

Research @ LCCEM

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The Laboratory of Crystallography and Structural Characterization of Materials (LCCEM), located at the Center for Natural and Human Sciences (CCNH) of the Federal University of ABC (UFABC) has been in existence since November 30th, 2011. Since then, 4 postdocs, 5 PhD theses, 4 Master dissertations and more than 10 undergraduate students finished their studies on X-ray powder diffraction and Crystallography.

During the last years, efforts to solve crystal structures of different materials by using X-ray powder diffraction data and different methodologies (simulated annealing, charge flipping) as well as qualitative and quantitative phase analysis, parametric Rietveld refinements and syntheses procedures to obtain new crystal forms (cocrystals and encapsulation of nanoparticles for drug delivery purposes) have been carried out.

The facilities include two X-ray powder diffractometers (shown in Figure 1), operating in transmission geometry with monochromatic radiations (Cu and Mo anode sources), an optical microscope with a hot-stage attached to it, a ball-mill reaction system among other computational and experimental items are available for the scientific community. To date, hundreds of researchers – from Brazil and abroad – have used the laboratory for collaborative research or even for their own scientific works. The body of students and the technical staff help new users to collect good-quality X-ray powder diffraction data.

In this talk I will discuss some of the results obtained during the last few years focusing on the crystal structure determination of pharmaceuticals, parametric Rietveld refinements applied to superparamagnetic iron oxide nanoparticles for potential biomedical applications and to recycled gypsum samples.



Figure 1: X-ray powder diffractometers available at LCCEM.

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