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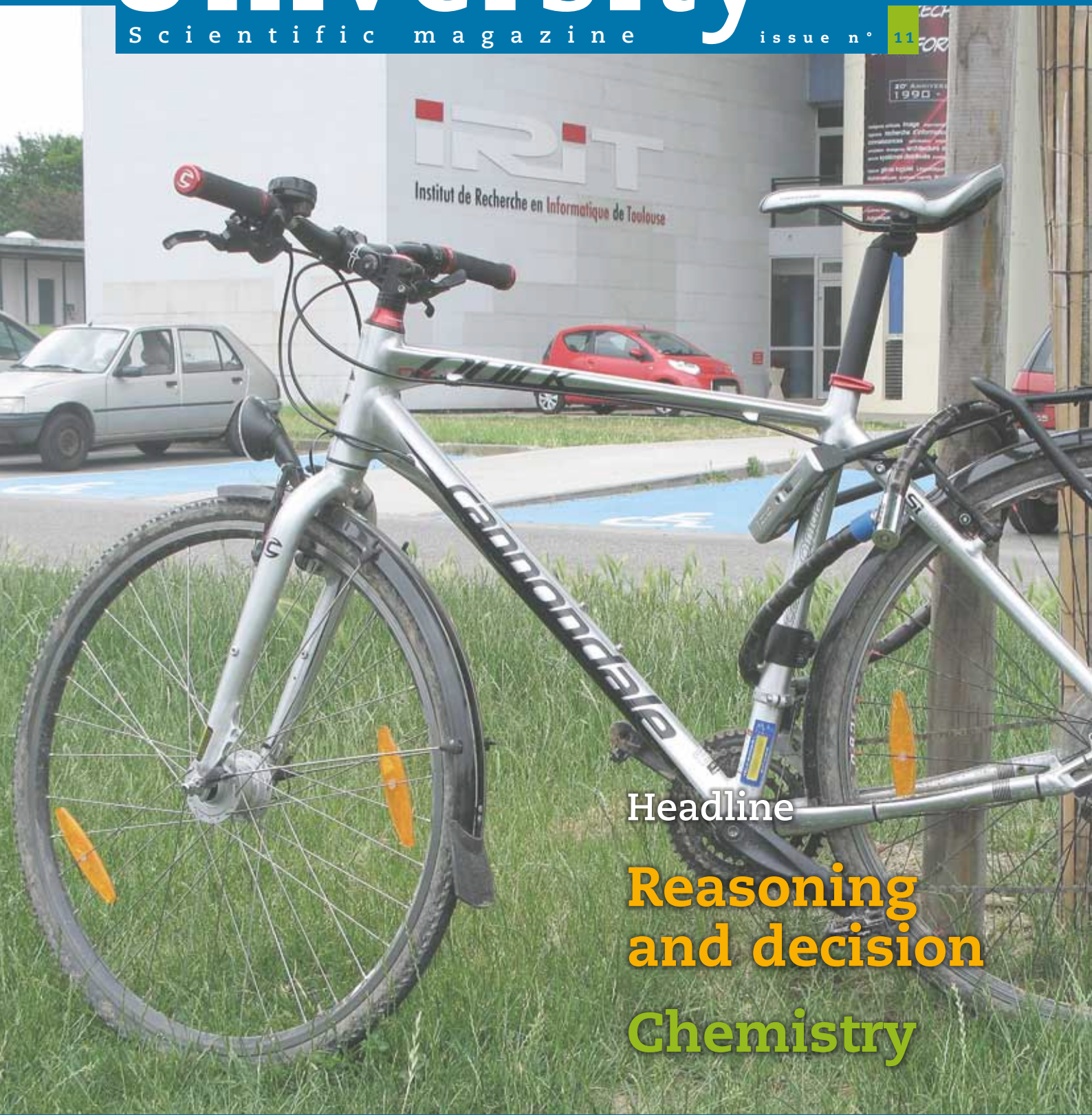

Headline

Reasoning and decision Chemistry

Université de Toulouse
Université Paul Sabatier
TOULOUSE III
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Instituts thématiques Inserm
Institut national de la santé et de la recherche médicale

The first headline of the present issue covers "reasoning and decision". The conceptual design of sophisticated machines that have the inherently human quality of reasoning is indeed an ambitious futuristic goal of researchers in this area. Such an achievement obviously requires a basic thorough knowledge of the human spirit, which primarily analyzes the physical reality of things, but which is also influenced by our beliefs, our objectives, our preferences, etc. So, this is obviously a multidisciplinary research domain, at the interface of computer science, human and social sciences, including psychology, linguistics, and economy. Such a research theme is not very well known, and yet, several research teams belonging to our university have already acquired international recognition in the field. In the following pages, we will learn more on the state of the art and challenges in this area.

The second headline is devoted to chemistry, keeping in mind that the United Nations has dedicated the year 2011 to chemistry. This is an excellent opportunity to highlight some prominent aspects of such a discipline, remembering that our university was named after Paul Sabatier, a prestigious world famous local scientist, who was awarded the Nobel Prize in 1912 for his pioneering discovery of *"a general method of hydrogenation by catalysis"*. During the past two decades, fundamental research in chemistry has met new challenges, and has extended its development at the interface with other disciplines. While continuously improving basic knowledge, chemistry is now also addressing important societal problems, such as health, nutrition, energy, sustainable development and climate change.
Enjoy reading our magazine.

Gilles FOURTANIER
President of Paul Sabatier University

Currently used abbreviations

UPS: Paul Sabatier University (Toulouse, France)
CNRS: French National Center for Scientific Research
INSERM: French National Institute for Health and Medical Research
INSA: National Institute of Applied Science
INRA: National Institute for Agricultural Research
INPT: National Polytechnic Institute of Toulouse
ANR: National Research Agency

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Security analysis for the example of a bicycle with two locks

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Reasoning and decision: human or machine?

How can a typically human activity such as reasoning be performed by machines? To answer this question we have to understand how our minds function. This is determined not only by physical reality, but also by our beliefs, goals and preferences.

>>> Andreas HERZIG, CNRS senior scientist at the Institut de recherche en informatique de Toulouse (IRIT, joint UPS/CNRS/UT1/UT2/INPT lab)

We don't know everything, our beliefs may be erroneous and we live in a world that changes all the time. Despite all these difficulties we are able to reason and to make decisions quite successfully. Our abilities to learn and to revise our beliefs are crucial for this.
We not only reason about nature and physical reality, but also about the other human agents in our environment and with social reality as created by man: society and its institutions, such as norms and conventions, things that are allowed and things that are forbidden, contracts, etc. Indeed, language and communication may be considered to be the first of these institutions: in dialogue we exploit the fact that others know the conventions of communication, allowing them to interpret what we say. An example of a convention is to avoid contradictions and to stay focused on the subject.

Anthropomorphism

What we have said up to now applies to human agents, and one might wonder what all this has to do with computer science. However, it appears that the central concepts in our discourse apply to artificial agents too. Such an anthropomorphic point of view was adopted in Artificial Intelligence right from its beginnings in the 60s and in multi-agent systems in the 80s.

Of course, how agents reason and decide is not only investigated in computer science, but originally in the humanities and in social sciences, viz. in psychology, philosophy, linguistics, cognitive science, and economy. It is therefore a multidisciplinary object of study, and the researchers of IRIT very often collaborate with linguists and psychologists of the Toulouse labs "Cognition, Langues, Langage, Ergonomie" (CLLE, université Toulouse 2) and the economists of the "Toulouse School of Economics" (TSE, université Toulouse 1).

