S

HUMAN RESOURCES AND MOBILITY (HRM) ACTIVITY

MARIE CURIE ACTIONS
Marie Curie Conferences and Training Courses

Series of Events (SCF)

and Large Conferences (LCF)

Project
" XX-IUCR FLORENCE "

B1. SCIENTIFIC QUALITY OF THE PROJECT *(MAXIMUM FOUR A4 PAGES)*

Crystallography, as "science that studies the regular shape of natural crystals", is with astronomy one of the oldest sciences. In fact, minerals and precious stones have long challenged human minds for the attractive symmetry and reflecting properties. Modern crystallography, however, has a more fundamental role as "science that determines the structural aspects of matter at the atomic and molecular levels and predicts properties and behaviour". Few other basic scientific discoveries have had wider applications than X-rays and the laws of their diffraction from crystals (Nobel prizes to Roentgen, von Laue and W. and L. Bragg, in 1901, 1914 and 1915, respectively). In less than a century, scientists have been able to understand the underpinnings of many fundamental processes, which occur in both living and unanimated entities and are strictly related to the three-dimensional atomic structure. Beside the analysis of organic, inorganic and mineral crystals, the continuous development of experimental, theoretical and computational tools has allowed to study increasingly complex systems. Some examples illustrate what crystallography has meant for the progress of the whole science and of molecular biology, in particular.

L.C. Pauling (Nobel, 1954), from the observation of hydrogen bonding in the structures of aminoacids, inferred the α-helix configuration of the polypeptide chains in proteins. Confirmation came soon after from M.F. Perutz and J.C. Kendrew (Nobel, 1962), who determined the structure of the first proteins, haemoglobin and mioglobin. At the same time, the double helix nature of DNA was ascertained by F.H.C. Crick, J.D. Watson, M.H.F. Wilkins (Nobel, 1962) and R. Franklin. Remarkably, the structure determination of DNA required fibre diffraction experiments, thus showing how the crystallographic methodology extends beyond crystalline state. With similar tools, K. Ziegler and G. Natta (Nobel, 1963) established important relations between structure and properties of synthetic polymers. Structure determination of pharmaceuticals opened the route to rational drug design after the work of D. Hodgkin (Nobel, 1964) on penicillin and vitamin B12. Today, the progress in the field allows knowing the structural features of target receptors and, also thanks to genomics, there are new perspectives to tailor efficient medicines for individual needs. Another breakthrough was the determination of the first virus structure, namely the tobacco mosaic virus, TMV (A. Klug, Nobel in 1982), which was followed from many others. Today, the crystallographic techniques, combined with high-resolution cryo-electron microscopy, allow the study of bacteriophages (Tao et. al, 1998), ribosomes (Yonath, Seitz *et. al.*), etc. As another example, the nature of a complex

photosynthetic reaction centre was elucidated from J. Deisenhofer, R. Huber and H. Michel (Nobel laureates in 1988). Even the most recent Nobel prize in chemistry (2003) has been awarded to a crystallographer, R. Mackinnon, for the fundamental characterization of ion channels and the biochemical activity of cell membranes.

Crystal structures of families of related compounds are essential for the understanding of the principles of chemical bonding and reactivity. An example is represented by the boranes studied by W.N. Lipscomb (Nobel, 1976), while his pupil, R. Hoffmann (Nobel 1981), correlated stereochemistry and electronic structure through Molecular Orbital theory, in organic, inorganic and solid state chemistry. Further understanding of the finer chemical and physical properties took place with the experimental determination of charge, spin and momentum densities, thanks to the new techniques for measuring accurate diffraction data at low temperatures (area detectors, synchrotron radiation, etc.). The studies are strictly connected to the progresses in computational quantum chemistry. Parallel development has occurred in the field of ultra-fast electron diffraction and has allowed A. Zewail (Nobel, 1999) to monitor fast chemical reactions occurring in femtoseconds (10^{-15} sec.). In material science, another crystallographer, G. Bednorz (Nobel, 1987), opened the route to the interpretation of superconductivity and to its potential applications.

