstead, M. M.; Balch, A. L. Isolation and Crystallographic Characterization of Tm3N@D-2(35)-C-88. *Fullerenes Nanotubes and Carbon Nanostructures* **2014**, *22*, 280. |