

Chemistry

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The strategy adopted by the Department aims to maintain a high level of expertise on the synthesis of inactive and radioactive compounds with impact on health, materials science and catalysis, allied to a wide range of specialized characterization techniques. The development and the application of nuclear and related methods, including chemical characterisation, light isotopes and absolute dating, to environmental studies and cultural heritage is also a major field of research in the Department. The activities of the Department are organized in five areas:

Solid State – the group focus its research activity on new materials with unconventional electrical and magnetic properties. The group combines a high expertise on preparative chemistry of molecule based conducting and magnetic materials and of intermetallic compounds with a wide range of specialized solid state techniques. A significant achievement of the group during 2004 was the enlargement of the study of the first series of isostructural spin ladder systems. Research on borides with interest to thermoelectric applications was other field of special relevance this year.

Inorganic and Organometallic Chemistry – the group is concerned with the synthesis, characterization and chemical reactivity of *4f* and *5f* compounds. Gas-phase ion chemistry studies of the actinides (An) by FTICR/MS were pursued. The work was now extended to Pa and for the first time the “bare” protactinyl, PaO_2^{2+} , was observed. Electron-transfer reactions of uranium(III) compounds showed to be a synthetic way to uranium (IV) and uranium(V) compounds. The oxidative coupling of methane (OCM) with a heterometallic lanthanide oxide, Eu-Ca-O, using CO_2 as oxidant agent, was achieved with the best yield and selectivity reported until now.

Inorganic and Radiopharmaceutical Chemistry – the research of the group is focused on the design, synthesis and characterization of novel specific radiopharmaceuticals for non-invasive molecular imaging and/or therapy. During 2004, new halogen – based radiotracers have been synthesized and evaluated as ER binding radiopharmaceuticals. Concerning metal-based radiotracers, the coordination of novel bifunctional pyrazolyl containing chelators to $-\text{[M}(\text{CO})_3]^+$ (M=Re, Tc) moieties was studied. Some of these chelators have been tested with success for the labelling of tumor-seeking peptides and for preparing complexes potentially useful as DNA metallointercalators.

Environmental Analytical Chemistry – the research is focused on *Instrumental Analytical Chemistry, Environmental Geochemistry, Isotope Hydrology And Archaeometallurgy*. During 2004, activities running under externally financed (FCT, IAEA) research

projects were enlarged by the approval of some new projects (6) in Earth Sciences, Isotope Hydrology and History and Archaeology. New studies were initiated in sedimentary geochemistry of lagoons, estuaries and interdune depressions of the SW coast and related watersheds and in the use of light isotopes ($\delta^{13}\text{C}$, $\delta^{15}\text{N}$ and $\delta^{18}\text{O}$) in organic matter as tracers of shelf sediments.

Cultural Heritage and Sciences – Geochemistry of the earth surface, mineralogy and absolute dating are the main research domains, applied to archaeometry, built patrimony and environmental geology. During 2004 an important increase of projects concerning archaeological ceramics of a wide range of chronologies, dating and geological materials occurred. This reflects an important feedback of the scientific community to the exertion made during the last years by the group, at a national level in these research fields.

To pursue these objectives the groups develop and maintain the best possible in-house capabilities: specialized solid state physics techniques, facilities for manipulation of radioactive compounds, FT/ICR mass spectrometry, instrumental neutron activation analysis, EDXRF spectrometry, two absolute dating techniques: radiocarbon and luminescence, and a tritium dating unit and an elemental analyser coupled to one of the two mass spectrometers for light isotopes. Five new projects headed by the Department were approved this year in the context of the National Scientific Infrastructure Programme. These projects will allow the acquisition of an INAA gamma-spectrometer with sample changer, a single grain luminescence reader, a SQUID magnetometer, an ICPMS, and an ESI-QITMS.

A major effort of the Department has been the education and training of young scientists. Undergraduate, MSc, PhD and Post-doctoral students account for roughly 50 % of our work force. Training of students and professionals of health is also undertaken due to our specialized existing facilities. Researchers of the Department have been involved in advanced training activities in collaboration with the university and in the context of international networks. A MSc course in Biomedical Inorganic Chemistry organized in collaboration with the university started this year.

These activities have been funded mainly by research projects supported by the Portuguese Science Foundation (FCT) and the European Commission, and by Protocols, Contracts and Services established with other private or public institutions and industry. During this year the main investment supported by ITN was the construction of a laboratory for animal experiments.

Structure of the Sector and Technical staff

Research groups in the Chemistry Sector

- Solid State
- Inorganic and Organometallic Chemistry
- Inorganic and Radiopharmaceutical Chemistry
- Environmental Analytical Chemistry
- Cultural Heritage and Sciences

Administrative and Technical staff

- E. C. FLORES
- M. F. MARQUES
- P. M. REIS
- M. F. CABRITA