Theories of possibility and logics of modality

The overall aim is to implement artificial agents in computers. How can one relate concept analysis and computer programs? For several years now, the researchers working on the "Reasoning and Decision" theme at IRIT have adopted a classical research avenue, viz. formal approaches, allowing for rigorous and verifiable proofs. Their main tools are possibility theory and modal logics, and the procedure is to start by formal modeling (including concept analysis). This is then followed by an investigation of the mathematical properties and the development of automatic or semi-automatic reasoning procedures.

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IRIT: Institut de recherche en informatique de Toulouse/ Toulouse Insitute of Computer Science Research

>>> Rodin's The Thinker at Saint Dié.
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>>> Nathalie Aussenac-Gilles, CNRS senior scientist, and Laure Vieu, CNRS scientist, researchers at the IRIT (UPS/CNRS/INP/UT1/UT2)

Language and representing knowledge

Reading a text, analyzing and summarizing it: these processes are not unique to humans anymore according to new work by researchers at the IRIT laboratory who are studying the automatic treatment of language

Among the first challenges faced by the Artificial Intelligence (AI) program was to reproduce the very human ability of producing and understanding linguistic messages. This is all the more difficult as such activity is thought of being a mark of human intelligence. Natural language processing makes linguistic analyses accessible to computer systems, from the handling of synonyms (lexical level), for instance, to the identification of verb complements (syntaxic level), finding what a pronoun refers to (semantic level) or the relation between two sentences (discourse level). This, in turn, is used for information extraction, machine translation, or automated summary production. Collaboration between linguists and computer scientists has proved very useful in this respect, and researchers in the NLP at IRIT have a long standing partnership with linguistic groups at Université Toulouse II (CLLE-ERSS and J acques Lordat Lab).

Information explosion

The path followed since the inception of the AI program has been tremendously transformed by the explosion of the amount of data available in natural language (whether written or oral) either published on the web or produced by companies or users. Managing this abundance opens up new avenues for testing hypotheses on languages, and the development of efficient tools for analysis. It also favours sharing of information, knowledge discovery and corroboration.

A major objective in the domain is to give some structure to the areas of knowledge that need to be formalized, by finding connections between relevant entities, their properties and the concepts they involve. This usually goes under the name of ontology. In the medical domain, many ontologies have been designed, often starting from thesaurii, such as MESH or UMLS, or from automated analyses of medical texts to jump-start the formalization process. These ontologies provide richer definitions of medical concepts, of relations between pathologies, treatments and anatomic aspects, etc. They are used to characterize the information available in patient files, good practice guidelines or scientific papers, for verification and corroboration, and more globally to fuel decision processes with recent research results.

Opinion mining

The main activity of our team contributes to the formalization of different elements that take part in the semantics of a text. Our work is concerned with the globality of a text or a discourse, how lexical and syntaxic elements combine but also how relations within and between sentences, paragraphs and other textual elements contribute to the construction of meaning. Research on ontologies includes these results to organize knowledge and build systems that can help to identify and extract information from texts. This also implies the development of tools to help model and maintain ontologies.

The end result combines knowledge and its linguistic expression. It is put to the test by a range of applications, mainly opinion mining (to understand such phenomena as corporate or private e-reputations, or product reviews), dialog analysis, text mining and automated ontology building. Our research also involves industrial partnerships (eg ACTIA Automotive, Synapse Development), institutional funding via ANR grants, for instance, for computer aided diagnostic of electronic failure, or geographical database integration.

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" You feel confused? You don't have a boyfriend? No social life? No dreams? You want to be more like sitcom actors? Then go for this TV show and watch it over and over again! "

>>> Caption:
In opinion mining of short texts, such as forum comments, the main goal is to find out if the author has a favorable opinion of the discussed topic. The example illustrates the limitations of algorithms based only on word spotting. The advice given in the article indicates a positive opinion of the show. However, taking into account the whole context and with sufficient background knowledge, it can be seen that " no social life " characterizes an audience for which the author has no respect, so that recommending the show for that particular audience actually leads to a negative opinion about the show itself.

Probability Theory alone cannot handle all facets of uncertainty

People constantly deal with pieces of information that are incomplete, uncertain, inaccurate, and sometimes inconsistent. To face this issue, scientists naturally resort to probability theory. But this approach does not take into account where uncertainty comes from.

>>> Didier DUBOIS and Henri PRADE, CNRS senior scientists at the Institut de Recherche en Informatique de Toulouse (IRIT, UPS/CNRS/UT1/ UT2/INPT

Probability theory as a tool for representing uncertainty has long existed, but it often does away with the fact that there may be several reasons for being uncertain. The main reason evoked is the variability of natural phenomena and of data coming from repeated measurements. Hence the frequentist's view of probabilities that is often taken for granted.

Thought lotteries

Another very common reason for uncertainty is the plain lack of information, which alone may prevent agents from knowing whether statements of interest are true or false. This kind of "poor" information often takes the form of an incomplete set of propositions in classical logic, or appears as an interval of possible numerical values of an ill-known quantity, or even as a set of attributes that does not allow for the precise description of an object. To understand such situations, we need another probabilistic concept, so-called subjectivistism, where a probability does not reflect an ideal frequency, but represents, in a betting framework, the price of a thought lottery that yields an euro if the concerned event occurs. This concept claims that it makes sense to represent any incomplete information situation by means of a unique probability distribution. But this view can be challenged: such a representation is not scale-invariant, and does not depend on the origin of uncertainty. It is more natural to represent incomplete information by means of a mere set of possible values, often called the "epistemic state" " in Artificial Intelligence.

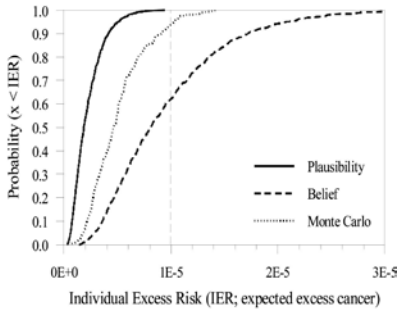
Uncertainty theories

It makes sense to be able to tell variability and incompleteness apart in the scope of information processing. Several new theories try to address this issue, such as possibility theory, evidence theory and imprecise probability theory. In such settings, instead of representing any information state by means of a unique probability distribution, sets thereof, or even random sets, are used. The confidence attached to an event occuring is then quantified by a probability interval, measuring certainty by its lower bound and plausibility by its upper bound. Sometimes such quantification is difficult to justify. All that can be said in some cases is that some events are more likely than others. One is then led to use qualitative representations of uncertainty, that turn out to be instrumental in dealing with exception-tolerant reasoning.

Possibilistic Logic

When information is incomplete, the human mind resorts to reasoning patterns that enable useful conclusions to be tentatively drawn despite incompleteness. Such conclusions can be questioned upon the arrival of new pieces of information. In this case, reasoning becomes non-monotonic and presupposes the truth of anything that is considered normal in the current informational context. This form of reasoning is not amenable to classical logic. It requires logic with embedded priorities, such as possibilistic logic. Such logic is also instrumental in the problem of merging partially inconsistent pieces of information.

