

Course description

Course Title Modern Methods of Structure Determination Métodos Modernos de Determinação Estrutural		
Type/Attendance Time Lecture + Tutorial + Laboratory: 2 afternoons per week	Credit points (ECTS) 12	Type of Examination Protocols and Presentation
Recommended Prerequisites none		
Content <ul style="list-style-type: none"> – X-ray diffraction: Physical background, crystallographic fundamentals (crystal systems, Bravais lattice, the reciprocal lattice, Miller indices, space group symmetry and nomenclature). – Single-crystal X-ray diffraction: Structure solution with Patterson and direct methods, structure refinement, graphic representation of the results, structure discussion. – Independent structure determinations of multiple single-crystal data, composition of a publishable manuscript of one of these structures. Representation of the structure in a presentation-like setting. – X-ray diffraction of powders: (Debye-Scherrer, Guinier, automatic powder diffractometer), determination of lattice constants, calculation of powder diagrams, phase analyses. – Application of structure databanks (ICSD, JCPDS, CSD) – Structure determination in the gas phase: Electron diffraction on gases (GED), rotational spectra – Solid-state NMR spectroscopy – EPR (electron paramagnetic resonance) spectroscopy 		
Conteúdo <ul style="list-style-type: none"> – Difração de raios X; – Difração de raios X em monocristal; – Determinação estrutural independentes de dados múltiplos de monocristal; – Difração de raios X de pó; – Aplicação de estruturas de banco de dados (ICSD, JCPDS, CSD); – Determinação estrutural na fase de gás; – Espectroscopia de RMN no estado sólido; – Espectroscopia de EPR (ressonância paramagnética eletrônica); 		