Chemistry

The chemical industry is developing new markets, notably by capitalizing on green growth, to compensate traditional activities.

In fine chemistry, technological developments concern, for example, synthesis from renewable raw materials and chemical derivatives used in the discovery process of biological targets.

In specialty chemistry, manufacturers aim to diversify their sources of raw materials, often from the sea, forest, plants etc. and look for usage properties such as biodegradability and resistance to biological agents, put on the market molecules with reduced toxicity and develop clean solvents.

Finally, nanotechnology is primarily involved in the development of new catalysts with greater efficiency, stability and recyclability.

The benefits of synchrotron light at SOLEIL

- Real time monitoring of chemical reactions, with a temporal resolution down to the millisecond.
- Tunability of the energy to access all the chemical elements in the periodic table.
- Operation of a microbeam to perform chemical imaging by scanning for spatial localization of chemical elements and functions.

- Access to the local chemical structure around a given atom (type and number of neighboring atoms, interatomic distances) by the specific technique EXAFS.
- Speciation (determination of the oxidation state) of chemical elements by the specific XANES technique in a wide range of spatial resolutions (from mm to µm).

Main synchrotron applications for the sector:

- Identification and monitoring of transient phases.
- Monitoring the nature and state of oxidation of reactants in catalytic reactions.
- Crystallization and microstructure of polymers and micro-morphology of foams.
- Monitoring the synthesis and shaping of plastics, elastomers and composites.
- Testing for fatigue, thermal and mechanical aging, under irradiation.

Chemistry contact:
Philippe Deblay: +33 (0)1 69 35 90 05
industrie@synchrotron-soleil.fr

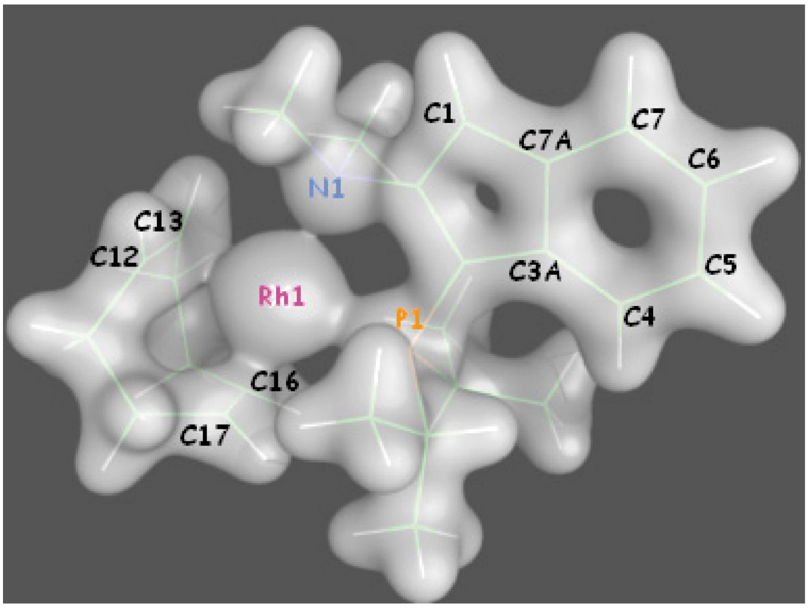
Chemistry

Metal-ligand interactions in a new rhodium complex

The determination of the physicochemical properties of rhodium complexes Rh (I) represents a key step in the analysis of their structure-function relationships and provides information vital for a better understanding of their catalytic properties; these complexes are involved notably in organic syntheses used in some industrial chemistry processes.

The first high-resolution X-ray diffraction experiments performed at 30 K on the CRISTAL beamline determined the crystal structure and the electron density distribution of the rhodium complex $C_{25}H_{37}NPRh$. The electron density around the rhodium atom, whose determination was the main difficulty of the experiment, is very well defined. The figure shows the distribution of electron density between the rhodium atom and its ligands.

It is observed that the rhodium-phosphorus interaction (Rh1-P1) is larger than that involving the nitrogen atom (N1). In addition, topological analysis around the rhodium atom has revealed the nature of the interactions between the atom and the six atoms of its coordination sphere. This approach made it possible to identify two types of Rh-C = C interactions, in contrast to results expected from a simple geometric analysis.



Three-dimensional representation of the total (static) electron density of the $(C_{25}H_{37}NPRh)$ complex.

Christophe Pichon, Head of the Department of Material Characterization at IFP-Énergies Nouvelles.

The primary mission of IFP-Energie Nouvelles, a public-sector R&D, training and information body, is to develop future technologies in the energy, transport and environmental fields.

SOLEIL serves as a tool complementary to those in our laboratories for physicochemical characterization of materials and products of interest in our sector: heterogeneous catalysts, adsorbent materials, polymeric or metallic materials, rocks, cement, gas, petroleum products or those resulting from the processing of biomass...

Today IFP-Énergies Nouvelles uses mostly synchrotron radiation for the characterization of structure (local or wider structure or electronic structures) of systems of interest to its areas of business, by means of X-ray diffraction and absorption based techniques. However, as SOLEIL's performance is improving in terms of photon flux and in operating micro-beams and sample environments, access to new techniques (high-resolution XPS, X-ray microtomography, IR microscopy, etc.) could prove useful for the scientific activities of IFP-Énergies Nouvelles.