For more than 20 years, our team has been working on the construction of formal frameworks that are wide enough to enrich the expressive power of traditional approaches to uncertainty, both probabilistic and logic-based. For the last 10 years or so we have cooperated with public research laboratories in the area of environmental risk analysis, such as BRGM or IRSN. In risk analysis, the usual methodology is first to build a mathematical model of some potentially hazardous phenomenon. Then in a second step, we must check on the basis of data collected on-site in an area of concern, whether the probability of a risky event is above some acceptable, say, pollution, threshold. But the collected objective data are often incomplete and part of the information must come from expert opinion. We have developed risk analysis methods based on imprecise probabilities encoded as possibility distributions, so as to separately handle uncertainty due to known variability and uncertainty due to lack of data.



>>> Results for risk calculation application

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Game theory, emotion and trust: from social sciences to artificial intelligence

In recent times, game theory has begun to take into account both motivations and more and more complex emotions such as trust, guilt or shame. These are useful concepts for designing robots similar to humans.

>>>Dominique LONGIN and Emiliano LORINI, CNRS senior scientists at the IRIT (UPS/CNRS/UT1/UT2/INP).

During the last century, game theory became the dominant paradigm in social sciences for modeling and for explaining social interaction between human agents and economic agents (states, companies, banks, etc.). The goal of this theory is to explain and predict social actors' choices in strategic interaction contexts, that is, when the choice of a given agent depends on what other agents decide to do. Classical game theory is based on a very simple conceptual frame including the concepts of preference and action. But following the work of the economists John Charles Harsanyi and Robert Aumann, game theory began to include the concepts of knowledge and belief in order to model strategic interaction situations with incomplete information. More recently, the concepts of emotion and trust have become central to this theory. Empirical evidence and psychological theories show that emotions such as guilt, shame or regret affect human strategic decisions. Furthermore, it has been proved that trust plays a crucial role not only in individual decision making but also in social interaction by fostering cooperation.

Reasoning from emotions

In recent years, game theory has become the most used theoretical framework in the area of multi-agent systems (MAS). MAS are a part of artificial intelligence (AI), whose goal is to develop interaction models between artificial autonomous agents (for instance, models of cooperation and coordination, negotiation models, etc.). Similarly, emotion and trust have become central themes in the area of AI. Computational models of autonomous cognitive agents capable of reasoning by taking into account human users' emotions, and whose decisions are influenced by their own emotions, already exist. Several models of trust have been proposed in the area of MAS: statistical and socio-cognitive models of trust and reputation models. These models provide formal and

>>> "Les tricheurs" (Caravaggio, Kimbell Art Museum)

abstract specifications that can be used for developing several applications such as web services, reputation systems (EBay for instance), semantic web, embodied conversational agents and cognitive robotics.

Facial expressions

Work at the LILaC group at IRIT aims to develop logical models of social interaction based on game theory and on psychological theories of emotion and of trust. These models can be exploited as a base for implementing artificial agents capable of reasoning from concepts of emotion and trust during interaction with a human user or with other agents and whose strategic decisions are influenced by their emotions. For instance, a logical model of emotions based on counterfactual reasoning, such as regret or guilt, has been developed. This model has been recently used in the ANR project CECIL for expressing such emotions in a multimodal fashion (for example, facial and vocal expressions, and gestures).

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My computer knows me so well

How much can computers learn to know us ? Machine learning is a research area where considerable progress has been made in the last 30 years.

>>> Jérôme MENGIN,
UPS assistant professor,
researcher at IRIT (UPS/CNRS/INP/UT1/UT2)

Computers are now able to recognize their users' voice or handwriting. Computers have learnt to discriminate human features. Can a menu recommender system, for example, learn what its user likes in order to suggest dishes to her liking? As we can see, "knowing" the user in this case means knowing her culinary preferences.

Decision-making support

More generally, knowing the user's preferences must help improve the quality of the services offered by decision-making support systems or recommender systems. Such systems must often help a user choose some alternative among a huge number of possibilities, notably because of the combinatorial nature of the alternatives. The goal of the system is thus to guide its user in order to help her end up with her preferred alternative. The efficiency of the system for this task will be improved if it knows, at least partially, the user's preferences.

The notion of preferences has been studied in various domains, notably in psychology, social choice theory, micro-economics and decision theory. When studying preferences of individuals that are supposed to be rational, one can consider strict order relations: the relation "is preferred to" is then supposed to be irreflexive (M is never preferred to itself) and transitive (if M is preferred to N, itself preferred to O, then M is preferred to O).

Learning one's preferences

Of course, one can only learn a user's preferences if some data about her is available. Therefore, we assume that we are able to gather information about the user during her interaction with the system. In particular, we suppose that we can obtain pairwise comparisons between alternatives (between menus in our example). For instance, if at some point during the interaction with the system, the user modifies a menu that has been suggested, we can record that she preferred the second menu. It is these examples of the user's preferences that will be the basis of the learning process. The problem is now to generalize these specific preferences, in order to obtain a total order relation over the possible menus. This induced relation can then be used to predict the user's preferences when the system suggests new menus.

As in any machine learning problem, the choice of the type of model that one tries to learn is crucial. We can try to learn ranking functions that associate a numerical value to every alternative. The ADRIA (Argumentation, Decision, Reasoning, Uncertainty and Machine Learning) research group at IRIT studies the induction of rules of the form: "If the main course is fish, then white wine is preferred to red wine, whatever the starter". We try to learn an order relation that is the transitive closure of pairwise comparisons implied by such rules. Depending on the type of rules that are authorized, one obtains classes of models of preferences of various richness, that can be learnt efficiently or not.

In particular, the ADRIA group has characterized the complexity of learning separable preferences (when preferences over, for instance, the main course, the wine, the starter and the dessert do not depend on one another). We have also proposed algorithms to learn lexicographic preferences - when some components of the menu are more important than others. These results have been obtained in collaboration with researchers from the LAMSADE - University Paris-Dauphine and from Mahasarakham University in Thailand.

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System security: look for weaknesses

To find security flaws, programs now think like crackers.

>>> Yannick CHEVALIER,
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at the Institut de recherche en informatique
de Toulouse (IRIT, UPS/CNRS/INPT/UT1/UT2)

Consider two University of Toulouse students, Alice and Bob, who share a bike. They don't meet regularly, but devised an ingenuous protocol to use the bike. When Alice stops riding the bike, she puts her padlock on it. When Bob plans to use the bike, he also puts his padlock on it. This way, the next time Alice sees the bike with two padlock on it, she can safely remove hers, leaving Bob's padlock on. He will then later be able to use the bike. To sum up, Alice and Bob have devised a set of rules such that, as long as they adhere to it, they will be able to use the bike, and the bike cannot be stolen. Computer scientists use cryptographic algorithms instead of padlocks to secure communications on the internet instead of a bike, but the idea is the same. The security analysis of cryptographic protocols consists in assessing where the devised set of rules is sufficient to provide a claimed guarantee. In plain text, is Alice and Bob's confidence that their protocol protects their bike well founded ? While cryptographs are chiefly interested in a padlock's resistance (or rather on the security provided by a cryptographic algorithm), the members of the LILaC (**L**ogic, **I**nteraction, **L**anguage, and **C**alculus) work on logical flaws, i.e. Flaws that do not rely on lockpicking or on a shear, given the set of rules. More specifically, they search algorithms able to automatically find such flaws when they exist. For example, if Charlie knows Alice and Bob's protocol, he can wait until there's only Alice's padlock on the bike, put on another padlock looking like Bob's, and wait until Alice comes back and remove hers. Charlie will at this point be able to ride away with the bike.

