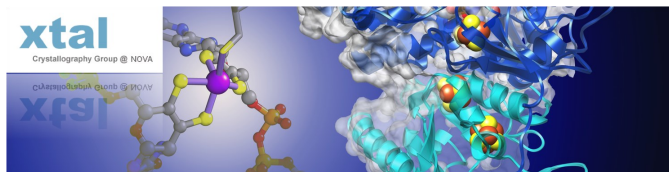


Single Crystal X-ray Structure Determination

The X-ray Diffraction facility provides the screening, testing and complete data collection from X-ray diffraction of single crystals. Dedicated software permits indexing, integration, scaling of data and 3D structure solution. The facility is equipped with a Bruker D8 Venture dual source X-ray generator (Mo and Cu microfocus X-ray sources) using the latest technology, a Photon 100 CMOS detector, and an Oxford cryo-system.

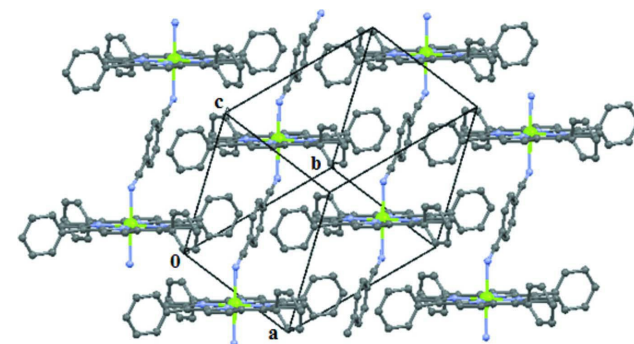


<http://sites.fct.unl.pt/xtal/home>

Single Crystal X-ray Crystallography Service
@ Chemistry Department
FCT-NOVA

Laboratório de Difracção de Raios-X 1.12
Departamento de Química
FCT-NOVA
2829-516 Caparica

xray.service@campus.fct.unl.pt
Phone: +351-21 294 83 00,
ext.10962, 10915



Single Crystal X-ray
Crystallography Service
Chemistry Department
FCT-NOVA

Service Responsible:
Dr. Ramesh Pandian
r.pandian@fct.unl.pt
Phone: +351-21 294 83 00, ext.10962, 10915

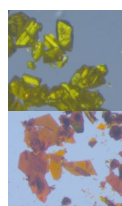
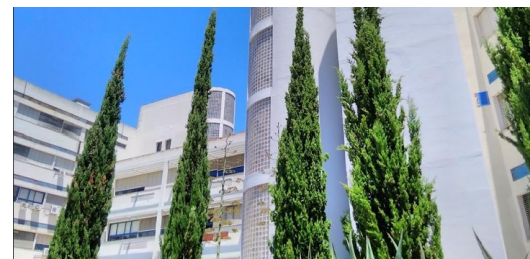
Contact:
Cecília Bonifácio
xray.service@campus.fct.unl.pt

Team Leader:
Prof. Maria João Romão
(mjr@fct.unl.pt)

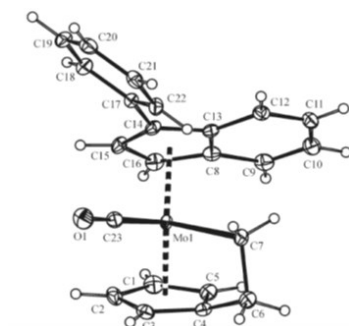


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Single Crystal X-ray Crystallography Service @ DQ-FCT-NOVA



Crystals are evaluated under the polarizing microscope and selected. Data is obtained in the in-house X-ray diffractometer (Mo and Cu micro-focus dual source) with the latest technology and collected on a CMOS detector, according to experimental requirements. Dedicated software permits indexing, integration, scaling of data and 3D structure solution.



"Reaction of Spiro [2.4]hepta-4,6-diene with Molybdenum(II) Indenyl Compounds: Effects of substitution in the Indenyl ligand" J. Honzicák, C.C. Romão, A. Mukhopadhyay, J. Vinklárek and Z. Padělková. *Organometallics*, 30, 717-725 (2011)

Services offered and Price list

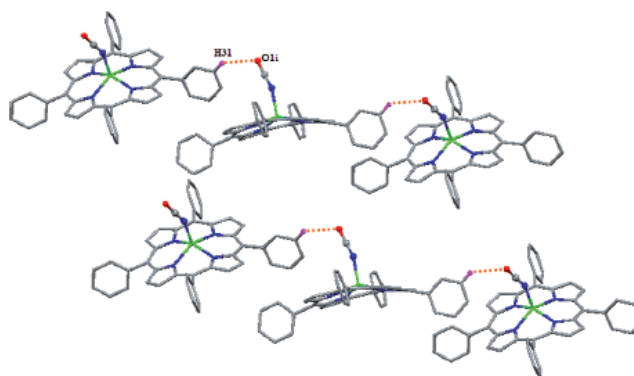
Crystal Evaluation, Selection and Mounting

Unit Cell and Space Group Determination only

Complete Data Collection Only

Complete Data Collection and 3D Structure Determination

Absolute Configuration Determination



"Exploring the Effects of Axial Pseudohalide ligands on the Photophysical and Cyclic Voltammetry Properties and Molecular Structures of Mg^{II} Tetraphenylporphyrin Complexes!" K. Ezzayeni, Z. Denden, S. Najmudin, C. Bonifácio, E. Saint-Aman, F. Loiseau and H. Nasri. *Eur. J. Inorg. Chem.* 5348-5361 (2014)

The 3D structure determination can be required under

Co-authorship or Service:

Services	FCT-NOVA	Other Universities and Public Institutes	Private Institutes, Companies, Industry
Crystal evaluation, selection and mounting	Free of charge	Free of charge	Free of charge
Unit cell parameters and space group determination only	35 Euros	45 Euros	55 Euros
Data collection only	50 Euros	70 Euros	100 Euros
Structure determination and refinement			
Routine	70 Euros	100 Euros	250 Euros
Non-Routine	100 Euros	150 Euros	350 Euros
Absolute configuration	100 Euros	100 Euros	100 Euros
Liquid nitrogen (Data collection)	0,86 Euros/L	0,86 Euros/L	0,86 Euros/L
500 € Package Discount	5%	5%	5%
1000 € Package Discount	10%	10%	10%
New users	Second structure free*	Second structure free*	Second structure free*

* same cost or less to the first structure (non-cumulative with other offers)

For other services please check our webpages:

<http://www.dq.fct.unl.pt/en/single-crystal-x-ray-structure-determination>

<http://sites.fct.unl.pt/xtal/pages/equipment-facilities>