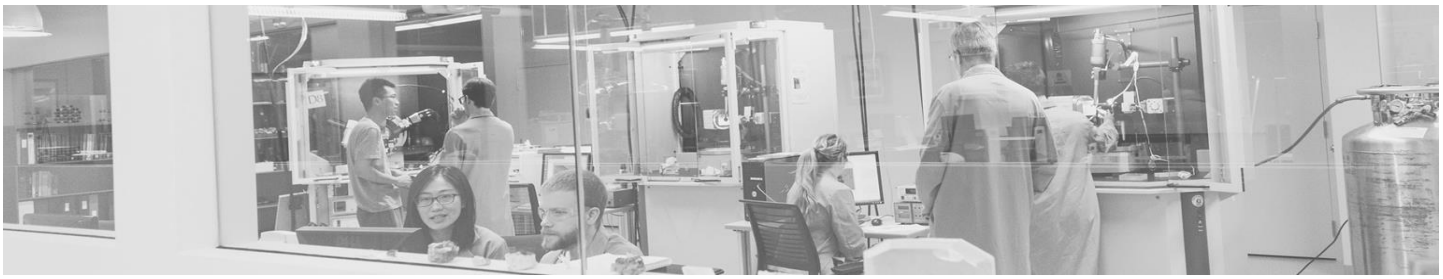
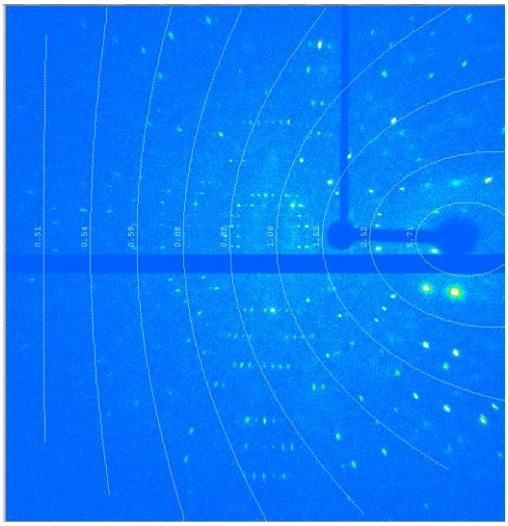
X-ray Crystallography Center

May 2017 Newsletter



Our new diffractometer has arrived!

Thanks to a grant from the National Science Foundation (CHE-1626172) and matching funds from the Emory College of Arts and Sciences, we have acquired and installed an ultra-high intensity X-ray diffractometer, the Rigaku XtaLAB Synergy system. This includes dual (copper and molybdenum) PhotonJet sources equipped with multilayer optics, and the recently introduced Rigaku HyPix-6000HE Hybrid Photon Counting (HPC) detector. The new technology of the microfocus source affords very strong, highly focused beam intensity with very low energy costs. The detector has zero-readout noise and a very high dynamic range so that reflections with very high and very low count rates can be measured simultaneously. The readout time is very low and we routinely measure data with 0.1 s exposures. The data collection, reduction, and structure determination is often complete in under 1 minute! This new instrumentation has already begun to significantly advance the research activities in the Department of Chemistry. The advanced hardware, including a high-brilliance source and a HPC detector with its small pixel size and zero background noise will assist in collecting data from very small crystals, poorly crystalline materials, biological materials and even protein crystals.



Emory X-ray Crystallography Center, Rm 163, Sanford Atwood Chemistry Center, 1515 Dickey Drive, Atlanta, GA 30322
T: +1 404-727-6140 E: john.bacsa@emory.edu http://xray.chemistry.emory.edu

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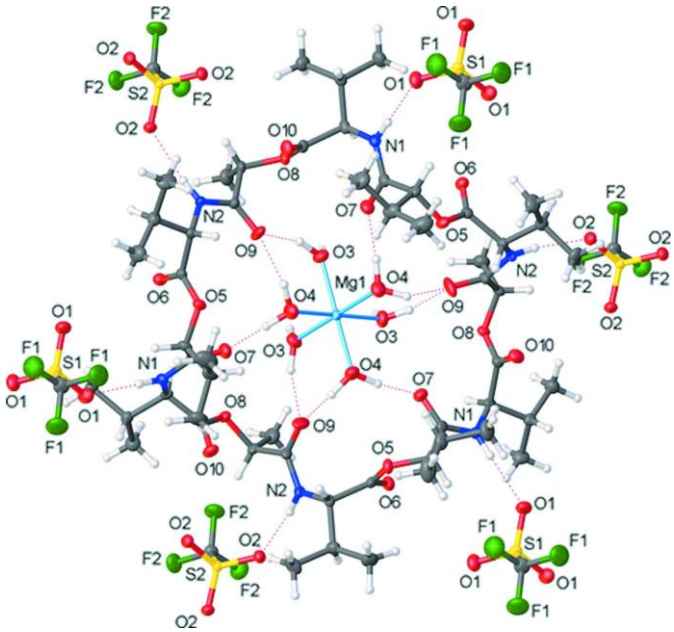
Science highlight: A new metal ion binding mode of valinomycin that incorporates a fully hydrated metal ion.

Valinomycin is an antibiotic produced by *Streptomyces fulvissimus* that transports K^+ ions through phospholipid bilayer membranes with a high selectivity over Na^+ ions. In these complexes, valinomycin adopts a bracelet conformation in which all six amide carbonyl groups accept intramolecular hydrogen bonds from neighboring amide N—H groups. The crystal structure of the $\{valinomycin[Mg(H_2O)_6]\}^{2+}$ complex revealed a new cation-binding mode of valinomycin which is considerably different from previously known valinomycin–cation complexes. The intramolecular amide hydrogen bonding in valinomycin is broken, and yet the complex retains a perfect threefold symmetry, accommodating one $[Mg(H_2O)_6]^{2+}$ ion through hydrogen bonding from the amide carbonyl groups to the Mg^{2+}-bound water molecules. This study showcases the versatile cation-binding ability of this natural product macrocycle, including a fully hydrated cation through hydrogen-bonding, not by direct coordination.



This work highlights our collaboration with Dr. Megumi Fujita. Dr. Fujita studies synthetic and natural ion receptors at the University of West Georgia, a predominantly undergraduate institution. Due to the comprehensive structural refinements and the novel binding mode, this structure was highlighted on the cover of the August 2016 issue of Acta Crystallographica Section C (Fujita, M., Kazerouni, A. M. & Bacsa, J. (2016). Acta Cryst. C72, 627-633; link).

Contact Dr. John Bacsa to discuss how the Emory X-ray Crystallography Center can support your research!

- We routinely determine the absolute configuration of light-atom chiral non-racemic compounds.
- Our powder X-ray analyses only require small amounts (µg quantities) of material and the applications include phase identification, unit cell refinements, and particle size analysis.
- Single crystal X-ray analyses include a publishable quality CIF and a complete structural report. We provide a detailed analysis of the results. You will receive a complete report of your structure as well as any relevant information that is needed for publication.

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