>>> A bike with two padlocks awaits the reader in front of the IRIT

Logical analysis

They work on a logical model of the system under scrutiny and of the goal properties. For example, a logical modeling of a function *f* (*e.g.* a decryption function) with one argument x would be a formula stating "*for any message x, either x cannot be computed by the attacker or f(x) can be computed by the attacker*". *Similarly, we state that a message f(m) must remain confidential by the logical formula "the attacker cannot compute f(m)*". These expressions are clauses of first-order logic. They express non-disjoint possible cases, and their meaning is that for every ground value of the variables at least one of the cases must be true. When there are several such clauses there is a risk that the cases are incompatible. For instance adding the clause "*the attacker can compute m*" yields an incompatible (logicians say *unsatisfiable)* set of clauses. What's interesting is that a set of clauses modelling a system together with its purported properties is unsatisfiable when one of the properties does not hold. Consequently, as logicians, our goal is to determine whether a set of clauses modelling a system is unsatisfiable.

Resolution

Though the problem is conceptually simple---it suffices to try all possible instances of each variable and see whether each clause is satisfied---it cannot be solved by a machine in general because there is an infinite number of possibilities for each variable. Alan Robinson has however devised a principle he named resolution that permits to speed up the examination of all possible instances. It is based on the combination of the cases occurring in the clauses. For instance, if a clause states that "*x* cannot be computed by the attacker or f(*x*) can be computed by the attacker" while another states that "*m* can be computed by the attacker", resolution on the first case of the first clause with the only case of the second clause yields a clause stating "f(*m*) can be computed by the attacker". Using the resolution principle one adds new clauses to a set of clauses. It is guaranteed that if the initial set of clauses is unsatisfiable, one will end up adding an unsatisfiable clause. But if the set of clauses is satisfiable, the computation goes on indefinitely.

Unification

This principle is based on the detection of when two clauses state a fact and its negation. One thus needs to be able to compute when two facts have common instances. This computation is called *unification*. While in the basic case this problem is simple, the security analysis of protocols depends upon additional equalities constructions, expressing for instance that the state of the bike with two padlocks is the same regardless of whether Alice or Bob puts her/his padlock first. The existence of such equalities makes unification unsolvable by a machine. Given that both detecting when two facts have common instances and detecting when a set of clauses is unsatisfiable cannot be solved *in general* by a machine, the work on security in the LILaC team consists in finding classes of sets of clauses and equality theories that are general enough to specify the systems analyzed and specific enough to be solvable by algorithms. For further information on how this can applied to find a flaw on Google's implementation of SAML, we refer the reader to our latest project website, *http://www.avantssar.eu !*

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Artificial Intelligence at work in negotiation

Which side to take in a trial? Which is the best medical decision to take? When choices are difficult, artificial intelligence can provide valuable assistance in dissecting the foundations of an argument. It becomes a theoretical tool for analyzing and formalizing the interactions between rational agents, for example, in negotiation.

>>> Argumentation in AI Group, ADRIA and LILAC teams: Leila Amgoud (research scientist, CNRS), Philippe BESNARD (CNRS), Claudette CAYROL (UPS professor), Sylvie DOUTRE (associate professor at UT1), Florence DUPIN de St-Cyr (UPS associate professor), Marie-Christine LAGASQUIE-SCHIEX (associate professor at UPS) in the Toulouse Institute of Computer Science Research (Institut de recherche en informatique de Toulouse, IRIT, UPS/CNRS/UT1/INP)

An opinion is justified by giving reasons that enforce or explain it. These reasons, called arguments, can take various forms, have different strengths, and are more or less relevant with regard to the thesis. Argumention is a process that consists of evaluating and comparing arguments and counterarguments in order to select the more acceptable ones.

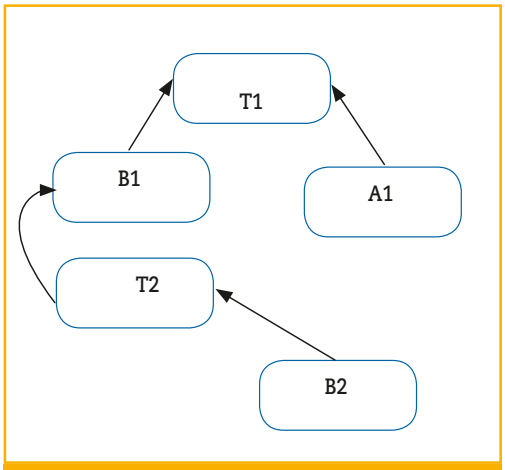
For an autonomous agent, it is a major component of reasoning, explanation of reasoning and decision support, especially in the presence of contradictory information.

The chances of reaching a consensus

Argumention also plays an important role in multi-agent interactions in general and in particular for negotiating. Negotiation-based reasoning enables agents to explain their choices with arguments. In the light of a new argument, an agent may revise its beliefs and preferences, increasing the chances of reaching a consensus.

How to appreciate an argument? This is the central issue on which the group "Argumentation in AI" of IRIT is working.

The work of this group covers both the formal aspects of argumention and the use of this formalism for reasoning and decision problems. Regarding the formal aspects, the group studies the interaction between different types of arguments, the methods of comparison and criteria for judging whether an argument is acceptable, and the dynamics of a system of argument, that is to say the change induced by the inclusion of a new argument or the deletion of an existing argument.



>>> **An argumention dialogue:** Tom (T1): "for going downtown, my car is a good mode of transport".
Bob (B1): "no, a car is a too dangerous mode of transport".
Tom (T2): "no, my car is equipped with airbags".
Bob (B2): "an airbag can explode!".
Anne (A1): "anyway, there's too much traffic to use the car"

Trials and medical decision

Formalisms are used to explain decisions, classify objects, and to model negotiation between agents. Although our research is usually very "upstream", it leads to many practical uses and affects many different areas. Argumentation is used, for example, to model and analyze legal arguments (the transcript of a trial). There exist also numerous applications in medicine; for example an argument-based formalism has been used to produce a tool managing the exchange of tissue between hospitals in transplantation (European project ASPIC). Finally, it is often used in trade negotiations on the web.

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Thinking fast without too much effort

Formal models of artificial intelligence require the development of algorithms that automatically solve the problems they pose. An essential requirement is that they do not consume too much computing time or too much memory.

>>> Martin COOPER and Olivier GASQUET, UPS professors and researchers at IRIT (UMR UPS/CNRS/INP/UT1/UT2)

The reconstruction of the shape of a 3D object from a 2D line-drawing is an example of a problem that can be modeled in terms of numerical, ordinal or structural constraints together with preferences (for flat surfaces and right angles, for example). Solving these constraints allows a program to reconstruct the object or to detect its physical impossibility.

The CSP ("Constraint Satisfaction Problem") has applications in many areas (such as in the aviation or automobile industries), but if constraint problems must be solved in real time, it is extremely difficult to guarantee a quick response time. Techniques known as "compilation" use off-line pre-processing to solve part of the problem (the model of the system to be diagnosed or the vehicle to be configured). Members of our research team work with industrial partners (Renault, Access Commerce) to integrate preprocessed structures into configuration systems for on-line sales.

Languages

In another line of research, the evolution of a discrete system can be modeled as a "transition system", the transitions marking the change from one system state to another. Examples include executing a program, using a computer-security protocol, driving a vehicle, or evolving information (knowledge) within an artificial agent. "Can the system get blocked? Does it contain unnecessary states? Is it possible to reach a state satisfying a given condition?". At IRIT we design formal "modal" languages in order to express such questions and to provide an automatic answer using calculations. Conversely, thanks to these modal languages, it is possible to describe the properties required of a system (this defines a modal logic). Appropriate algorithms can then determine the existence of a system, called a model, satisfying these requirements and even build such a model.

