POM-BASICS Summer School

"Polyoxometalate Chemistry for Fundamentals and Applications"

La Rochelle-France, June 13-15th 2022

Session 3 - Multiscale structural characterization techniques and modelling in POM chemistry

Part-1. Structural characterization in the solid state and in solution: opportunities and pitfalls

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Abstract of the course:

Part 1 of this session deals with the importance of complete and unequivocal structural characterization of novel POMs in the solid state and in solution. The focus will be on single-crystal X-ray diffraction (S-XRD) as a key solid-state technique, and multinuclear (e.g. ^{183}W, ^{31}P) nuclear magnetic resonance (NMR) as a key solution technique. Both analytical methods are highly complementary and should be used jointly, whenever possible, in order to evaluate if the POM solid-state structure is maintained in solution. Nevertheless, both S-XRD and NMR also have their limits and at times even POM experts can be mislead resulting in wrong assignments. Besides, some other complementary analytical methods will be discussed, while demonstrating their strengths and weaknesses, such as IR, Raman, powder XRD, SAXS, ESI-MS, thermogravimetric and elemental analysis. It will become apparent that the complete structural characterization of novel POMs can be a difficult task and that the use of several complementary analytical techniques is strongly advised, covering the solid-state, solution and gas phase. Furthermore, the experimental studies should be supported by theoretical studies, which will be discussed in Part 2 of this session.