

What modern crystallography can do for you: from bonding analysis to the evaluation of oxidation states

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CICLO CONFERENCIAS ISQCH 2025

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In practically all areas of chemistry, crystal structure determination still dominates using methods that are more than half a century old. However, there are now many ways to get more out of diffraction data for the benefit of chemists. Great progress has been made, especially with the integration of individual quantum chemical calculations into the structural model.[1] Today, for example, hydrogen positions can be obtained with a laboratory X-ray diffractometer with an accuracy that until recently required neutron diffraction experiments.[2] It is also possible to investigate the concepts of bonding theory experimentally, for example to draw conclusions about a dominant mesomeric structure.[3] Finally, X-ray diffraction data can even be used to obtain chemical information that is normally obtained by spectroscopy.[4] Considering that X-ray absorption spectroscopy is usually used to determine formal oxidation states, this opens up new possibilities for the chemists, at their in-house diffractometers. The presentation will give examples of all these methods and also show how you can use them yourself.

[1] *Chem. Sci.* **2021**, 12, 1675; [2] *Acta Cryst.* **2021**, B77, 785; [3] *Chem. Eur. J.* **2024**, 30, e202303762; [4] *IUCrJ*, **2022**, 9, 604.

**Dr. Michael Bodensteiner**

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Publications

[Google Scholar](#)

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Professional Experience**Head of X-ray Structure Analysis Department**

University of Regensburg, Germany — November 2011 - present

Structure determinations, management of technical staff, departmental budget, equipment maintenance and purchases, training of students and scientific staff, radiation safety officer.

Managing Director

OlexSys GmbH, Regensburg, Germany — September 2018 - present

Development and marketing of crystallographic software (Olex2) and a chemical management system (LabSafe), business management, personnel and process management, cooperation agreements.

Scientific Advisor

OlexSys Ltd, Durham, UK — January 2017 - August 2018

Consulting for the development of software for crystal structure determination (Olex2), structure reviews and workshops.

Scientific Employee

University of Regensburg, Germany — March 2007 - October 2011

PhD student in the group of Prof. Dr. Manfred Scheer, research focus on organometallic chemistry and chemical crystallography.

Education**Ph.D. in Chemistry**

University of Regensburg, Germany — March 2007 - April 2011

Dissertation: "Syntheses and Reactivity of Lewis Acid/Base-Stabilized Phosphanylalanines and X-Ray Structure Determinations."

Diploma in Chemistry

University of Regensburg, Germany — October 2001 - February 2007

Thesis: "Investigations on the Oligomerization of Lewis Acid/Base-Stabilized Phosphanylalanines."

Science and Technology Specialties

X-ray structure analysis, quantum crystallography, anomalous dispersion and absorption effects, synchrotron, crystallographic software development, inorganic chemistry

Other Activities

Chairman of the Working Group on Chemical Crystallography, member of various committees and commissions.