Tractable problems

It is not only important to discover algorithms and optimize them, but also to search for classes of problems that can be solved by these algorithms. Particular emphasis is placed on the identification of so-called tractable classes of problems whose solution time does not increase exponentially. A joint research project with the University of Oxford has identified several new tractable classes.

Our work has also given rise to the production of free software: Toulbar2 (in collaboration with INRA http://carlit.toulouse.inra.fr/cgi-bin/awki.cgi/ToolBarIntro), which is a complete program for solving valued constraint problems and LoTREC (http://www.irit.fr/Lotrec), which is a development platform for modal logic and model building.

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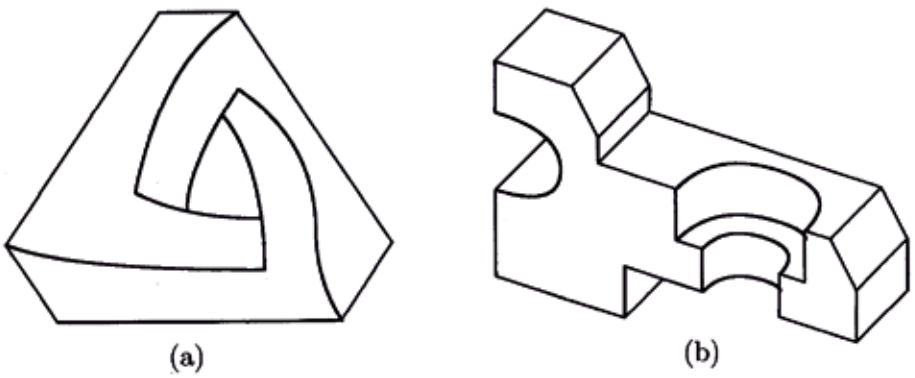

(a) An impossible object; (b) a possible object.

Chemistry Research, a crossroads of knowledge

2011 has been declared the International Year of Chemistry by the United Nations and was an excellent opportunity to demonstrate the latest research in the subject at the University Paul Sabatier in Toulouse. Paul Sabatier, after whom the University was named, received the Nobel Prize for Chemistry in 1912.

>>> Sylviane SABO-ETIENNE, CNRS senior scientist at the Laboratoire de chimie de coordination (LCC, CNRS and UPS) and Antoine BACEIREDO, CNRS senior scientist, head of the ICT and member of the Laboratoire d'Hétérochimie Fondamentale et Appliquée (LHFA, UPS/CNRS)

Chemistry plays a vital role in our lives and in almost all industrial and economic sectors and continuing advances in chemistry have led to significant changes in society over the last century. In keeping with the motto "Chemistry - our life, our future", the discipline helps provide appropriate responses to major issues affecting today's society, including: health, nutrition, energy, sustainable development and climate change. For these reasons, chemical research must be inventive, and based on fundamental research at the highest level. The reputation and influence of Toulouse chemists has been rewarded by many national and international awards and three elections to the French Academy of Sciences.

There are 300 permanent staff working in the area of molecular chemistry at Toulouse. The department is linked to the Institute of Chemistry of Toulouse (ICT-http://ict.ups-tlse.fr), which includes five chemistry laboratories (LCC LHFA, IMRCP, SPCMIB, PharmaDev) and two physical chemistry teams (CEMES and LPCNO). The ICT shares heavyweight equipment, available to the scientific community of Toulouse and a team of 20 engineers and technicians contribute to the powerful research platform, which provides an efficient support to research teams. The ICT platform is also developing new methodologies to meet the ever demanding needs of researchers.

The scientific teams of the ICT cover virtually all areas of chemistry, ranging from very basic studies to more applied aspects, and research at the interface of physics and biology.

To better understand this research activity, which aims to be at the highest international level, we can highlight four major recent advances:

>>> The team in charge of the ICT platform

New concepts, hetero- and organometallic-chemistry.
This research area aims to develop highly reactive molecules, based on original concepts, opening new perspectives in many areas, including synthesis and catalysis.

Supra- and macromolecular chemistry.
This area aims to develop new giant well-defined molecules, self-organization of molecules and polymers that have unique physical and biological properties with important future applications.

Interface between chemistry and physics.
This area aims to build new objects (molecules, molecular materials, nanoparticles) and develop their physical properties.

Chemistry for health.
This area aims to synthesize new biologically active molecules and study how they act.

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ICT: Institut de Chimie de Toulouse / Institute of Chemistry of Toulouse

LHFA: Laboratoire d'Hétérochimie Fondamentale et Appliquée/Laboratory for fundamental and applied heterochemistry

IMRCP: Laboratoire des Interactions Moléculaires et Réactivité Chimique et Photochimique/ Laboratory of Molecular Interactions and chemical and photochemical reactivity

LSPCMIB: Laboratoire de Synthèse et PhysicoChimie des Molécules d'Intérêt Biologique /Laboratory of Synthesis and Physical Chemistry of Molecules of Biological Interest

PHARMA-DEV: Pharmacochimie et pharmacologie pourle développementMedicinal Chemistry and Pharmacology Development

CEMES: Centre d'Elaboration de Matériaux et d'Etudes Structurales/ Center for Material Elaboration and Structural Studies

LCC: Laboratoire de Chimie de Coordination/ Coordination Chemistry laboratory

LPCNO: Laboratoire de Physique et Chimie des Nano-objets/ Laboratory of Physics and Chemistry of Nano-Objects

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The Interface with Physics

>>> Azzedine BOUSSEKSOU, CNRS senior scientist at the Laboratoire de chimie de coordination (LCC, joint CNRS/UPS lab)

For several years, research at the interface between chemistry and physics has advanced dramatically: molecular magnets, conduction and molecular bistability are new areas, to name but a few. The materials developed in the Toulouse laboratories have already led to more than fifty patents, showing that chemistry in Toulouse can lead to a wide range of applications for society.

The convergence of chemistry and physics has spawned a multitude of functional molecular assemblies including single molecule commutation. Researchers at CEMES have demonstrated for the first time a reversible conformational change between two stable states of a copper complex adsorbed onto a Cu(111)/NaCl surface, induced by a tunnel bias. The molecular bistability in these systems stems from the rearrangement of the coordination sphere surrounding the metallic ion induced by the storage of a single charge. This system can be considered as a new single molecule electro-mechanic actuator.

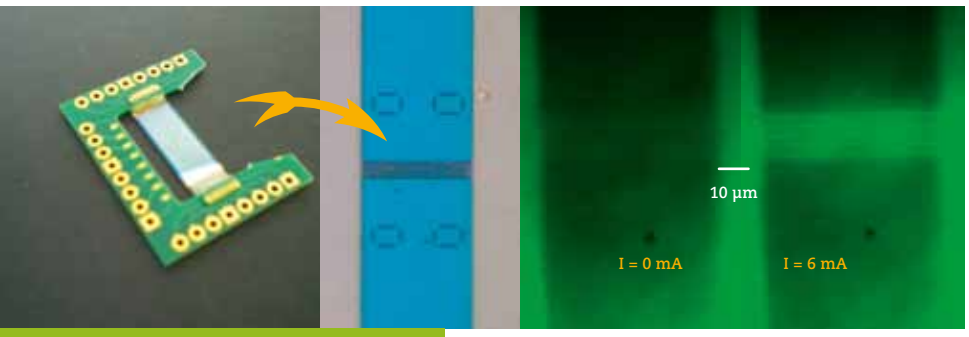
Materials with variable porosity

A second research area concerns the related fields of molecular magnetism and coordination chemistry. Porous, supramolecular magnets are being constructed at the LCC. The characteristic properties (critical temperature, coercive field) of these three dimensional architectures can be significantly modified by adsorption of guest molecules in the network. This approach to assembling molecular building blocks has also been applied to the synthesis of supramolecular or fluorescent materials with variable degrees of porosity.

