

UWI-LAAAMP
Caribbean Crystallography School
Inaugural Edition

UWI Mona Campus, Jamaica, 2-7 June 2025

Lecturers

Andrea Araya-Sibaja (AA)	Yinka Olatunji-Ojo (YO)	Michele Zema (MZ)
Javier Alcides Ellena (JE)	Ashley Schmidt (AS)	Jermaine Smith (JS)
Graciela Diaz de Delgado (GDD)	Marvadeen Singh-Wilmot (MSW)	Zeyar Min (ZM)
Ilaria Gimondi (IG)	Leopoldo Suescun (LS)	
Lucia Maini (LM)	Serena C. Tarantino (SCT)	

GROUPS (ca 7 students/group): **BLUE**; **GREEN**; **PURPLE**; **BROWN**.

PROGRAMME

Sunday, June 1, 2025

Arrival of participants and evening networking event at The Jamaica Pegasus Hotel

Monday, June 2, 2025

Morning

08:30-09:30 Registration of participants

09:30-10:30 MSW (Master of Ceremony) Welcome speeches from authorities and main partners

- 09:30-09:45 **MSW** Welcome and introduction
- 09:45-09:50 **UWI Dean**
- 09:50-09:55 **UWI HoD Chemistry**
- 09:55-10:00 **UNESCO Office for the Caribbean**
- 10:00-10:05 **IAEA** pre-recorded video
- 10:05-10:10 **AA LACA**
- 10:10-10:15 **LM** UniBO Global South
- 10:15-10:20 **GDD** ISC RFP-LAC and IUCr
- 10:20-10:30 **MZ LAAAMP**

10:30-11:00 Coffee break

11:00-11:30 MSW, MZ, LS Crystallizing the CCS network

11:30-13:00 MZ *History of crystallography and introduction to crystal symmetry* (1.5h)

13:00-14:00 Lunch

Afternoon

Chair: JE

14:00-15:00 MSW *Principles of crystallization and crystal growth* (1h)

15:00-16:00 AS *The D8 Quest Eco diffractometer and crystal mounting techniques* (1h)

16:00-16:20 Coffee break

16:20-16:30 Groups formation: **BLUE**; **GREEN**; **PURPLE**; **BROWN**.

16:30-18:30 Laboratory activity (2h)

In the lecture room (LS, LM; MZ, SCT, GDD):

16:30-17:30 **BLUE** and **GREEN**: *Symmetry in crystals with exercises [symmetry operations; lattices]*

17:30-18:30 **PURPLE** and **BROWN**: *Symmetry in crystals with exercises [symmetry operations; lattices]*

In the chemistry lab (MSW, AA; JS, ZM):

16:30-17:30 **PURPLE**: *Crystal growing techniques*

17:30-18:30 **BLUE**: *Crystal growing techniques*

In the XRD lab (AS, JE; MZ, JS, ZM):

16:30-17:30 **BROWN**: *Crystal selection and mounting, XRD data collection*

17:30-18:30 **GREEN**: *Crystal selection and mounting, XRD data collection*

Tuesday, June 3, 2025

Morning

Chair: AA

08:30-09:30 **LM** *Point and space groups in crystals* (1h)

09:30-10:30 **LS** *The International Tables for Crystallography Vol. A* (1h)

10:30-11:00 Coffee break

11:00-13:00 **Laboratory activity** (2h)

In the lecture room (LS, LM; MZ, SCT, GDD):

11:00-12:00 **PURPLE** and **BROWN**: *Determination of plane and space groups with exercises*

12:00-13:00 **BLUE** and **GREEN**: *Determination of plane and space groups with exercises*

In the chemistry lab (MSW, AA; JS, ZM):

11:00-12:00 **GREEN**: *Crystal growing techniques*

12:00-13:00 **BROWN**: *Crystal growing techniques*

In the XRD lab (AS, JE; MZ, JS, ZM):

11:00-12:00 **BLUE**: *Crystal selection and mounting, XRD data collection*

12:00-13:00 **PURPLE**: *Crystal selection and mounting, XRD data collection*

13:00-14:00 Lunch

Afternoon

Chair: SCT

14:00-15:00 **AS** *Cell determination and data collection strategies using Apex6* (1h)

15:00-16:00 **JE** *X-ray diffraction, Bragg's law, Reciprocal space* (1h)

