



FIRST Newsletter

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D8 QUEST ECO – Undergraduate Research and Teaching at Radford University

Michael Ruf, Sr. Manager SC-XRD, Bruker AXS LLC, and Vernon Smith, SC-XRD Business Development Manager, Bruker AXS GmbH

Training sessions are extraordinary moments spent with our customers and visiting with the Radford University, Virginia was no exception. Dr. Michael Ruf, Bruker Senior Manager of Single-Crystal X-Ray Diffraction (SC-XRD), visited the Chemistry Department, and together with Dr. George Harakas, Associate Professor, demonstrated that it doesn't take a huge investment to succeed in ambitious research goals and to contribute to better teaching and learning – opening new horizons for students and experienced crystallographers alike.

Dr. George Harakas, Associate Professor at Radford University, has been teaching Inorganic Chemistry since 2015. He is working on synthetic organo-metallic chemistry and his primary interest is in the synthesis of unique transition metal clusters and transition metal-main group compounds. Transition metal clusters can be used as precursors for applications such as heterogeneous catalysis, desulfurization of fossil fuels, and magnetic materials. Bruker provided X-ray crystallography training to Professor Harakas and our [D8 QUEST ECO](#) diffractometer keeps impressing with its research-quality data and low cost of ownership.

“The D8 QUEST ECO has made it possible for us to have a research quality instrument without the high cost of the infrastructure needed for most diffractometers,” commented Dr. George Harakas.

The balanced design and functionality of the software, between accessibility for novices and very advanced features for more experienced users, makes it perfect for the academic environment, without compromising usage by advanced researchers.

The new [STRUCTURE NOW](#) plug-in for automated structure determination applies the latest artificial intelligence technology to automate structure determination. *“I really like the new STRUCTURE NOW capability,”* continued Professor Harakas. *“Having data collection and structure solution running simultaneously is very impressive.”*

Contributing to a more advanced and comprehensive course curriculum

Delivering training at the Chemistry Department of Radford University accomplished much more than simply teaching how to use Bruker diffractometers. Being able to demonstrate all the potential of the D8 QUEST ECO opened new horizons and contributed to a more solid and competitive curriculum for the Advanced Inorganic Chemistry course.

Professor Harakas is now planning to incorporate both single-crystal and powder X-ray diffraction into his Advanced Inorganic Chemistry classes.

“The training was great! Bruker helped me sort out the structure of a compound on an ongoing research project. Furthermore, the instruction on collecting powder X-ray data was very productive.”

Professor George Harakas

Unexpected achievements powered by advanced and specialized instruments

The first article published using the Bruker D8 QUEST ECO diffractometer with [PHOTON II](#) detector at the Department of Chemistry of Radford University was on the reaction of $\text{Na}_2\text{Fe}(\text{CO})_4$ with an excess of MnCl_2 in tetrahydrofuran (THF) producing $[\text{Fe}_2\text{Mn}(\text{C}_4\text{H}_8\text{O})_2\text{Na}_2(\text{C}_4\text{H}_8\text{O})_5(\text{CO})_8]_n$ or $\text{C}_{36}\text{H}_{56}\text{Fe}_2\text{MnNa}_2\text{O}_{15}$.

The compound is a xenophilic dianion with short iron-manganese bond lengths. The sodium cations of the dianion are coordinated to THF ligands and have isocarbonyl interactions, forming a polymeric (two-dimensional) structure in the crystal. One of the THF molecules was modeled with the carbon atoms being statistically disordered.

The results were published in August 2021 and can be found on IUCrData [here](#).

“The instrument is fantastic! [...] Last year I published my first structure using the ECO.”

Professor George Harakas

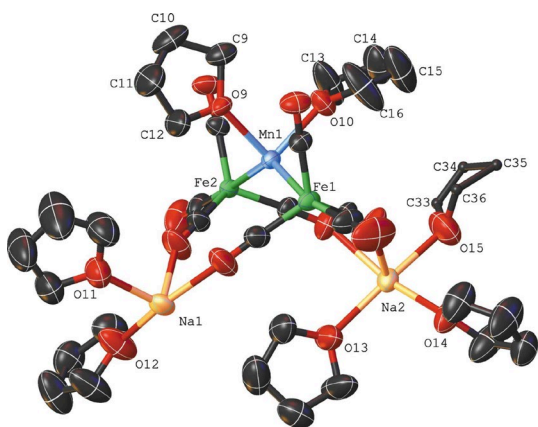


Figure 1. The asymmetric unit of the title compound, with displacement ellipsoids drawn at the 50% probability level. One tetrahydrofuran molecule coordinating Na_2 is statistically disordered.

Source: referred article

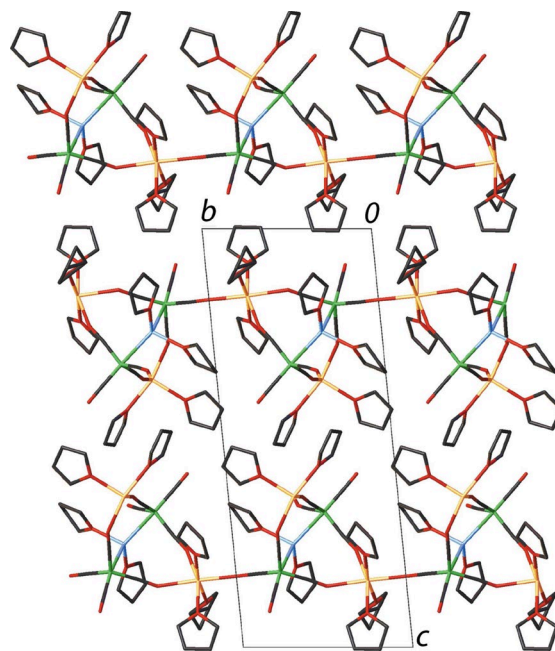


Figure 2. Packing diagram of the title compound, viewed along the a axis, highlighting the stacking of layers. Source: referred article

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The article Poly[octacarbonylheptakis(tetrahydrofuran)diiron manganese disodium(2 Mn—Fe)] [Harakas & Whittlesey (2021). IUCrData, 6, x210845, <https://doi.org/10.1107/S2414314621008452>] is published under an open-access license, so you are free to reuse it without restriction provided there is attribution for the article.

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