The specificity of organometallic chemistry allows for a high level of synthetic control over the morphology of nanoparticles (Nps). As a consequence, preparations of such Nps in powder or colloidal suspension may be integrated into devices for a variety of applications. Thanks to the development of impeccably controlled syntheses, it is now possible to modulate the physical properties of Nps, for example by modifying their surface chemistry. This rewarding collaboration between chemistry and physics enabled the use of these Nps in various domains, including varistance, gas sensing, integrated induction, microelectronics and magnetic information storage. There is also great potential for these materials in biological applications such as MRI and biosensing.

Fully Molecular Devices

Electric transport of conducting and molecular wires is an emerging area of research, and one in which the laboratories of Toulouse are very active. The ultimate goal is to produce "all molecular" devices. Thus, following the discovery of molecular supraconductivity a few years ago at the LCC, researchers are today interested in the development of thin films or Nps based on molecular conductors/supraconductors. Recently this aim has culminated in a spectacular result: the observation of a supraconductive transition in thin films, previously only observed in single crystals. Furthermore, the Nps of these conductors are currently employed in the development of composite materials with applications in the electromagnetic protection of satellites. Finally, a novel approach for thermal imaging by micro- and nano-thermometry based on spin crossover molecular materials has been recently developed and patented. The concept is grounded in the design of hybrid materials that combine optical bistability and fluorescence. This approach has led to the creation of micro-and nanometric hot spot cartographic devices with high spatial resolution, opening important avenues for exploitation in microelectronics and biology.



>>> Electronic device including nickel microwires covered by fluorescent doped spin crossover Nps before (low spin state) and after (high spin state) the application of a bias of 6mA. Clearly, the fluorescence intensity of the fluorophore is modulated by the spin state of the material.

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Chemistry and Health

The development of new molecules of biological interest is one of the main scientific strengths of the Institute of Chemistry research programs at Toulouse. Both natural and synthetic molecules are being developed for applications in medicine, diagnostic imaging and bioanalysis. This research is based on strong and diverse skills, ranging from synthetic organic chemistry to mechanistic studies, basic methods of bioinformation technology and bioimaging and analysis.

>>> Michel BALTAS, CNRS senior scientist, head of the Laboratory of Synthesis and Physical Chemistry of Molecules of Biological Interest (LSPCMIB, joint UPS/ CNRS lab)

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Natural products and synthetic molecules

The PNASM LSPCMIB team has designed original molecules inspired by natural cinnamoyl derivatives of phytochemical origin. The designed molecules were found to be active in the field of cardiovascular diseases and tuberculosis. The proper functionalization of the molecules was carried out through reactions that are compatible with automation as well. The features introduced in these structures give these molecules complementary *in vivo* properties (cytoprotection, carbonyl scavenger function), which place them among the most active of all known compounds against the formation of thrombotic plaques. The team also showed that other original chemical series can also be synthesized (via reactions compatible with automation) from cinnamic acid showing strong anti-tuberculosis activity, particularly against resistant strains.

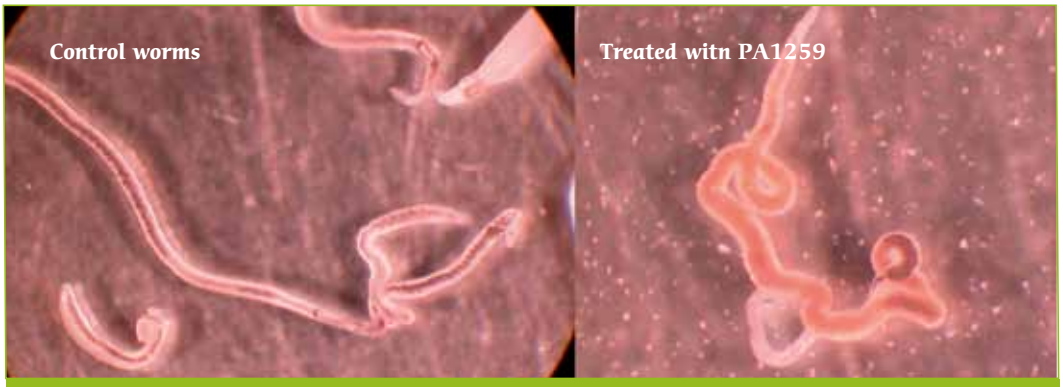
The "Metals in Biology and Medicinal Chemistry" team of the LCC has developed new inhibitors of *Mycobacterium tuberculosis* InhA, based on the core of the active metabolite of isoniazid, a major anti-TB drug (CNRS-UPS patent pending). The team also prepared promising compounds able to bind to quadruplex DNA, recently discovered as a target for cancer treatment, and binuclear complexes based on platinum and copper that are capable of producing non-repairable damage on DNA. These molecules are also excellent tools for understanding the mechanisms of cell survival. The work of the "Natural Substances" team at PHARMA-DEV conducted in Guyana on the traditional treatment of malaria has led to the isolation of a molecule that is active at all stages of the cycle of the malaria parasite (Plasmodium), something that has rarely been observed. The "Redstress" team at PHARMA DEV has discovered the indolones-N-oxide (radical scavengers) family of compounds that are active *in vitro* and *in vivo* against the parasite that causes malaria.

Mechanistic Studies

The PEP team of the IMRCP Laboratory is conducting research into the mechanisms of photosensitivity of biological targets through new sensitizers and photoactivatable probes for better therapeutic strategies. The team found that dihydropterines very efficiently trap singlet oxygen by being oxidized to pterins, compounds involved in important biological functions (immune responses) and diseases (depigmentation of the skin and sensitivity to UV radiation). In addition, the team identified the mechanisms by which complex polypyridyl ruthenium(II) compounds alter their reactivity with DNA in the presence of some proteins involved in cellular regulation. The "Chemical Biology" team at LCC has recently shown significant differences in binding copper(II) on human beta-amyloid peptide (directly linked to Alzheimer's disease) and in mice, where the disease does not exist. Teams from LSPCMIB, as well as LCC PHARMA-DEV, have several research programs studying the mechanisms of action of natural and synthetic biologically active compounds, particularly those with antitumor, antiatherogenic, antituberculosis and antimalarial activity. Finally, the "Metals in Biology and Medicinal Chemistry" team of the LCC has discovered new trioxaquines that are active against schistosomes parasitic worms. The action of these chemicals on the parasite hemozoin was confirmed by microscopy (photographs).

