

SUMMER SCHOOL 2024  
**SPECTROSCOPY AND ELECTRONIC STRUCTURE  
OF TRANSITION METAL COMPLEXES**

**SUNDAY 22/9**

12:00 - 13:30 Registration  
13:30 - 14:00 Welcome  
14:00 - 15:30 **Introduction to Computational Chemistry**  
(Dimitrios Pantazis)  
15:30 - 16:00 Coffee break  
16:00 - 18:30 **Introduction to ORCA** (Frank Wennmohs)  
& **ORCA practical**  
18:30 - 21:00 Dinner and welcome reception

**MONDAY 23/9**

09:00 - 10:00 **Group Theory** (Serena DeBeer)  
10:00 - 10:30 Coffee break  
10:30 - 12:00 **Ligand Field Theory** (Serena DeBeer)  
12:00 - 13:30 Lunch (KoFo)  
13:30 - 15:00 **Optical Spectroscopy** (Frank Neese)  
15:00 - 15:30 Coffee break  
15:30 - 17:00 **X-ray Spectroscopy** (Serena DeBeer)  
17:00 - 18:00 Start of **Poster Session** (CEC)  
18:00 - 19:30 Dinner & **Poster Session** (CEC)

**TUESDAY 24/9**

09:00 - 10:30 **Vibrational Spectroscopy** (Maurice van Gastel)  
10:30 - 11:00 Coffee break (**Group Photo?**)  
11:00 - 12:30 **Practical: Vibrational Spectroscopy** (Maurice van Gastel)  
12:30 - 14:00 Lunch (KoFo)  
14:00 - 15:30 **Facility Tours in Small Groups: 1) Raman, 2) UV-Vis  
RFQ/Stopped Flow, and 3)/4) Both X-ray Labs**  
15:30 - 18:30 **Practical: Excited State Spectroscopy** (Dimitrios  
Manganas)  
18:30 - 20:30 Dinner & **Poster Session** (CEC)

**WEDNESDAY 25/9**

09:00 - 10:30 **Spin Hamiltonians** (Frank Neese)  
10:30 - 11:00 Coffee break  
11:00 - 12:30 **Magnetochemistry** (Daniel SantaLucia)  
12:30 - 14:00 Lunch  
14:00 - 15:30 **EPR Spectroscopy** (Alexander Schnegg)  
15:30 - 16:00 Coffee break  
16:00 - 18:00 **Practical: Magnetochemistry** (Daniel SantaLucia)  
18:00 - 19:30 Dinner

**THURSDAY 26/9**

09:00 - 10:30 **Practical: Simulation of EPR spectra**  
(Alexander Schnegg & George Cutsail)  
10:30 - 11:00 Coffee break  
11:00 - 12:30 **Practical: EPR calculations** (Dimitrios Pantazis)  
12:30 - 14:00 Lunch  
14:00 - 15:00 **MCD Spectroscopy** (Frank Neese)  
15:00 - 15:15 Coffee break  
15:15 - 16:15 **Mössbauer Spectroscopy** (Daniel SantaLucia)  
16:15 - 16:30 Coffee break  
16:30 - 18:30 **Practical: Mössbauer Spectroscopy** (Daniel SantaLucia)  
18:30 - 19:30 Dinner

**FRIDAY 27/9**

09:00 - 11:30 **Facility Tours in Small Groups: 1) SQUID/MCD, 2)  
Mössbauer, and 3)/4) Both EPR Labs**  
11:30 - 12:30 Open Q & A Session  
12:30 - 13:00 Survey  
13:00 - 14:30 Lunch  
15:00 Start of the Eckhard Bill Symposium