16:00-16:30 Coffee break

16:30-18:30 **Practical activity** (2h)

In the computer room (AS; MZ, JE, LS, AA, LM, SCT, GDD, JS, ZM):

16:30-18:30 **ALL GROUPS**: *Tutorial on Apex6*

Wednesday, June 4, 2025

Morning

Chair: GDD

08:30-10:30 **Practical activity** (2h)

In the computer room (IG and YO):

08:30-10:30 *Tutorial #1 on the use of the Cambridge Structural Database*

10:30-11:00 Coffee break
11:00-12:00 **SCT** Structure factors (1h)
12:00-13:00 **JE** Structure solution methods (1h)

13:00-14:00 Lunch

Afternoon

Chair: MZ

14:00-15:00 **AS** Data integration, scaling and space group determination using Apex6 (1h)
15:00-16:00 **LM** Structure refinement step by step – live demo with real data (1h)
16:00-16:30 Coffee break
16:30-18:30 **Laboratory activity** (2h)

In the computer room (LM; JE, MZ, LS, GDD):

16:30-18:30 **ALL GROUPS:** Structure refinement with SHELXL

In the XRD and chemistry labs (AS, MSW, AA; JE, SCT, JS, ZM):

16:30-18:30 Activity continues as needed

Thursday, June 5, 2025

Morning

Chair: LM

08:30-10:30 **Practical activity** (2h)

In the computer room (IG and YO):

08:30-10:30 Tutorial #2 on the use of the Cambridge Structural Database

10:30-11:00 Coffee break

11:00-12:00 **JE, IG** Structural computing and analysis using Mogul and Crystal Explorer - live demo with real data (1h)

12:00-13:00 **LS** Use of ITA for structural analysis: a case study

In the XRD and chemistry labs (AS, MSW, AA; LM, MZ, SCT, JS, ZM):

11:00-13:00 Activity continues as needed

13:00-14:00 Lunch

Afternoon

Excursion

Friday, June 6, 2025

Morning

Chair: IG

08:30-09:30 **AA** Polymorphism in organic crystals (1h)

09:30-10:30 **SCT** Polymorphism and phase transitions in inorganic crystals (1h)

10:30-11:00 Coffee break

11:00-13:00 **Laboratory activity** (2h)

In the computer room (LM; JE, MZ, LS, GDD):

11:00-13:00 Structure refinement with SHELXL: new data

In the XRD and chemistry labs (AS, MSW, AA; JE, SCT, JS, ZM):

11:00-13:00 *Activity continues as needed*

13:00-14:00 Lunch

Afternoon

Chair: MSW

14:00-15:20 **Students' presentations** Each group nominates their delegates to present the results of their work (20 min/group)

15:20-16:00 **All lecturers and students** Q&A session on the works presented by groups

16:00-16:30 Coffee break

Chair: LS

16:30-18:30 *Special topics: A crystallography symposium in 2 hours*

16:30-16:45 **MSW** MOFs

16:45-17:00 **LM** Organic molecular materials

17:00-17:15 **GDD** Polymorphism in pharmaceuticals

17:15-17:30 **AA** Bioactive compounds: from crystal engineering to drug delivery

17:30-17:45 **JE** Quantum crystallography

17:45-18:00 **MZ** Single-crystal X-ray diffraction at variable T and P

18:00-18:15 **SCT** Spinel

18:15-18:30 **LS** Perovskites

Saturday, June 7, 2025

Morning

Chair: MZ

08:30-09:30 **GDD** Structure validation, preparation of CIF file, CIF tools (1h)

09:30-10:30 **All lecturers and students** Roundtable

10:30-11:00 Coffee break

11:00-13:00 **Laboratory activity** (2h)

In the computer room (LM; JE, GDD, MZ, LS):

11:00-13:00 *Structure refinement with SHELXL: new data*

In the XRD and chemistry labs (MSW, AA; JE, SCT, JS, ZM):

11:00-13:00 *Activity continues as needed*

13:00-14:00 Lunch

Afternoon

14:00-15:00 **GDD** IUCr-sponsored lecture: *Publishing with IUCr Journals* (1h)

15:00-16:00 **MSW** Presentation of certificates of attendance and awards (ICDD; AIC; RSC; IUCr; UNESCO Office for the Caribbean)

16:00-16:30 **MSW and MZ** Closing remarks