Diagnostic imaging, bio analysis

The "SOMAB" team in LSPCMIB (chemical, biological and medical imaging), has developed new molecules capable of complexing transition metals (Tc, Re), lanthanide ions (Gd, Eu, Tb, Yb), or related ions (In, Y). These metal complexes exhibit high stability in biological media, making them particularly interesting for applications in optical imaging, MRI or radionuclear imaging. In addition, the team has developed original



Schistosomes (worms responsible for schistosomiasis disease) controls and treated with trioxaquine. © J. Boissier

organic architectures where two different metals (Tc/Re, Gd/Re ...) can be complexed in a single structure , thereby leading to bimodal organometallic probes. These systems are useful for two distinct imaging modes (for example, Tc-99m/scintigraphy and Re/optical imaging) and can combine the advantages of each of the two techniques in terms of sensitivity and resolution for in vitro and in vivo use. Using micro- and nano-technology techniques, the Redstress PHARMA-DEV team has developed an integrated microfluidic device (lab on a chip) to work on very small sample volumes and integrate complex processes leading to portable systems for bioanalysis (sorting, counting cell subpopulations as markers of early disease). Finally, the "Nanostructures and Organometallic Chemistry" team at LCC and the "Sensors and Biosensors" team at LGC (Laboratory of Chemical Engineering) have designed new interfaces modified with electroactive nanoparticles as biomarkers of oxidative stress, with better properties in terms of sensitivity and selectivity.

Contributors to this article: Geneviève Pratviel (LCC) and Françoise Nepveu (Pharma-dev)

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headline

New Concepts, Main-Group and Organometallic Chemistry

The Toulouse site is extremely active in Main-Group and Organometallic Chemistry. The groups working in these two areas have a unique expertise in the design of highly reactive molecules and the establishment of new concepts, both leading to a wide variety of applications in synthesis, catalysis, materials, life sciences…

The various topics developed at the ICT and more particularly in the two laboratories, LHFA and LCC, are spread over four areas:
1) New concepts: highly reactive molecules (carbenes, ylides, low-valence main-group elements…) and new bonding modes (non classical metal/ligand interactions).
2) Activation of small molecules with some key targets: hydrogen, methane, carbon dioxide.
3) Catalysis: challenging reactions of industrial relevance such as hydroamination, methanol carbonylation, C-C bond formation via C-H activation, selective silylation and borylation, enantioselective catalysis, non conventional media (water, ionic liquids) and mild conditions.
4) Mechanistic investigation: to gain a better knowledge of any elementary step of a catalytic cycle, to characterize key intermediates, to determine kinetics and thermodynamics, to control and optimize selectivity and activity.

This research can only be performed thanks to the excellent ICT technical platform. Moreover a strong synergy between experimentalists and theoreticians is helping to rationalize the results and predict some new key targets.

Ylides and Main group elements: Stabilization of species bearing formal charges, and applications in synthesis

Phosphonium sila-ylides: the heavier congeners of Wittig reagents have been recently synthesized for the first time. They are highly reactive species exhibiting behavior similar to transition metal complexes, opening new perspectives in catalysis.

Low valent compounds: extremely active pi-systems

Compounds featuring cumulated P=C and Ge=C double bonds : a phospha-germa-allene. The presence of the main-group elements induces peculiar reactivity. Instead of the common 1,2-addition reactions, a 1,3-dipole behavior has been seen for acetylenic derivatives. Upon [3+2] cycloaddition, a cyclic phospha-germa-carbene is obtained. This derivative, which appears as a heavier analog of the carbenes isolated so far, has original properties.

>>> Pressure NMR tube (NMR = Nuclear Magnetic Resonance) for in situ monitoring of the catalyzed hydrogenation of benzonitrile.

Truly odd metal / ligand interactions: coordination of Lewis acids

While transition metals normally tend to surround themselves with electron-donating ligands, Lewis acids, archetypal electron-deficient moieties, have been shown to also behave as ligands to form coordination complexes. This umpolung (polarity reversing) behavior involves unprecedented interactions between the metals and the main-group elements (boron, gallium, silicon…) and leads to original geometric and electronic properties.

Hydrogen in catalysis and energy

Paul Sabatier, the father of the catalyzed hydrogenation process, received the Nobel Prize of Chemistry in 1912 and gave his name to the Faculty of Science, now belonging to the University of Toulouse. Almost 100 years later, hydrogen is still attracting a lot of interest in two main fields: catalysis and energy.

Two recent achievements at LCC illustrate this domain: Nylon synthesis is one of the most important industrial

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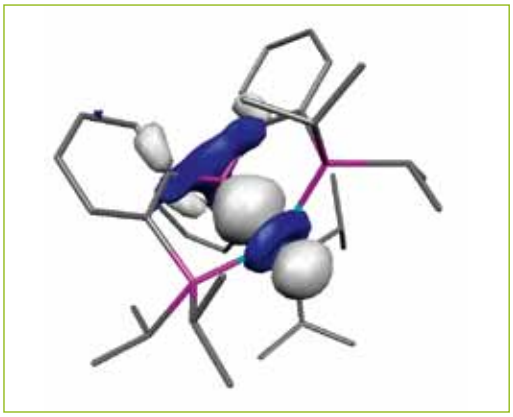
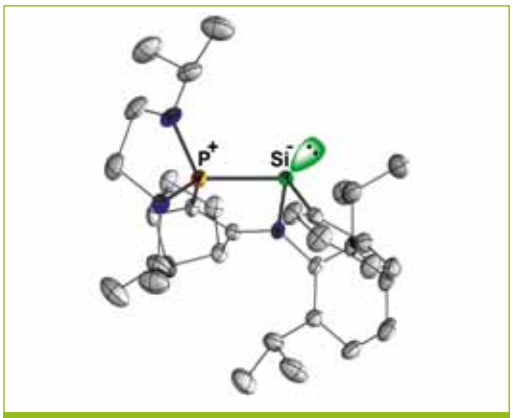
processes. As a key step, it involves hydrogenation of a nitrile function. Mechanistic investigation on a model substrate, benzonitrile, allowed us to develop a process that operates under mild conditions (room temperature and low pressure of H_2). The catalyst precursor is a sigma ruthenium complex which is able to coordinate dihydrogen in a reversible manner. The second example deals with the use of hydrogen as an energy carrier. Can we consider hydrogen as "the fuel of the future"? Again, sigma ruthenium complexes play a key role: ammonia borane (H_3NBH_3), an attractive molecule to produce H_2, can be dehydrogenated, and for the first time, aminoborane (H_2NBH_2), a very elusive compound, has been trapped and clearly identified as a key elementary step in the dehydrogenation process.





>>> *Bottom:* X-ray diffraction structure of a phosphonium sila-ylide. *Top:* Molecular orbital involved in the coordination of a Lewis Acid to a transition metal.

Methane functionalization

Methane is the main component of natural gas. A real breakthrough would be to functionalize this abundant molecule instead of burning it or just producing H_2. The C-H bonds of alkanes, and particularly of methane, are strong and difficult to activate. In the frame of an ERA chemistry program, the first catalyzed functionalization of methane into esters was performed under very mild conditions. The catalyst is a silver complex decorated with a highly fluorinated ligand, which makes it very reactive and soluble in supercritical CO_2, a crucial solvent for this reaction. It is a remarkable reaction whose mechanistic as well as selectivity properties are currently being investigated at LCC.

Hydroamination and atom-economy

The intermolecular hydroamination of non-activated olefins is another great scientific and economical challenge tackled by the chemists at Toulouse. It is an atom economical transformation (no by-product, no waste) to obtain amines, important industrial intermediates for the production of a vast array of consumer products. An efficient catalysis of this process by platinum complexes has been discovered and the detailed investigation of the catalytic mechanism will help us improve it.

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Supramolecular systems

>>> Monique MAUZAC, CNRS senior scientist, head of the Laboratoire des Interactions Moléculaires et Réactivité Chimique et Photochimique (IMRCP, UPS/CNRS). Montserrat GÓMEZ, professor at UPS, SYMAC team member at the Laboratoire Hétérochimie Fondamentale et Appliquée (LHFA, UPS/CNRS)

Making larger structures via low or high energy interactions, leads to a wide diversity of chemical systems or nanomaterials with various applications. Toulouse researchers are involved in several projects concerning chemistry at the nano- and micro-meter scales, that is, in the conception and study of chemical objects that are larger than a single molecule. As such, it has been recognized as a European research training site.

