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## **Magnetic Structure Determination from Neutron Diffraction Data, July 22-25, 2024**

**KSU Event Center (Kennesaw State University 3333 Busbee Drive MD#3301 Kennesaw GA 30144)**

**Monday July 22, 2024 [KSU Event Center, Room #300]**

<b>Time</b>	<b>Event</b>	<b>Presenter</b>
8:30 – 9:00am	Registration/Breakfast	
9:00 – 9:30am	Welcome and workshop overview	TBD (KSU)
9:30-10:30am	Overview of ORNL neutron facilities and instruments	Clarina dela Cruz
10:30 – 10:45am	Break	
10:45 -11:15	Proposal writing for neutron beamtime at ORNL	Clarina dela Cruz
11:15 – 12:30	Neutron scattering as a tool for magnetic structure determination (Magnetic structure factors, form factors, k-vector & experimental techniques)	William Ratcliffe
12:30– 1:30 pm	Working LUNCH: Overview of software tools for magnetic diffraction	Ovi Garlea
1:30 – 2:30 pm	Magnetic symmetry-based modeling of magnetic structures	J. Manuel Perez-Mato
2:30 – 3:45pm	Representation theory in magnetic Structure Analysis/ Representation theory vs Magnetic Space group approach.	Branton Campbell
3:45 – 4:00pm	Break	
4:00 – 5:15 pm	Hands on demonstration of Bilbao Crystallographic server: MAXMAGN, MVISUALIZE, k-SUBGROUPSMAG, MAGNDATA database etc	J. Manuel Perez-Mato
5:15 – 6:15 pm	Introduction to Fullprof / Example of Fullprof refinement of commensurate structures from CW powder diffraction data -part 1 (refining crystal structure)	Stuart Calder



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## Tuesday July 23, 2024 [KSU Event Center, Room #242]

Time	Event	Presenter
8:30 – 9:00 am	Breakfast snack /Questions from previous day	Everyone
9:00 – 10:00 am	Hands-on example of Fullprof refinement of commensurate structures from CW powder diffraction data [Fullprof/Bilbao Magnetic Space Groups] -part 2	Stuart Calder
10:00 – 10:15 am	Break	
10:15 -11:30 pm	Hands-on example: Fullprof refinement of commensurate structure from TOF data (Fullprof/ magnetic space group approach (BCS))	Qiang Zhang
11:30 – 12:00 pm	Multi-k magnetic structures from powder data -part1	Ovi Garlea
12:00 – 1:00 pm	Working LUNCH (Lightning science talks)	
1:00 – 1:45 pm	Multi-k magnetic structures from powder data - part 2	Ovi Garlea
1:45 – 3:00 pm	Hands-on example: Fullprof refinement of single crystal data (commensurate structure with magnetic space group approach)	Huibo Cao
3:00 – 3:30 pm	Multi- magnetic domains and multi-k magnetic structure in fitting single-crystal data	Huibo Cao
3:30–3:45 pm	Break	
3:45 – 5:15 pm	Introduction to ISOTROPY and hands-on examples	Branton Campbell
5:15–5:45pm	Demonstration: AMPLIMODES refinement with Fullprof [Fullprof & isotropy]	Ovi Garlea



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Time	Event	Presenter
5.45 – 6.00pm	Student questions from the day	EVERYONE

## Wednesday July 24, 2024 [KSU Event Center, Room #242]

Time	Event	Presenter
8:30 – 9:00 am	Breakfast snack / Questions from previous day	Everyone
9:00 – 10:30 am	Hands-on example: Example of Fullprof refinement of commensurate structures from CW powder diffraction data [Fullprof & SARAh]	Stuart Calder
10:30 -10:45 am	BREAK	
10:45 am -12:00	Symmetry of incommensurate magnetic structures: magnetic superspace groups/ Isotropy examples	Branton Campbell
12:00 -1:00pm	LUNCH (Sample environment available on diffraction instruments)	Stuart Calder
1:00 – 2:30	Fullprof incommensurate structure from powder data (superspace group)	Ovi Garlea
2:30 – 4:00 pm	Hands-on example: Fullprof refinement for incommensurate magnetic structures from CW powder data (basis vectors/irreps)	Ovi Garlea or Stuart Calder
4:00 – 4:15 pm	Break	
4:15 – 5:45 pm	Fullprof refinement of single crystal data (incommensurate structure with irrep approach)	Huibo Cao
5.45 – 6.00pm	Student questions from the day	EVERYONE



## Thursday July 25, 2024 [KSU Event Center, Room #242]

Time	Event	Presenter
8:30 – 9 am	Breakfast snack / Questions from previous day	Everyone
9:00 – 9:45 am	Fullprof: Future developments. Questions and discussions	Juan Rodríguez-Carvajal
9:45 – 10:45 am	How to report magnetic structures in publications and submit mcif files to MAGNDATA (tutorial)	J. Manuel Perez-Mato
10:45 – 11:00 am	Break	
11:00 – 12:00 am	Prepare a mcif files from a publication on your own (groups working independently on examples of published structures) – part1	J. Manuel Perez-Mato /Everyone
12:00 – 12:45 pm	Working Lunch (mCIF and MAGNDATA discussion)	
12:45 – 1:15 pm	Prepare a mcif file from a publication on your own (groups working independently on examples of published structures)- part2	J. Manuel Perez-Mato /Everyone
1:15 – 2:00 pm	Introduction to GSAS-II/ Magnetic structure in GSAS-II	Yuanpeng Zhang
2:00 – 3:30pm	Example of GSAS-II refinement of magnetic structure from CW powder data	Keith Taddei
3:30 - 3:45 pm	Break	
3:45 – 5:15pm	Example of GSAS-II refinement of magnetic structure from TOF data	Qiang Zhang
5:15–5:30pm	CLOSEOUT: Questions and discussion	EVERYONE