

Action CM0802

2008 - 2012

European Phosphorus Sciences Network - PhoSciNet -

Participating countries: AT, BE, BG, CH, DE, ES, FI, FR, GR, HU, IT, NL, NO, PL, RO, SE, SK, TR, UK

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CMST



www.cost.esf.org/domains_actions/cmst/Actions/European_Phosphorus_Sciences_Network
www.phoscinet.org



Figure 1: PhoSciNet researchers participating in the European Workshop on Phosphorus Chemistry in Florence (2009)



Figure 2: PhoSciNet is a platform for interdisciplinary discussions related to high-level scientific research on phosphorus sciences

Objectives:

- The main objective of the Action is the understanding of structure–reactivity correlations and properties of novel phosphorus compounds according to their potential applications in materials science, catalysis, and bioscience-related fields.
- **1. Materials:** Develop fundamentally new classes of phosphorus-based materials employing a bottom-up approach based on suitable phosphorus-containing molecular building blocks by using the predictive power of structure–property relationships.
- **2. Catalysis:** Synthesise and apply novel P-based ligands for efficient chemo-, regio- or stereoselective catalysis with emphasis on environmentally friendly methods for compounds having an industrial or biological interest.
- **3. Bioscience-related Topics:** Develop bio-active organophosphorus compounds, e.g., for diagnosis and treatment, to acquire an understanding of specific biological processes.
- **4. Basic-applied Research:** Develop highly functionalised, high-potential phosphorus compounds with new bonding modes, new bonding concepts, and unusual reactivities. With the applicability of these compounds becoming apparent, this knowledge will be implemented in the Working Groups 1-3.
- **5. Methods Development** and application of state-of-the-art synthetic, spectroscopic and theoretical methods to support and complement the experimental research. Structure-reactivity correlations will be employed to manipulate reactivities and properties of novel phosphorus compounds to enable their applicability in Working Groups 1-3.

Working Group 1: Materials Science and Nanoscience

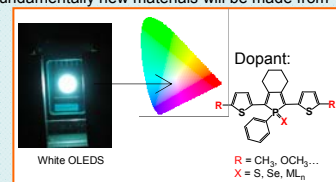
The WG materials research is based on a “bottom-up” approach: Fundamentally new materials will be made from progressive phosphorus-based building blocks.

Research Areas:

- P-containing polymers (chiral, P-C cages)
- Polymer doping for catalysis
- Electronic, optical, magnetic properties [e.g., OLEDs (white)]
- Metal-phosphide nanoparticles (e.g., from P₄)

Methods of Achievement:

- Develop (in)organo(metallic) building blocks
- Predict structure–property relationships
- Integrated synthetic–theoretical approach



Working Group 2: (Asymmetric) Catalysis

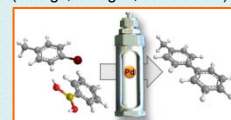
Research in catalysis is of utmost importance in applied sciences, involving many fields of chemistry, especially organophosphorus and organometallic chemistry and biosciences.

Research Areas:

- Switchable “smart” catalysts (light, electrochemically, heat; modification of cone angles, donor/acceptor properties)
- Sculptured, tailor-made P ligands for homogeneous catalysis with pre-designed shapes (P rings, P cages, dendrimers) and properties (water-soluble, ionic liquids)

Methods of Achievement:

- Synthesis of novel tunable (chiral) ligand systems
- Exchange of knowledge on catalytic processes
- Synthesis of novel (biologically active) compounds
- Energy-efficient, waste-free, non-toxic, non-hazardous conditions



Working Group 3: Bioscience-related topics

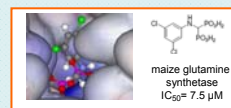
Research is focussed on two main directions which deal with the development of new drugs through phosphine-based catalysis and on the synthesis of biologically active phosphorus compounds for medicinal applications.

Research Areas:

- Water-soluble P ligands as transport agents to cross cell membranes
- P-containing drugs (non-steroidal anti-inflammatory agents, metal phosphines,...)
- P-containing macrocycles or chelate ligands for imaging agents

Methods of Achievement:

- Synthesis of bio-active molecules
- Interaction with bio-medicinal sciences



Working Group 4: Novel high potential phosphorus compounds for non-typical applications

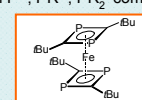
Targets are highly functionalised novel phosphorus compounds, which often defy common analogies (phosphorus-carbon diagonal relationship, isolobal concept) and exhibit new bonding modes to display unusual reactivity. Strong interaction between this WG and WG1-3 is envisaged as is apparent from the emerging applications of some of these compounds.

Research Areas:

- Highly functionalised P compounds (P anions/cations/radicals, rings, P=X / P≡X bonds; metal P³⁻, PR²⁻, PR₂⁻ complexes)
- Tuning the reactivity of compounds, intermediates, and metal complexes
- P₄ activation; design of P-based ligands and macrocycles

Methods of Achievement:

- Synthesis of ‘unusual’ compounds with ‘unusual’ reactivity
- Interaction of basis research with materials science, catalysis, and bio-sciences



Working Group 5: State-of-the-art synthetic, spectroscopic, and theoretical methods

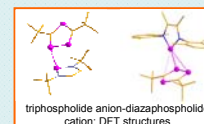
New experimental techniques will be developed, and existing ones and the necessary theoretical and software tools will be improved, aiding all the other WG activities in reaching their goals. Sharing of expertise within PhoSciNet will be stimulated.

Research Areas:

- High-level theoretical calculations (ab initio, density functional theory, QM/MM) calculate structures of (macro)molecules, intermediates, complexes, and catalysts
- predict and support reactivities, stabilities, and (opto-)electronic properties
- calculate electron densities and spectroscopic data (IR, UV, NMR, CV, EPR,...)

Methods of Achievement:

- Understand structure–reactivity relationships
- Relate reactivities and properties of novel compounds/intermediates to materials science, catalysis, and biosciences



Main Achievements:

- PhoSciNet has united researchers working in synthesis with those focussing on applications in materials science, catalysis and biosciences, with strong involvement of theoretical groups to understand structure–reactivity correlations. More than 60 research groups are presently involved in PhoSciNet to explore the undervalued potential of phosphorus in many contemporary topics of basic and applied research.
- Each research group participates in PhoSciNet with an average of at least four researchers, i.e., experienced scientists, early-stage researchers and doctoral candidates. Through the interaction between the research groups in different EU countries, they acquire an understanding of the different procedures and cultures and are part of high-level scientific research on an international platform.
- Several senior scientists participate with their research teams in more than one Working Group, to encourage focussed research interactions spanning the different research topics of the five Working Groups’ activities.
- Excellent experimental and technical facilities are available at the participating institutions to achieve the research objectives within PhoSciNet. They also allow transfer of techniques and applications and sharing best-practice procedures (e.g., during STSMs) to advance European scientific/technological know-how.
- Industrial partners are involved in PhoSciNet to enable industrial applications and to ensure technology transfer.