Carbon nanotubes and metallic nanoparticles

The molecular approach developed at LCC allows us to modulate the size and shape of metallic nanoparticles (MNP). These nanometric materials have applications in different fields, in particular catalysis. LCC and LHFA have made efficient nanocatalysts for hydrogenation (Pt) and C-C coupling (Pd) reactions. Indeed, the preparation of composite nanomaterials comprising metallic oxide nanoparticles in a silica matrix (by LCC), has led to the development of catalytic filters for gas sensors.
The complementary skills of these two labs have led to new catalytic systems assembling metallic nanoparticles and multiwall carbon nanotubes (MWCNT) exhibiting original catalytic properties. The pre-development for the production of these MWCNT has been developed at the LCC, in collaboration with Arkema and LGC. Tuning the surface chemistry of MWCNTs allows us to selectively introduce MNP into the inner cavities of MWCNTs or fix MNP on the MWCNT surface, leading to different catalytic behaviors. Selective and efficient catalysts have also been obtained by supporting catalytic ionic liquid phases on functionalized MWCNT. With regard to other areas, the SPCMIB lab in collaboration with CIRIMAT has developed the functionalization of double-wall carbon nanotubes (DWCNT) for biomedical applications (imagery, vectorization, implants for tissue engineering).

Supramolecular chemistry, ionic liquids

Supramolecular self-assemblies in which molecules interact with each other via low energy interactions are largely studied in the IMRCP laboratory, for example to develop "green" bioactive formulations. A key step in the development of a drug from an active ingredient is in fact the choice of the best formulation. A new concept was established by implementing so-called bioactive formulations, based on supramolecular self-organization in which the active ingredient is an amphiphile that reduces the number of ingredients in the final product. At the same time, specific therapeutic activity is achieved, thanks to the nature of the supramolecular self-assemblies formed, such as micelles. Several products have been developed, especially from active amphiphilic molecules derived from rhamnose. One of them, easily obtained from renewable resources (seeds from Brazil) and marketed by Pierre Fabre as Selectiose ®, can successfully treat many inflammatory conditions associated with skin allergies such as eczema. A second product, Effectiose ® has been recently marketed against acne.
Ionic liquids are salts often made up of an organic cation and an inorganic anion, liquids at room temperature and highly organized structurally. They have multiple properties: they are non-volatile, stable at high temperatures, non-flammable, good conductors, recyclable ... and can be used in a vast number of fields. The SPCMIB, IMRCP and LHFA labs are involved in developing and utilizing these new solvents, prepared from renewable sources and sustainable technologies. The labs are interested in new strategies for synthesizing molecules exhibiting biological activity and in auto-assembling molecules or amphiphilic polymers in ionic liquids. These solvents also allow for stable metallic nanocatalysts forapplications in organic synthesis (LHFA in collaboration with Solvionic).

Dendrimers, nano-engines, polymers

Dendrimers are branched, perfectly defined and highly functionalized macromolecules. They belong to the family of polymers because of their repetitive structure, but are synthesized layer by layer and not by polymerization. The presence of many terminal chemical functions that are easily accessible gives them unique properties. The LCC team is specialized in the synthesis and study of the properties of phosphorus dendrimers that have very diverse applications, from catalysis to biology/medicine. For detection and diagnosis, dendrimers bring an increased sensitivity, a perfect reproducibility and an excellent stability. The start-up DendrisTM created in 2009 at the Center Pierre Potter of the Cancéropôle of Toulouse, aims to produce "ready to use" diagnosis kits in the fields of health, agriculture and the environment.
Moreover, the application of near-field microscopy techniques (CEMES) has allowed the synthesis of

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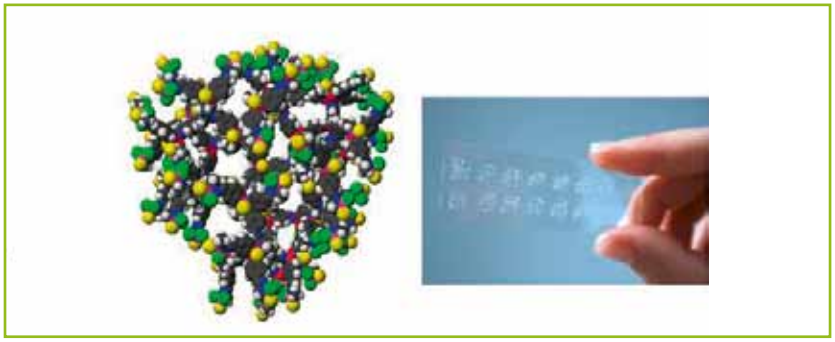

>>> from a phosphorus-based dendrimer to a Biochip @DENDRIS

molecular-devices such as rotors, motors, memories and logic gates.
In order to replace metal-based catalysts in polymerization processes, carbenes were recently developed and successfully employed as organocatalysts for the synthesis of silicones and polyurethanes. Following the same trend, sulfonic acids were shown to catalyze the polymerization of cyclic monomers. The resulting biodegradable polymers with a controlled size could be incorporated into more complex macromolecular architectures. All these research projects are backed-up by industrial partners (Rhodia, Arkema, Bluestar Silicones, Map). The RAFT/MADIX controlled radical polymerization process (LHFA, Rhodia funding) is an alternative synthetic strategy that can yield well-defined functional copolymers with controlled architectures. It exploits xanthates as reversible chain transfer agents. Other methods (LCC) based on organometallic chemistry (reversible cleavage of a metal-carbon bond) are suited for the control of "difficult" monomers and help extend the range of available technologies.
Polymers can be considered either as bulk materials or as a matrices for making composites. Inorganic nanoparticles, with controlled geometry and size, can be incorporated in the polymeric medium or formed in situ (IMRCP, LHFA, LCPNO). The obtained materials possess properties that can be modified by light, temperature, solution acidity, magnetic fields ... Materials from a liquid crystalline polymer matrix and cobalt nanoparticles have been synthesized that respond to very low 50 mT magnetic fields at room temperature. Block copolymers (IMRCP, LHFA) were obtained in order to stabilize metal particles or for applications such as photodynamic therapy used for cancer treatment. Copolymers bearing small DNA parts are also interesting nano-objects with recognition properties that can be used in biochemistry. Lastly, a study by the InNaBioSanté foundation (IMRCP, LAAS), aims at detecting cancerous biomarkers using an electronic device containing an imprinted polymer and a detection process.

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Research at Paul Sabatier University

Research at Paul Sabatier University is spread across 62 laboratories, most of which are joint labs with the CNRS, INSERM, IRD, INRA and CNES.
2550 researchers and assistant professors, and 1200 technical and administrative staff work in these laboratories.
1600 PhD students are enrolled at UPS, in 11 doctoral schools of which 6 are run by UPS.

The four main poles of research are:

> **MST2I** (Mathematics and Science and Information and Engineering Technology): 9 labs and 5 federations
> **UPEE:** (the Universe, Planet, Space and Environment): 7 labs, 1 observatory
> **SM (Materials Science):** 12 labs and 2 federations
> **SV (Life Sciences):** 26 labs and 5 federations

To these four major poles, add the **CIGEDIL** (Communication, Information, Management and Languages Didactics): 3 labs and one federation

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