The rich production of the crystallographic research prompted, since 1965, the deposit of the results in databanks, which are now basic tools for all branches of science. The Cambridge Structural Database contains today about 300 thousands entries of organic and organometallic compounds. Similar importance has the Inorganic Crystal Structure Database (ICSD), which catalogues inorganic materials and minerals. Most impressive is the exponential growth of the Protein Data Bank (entries > 20.000) which supplies a sound structural basis for the development of proteomics. In illustrating the state of the art, those people, who provided the theoretical tools for straightforward structure determinations, must be mentioned. The basic “phase problem in crystallography” was solved by H. Hauptman and J. Karle (Nobel, 1985) with the application of statistical methods. After their seminal work, the “direct methods” were perfected to solve routinely small and medium size molecules and, today, they apply also to complex proteins, which hide the secrets of life. The latter task is also facilitated by the major improvements in crystallization techniques, the high technology of the new detectors, the availability of synchrotron radiation, etc.

The above are just a few examples of the contribution of crystallography to basic and applied sciences. The richness of interests does not affect the identity of crystallography as a science. The community is numerous (> 8000 researchers in at least 70 countries), solid and homogeneous thanks to the concerting role of the International Union. This started its activities in 1946, under the coordination of an international Executive Committee, and produces, since then, a series of prestigious publications (Acta Crystallographica, special volumes, technical manuals, *etc*.) for the diffusion and teaching of the discipline. Today, the cultural dissemination is guaranteed *via* web and related on-line technologies. Other institutional tasks of IUCr are the standardization of the methods, units, nomenclature and symbols, focusing on the relations between crystallography and the other sciences. The cohesion of crystallographers is testified, every three years, by the multitude of participants to the world congress (2500, on average). For this reason, the choice of the host town is a very selective procedure. The potential hosts must document their interest, competence, organizing capabilities, facilities, etc. Because of the alternation of the continents, Europe can host the congress not more than once per decade (an exception to the rule was for Geneva-2002 which replaced Jerusalem). To gain the nomination for 2005, the Italian crystallographic community has pledged itself since 1996 and in 1999 Florence won the nomination after competition with Nagoya (Japan). Beside all of the practical aspects faced by the local organizers, a committee of 23 international experts, covering all branches, is at work to set up the scientific program of the XX IUCr Congress within the summer of 2004. There will be more than 500 speeches (subdivided in about 30 keynote lectures and 100 microsymposia) to focus on the achievements as well as on the new trends in crystallography. General topics will be the experimental techniques, the methods for structure determination also from powders, the structure-properties relationships, crystal engineering, crystal growth, structural characterisation of materials, polymorphism and isomorphism, structure at extreme temperatures and pressures, crystallography and mineralogy, nanomaterials, life-science, etc. To provide an idea of the excellence and variety of the program, we report here a provisional list of subjects: 1) Aperiodic crystals (quasi crystals and incommensurate crystallography). 2) Biological Macromolecules (crystallography of proteins and its role in elucidating biological mechanisms. The 2003 Nobel Laureate, R. Mackinnon will be invited for a keynote lecture). 3) Charge, spin and momentum densities (combination of X-Ray and electron diffraction methods with quantum chemistry to analyse chemical bonding and properties). 4) Powder diffraction (synchrotron and neutron sources for academic and industrial applications,

e.g. structure solution, nano-materials, drug design, mining and mineral processing, environment, forensic science, astrophysical studies, etc.). 5) Small Angle Scattering (high resolution tomography and 3D visualization methods). 6) Structural chemistry (basic relations between structure, properties and reactivity; the Nobel Laureate R. Hoffmann will highlight achievements and perspectives). 7) Synchrotron radiation (micro-diffraction, inelastic X-ray scattering in biology). 8) High pressure (new materials also of biological relevance, liquids and amorphous systems; crystallography at conditions of earth- and planetary interiors). 9) Electron diffraction (cryo-microscopy in biological applications and diffractive imaging with electrons and X-rays. To illustrate the latter theme, A. Zewail, Nobel 1999, will be invited. 10) Inorganic and mineral structures (structure/properties relationships in minerals and compounds of technological interest). 11) Neutron scattering (functional materials for biological, fuel cell, battery and geo-science applications). 12) Crystal growth and characterization materials (materials for the storage and conversion of energy; in situ characterisation during crystal growth). 13) Crystallographic computing (advances of the methods in protein crystallography, powder diffraction, quasi crystals and incommensurate structures, charge density studies, structure prediction, etc.). 14) XAFS (complementary information from the combination of x-ray absorption and classic absorption (EXAFS)). 15) Some topics of interest, also for the general public, concern the impact of crystallography on everyday life. A microsymposium on the techniques for diagnosis and preservation of cultural heritage seems particularly adequate for Florence as well as another one on the beautiful and symmetric nature of crystals and their impact on art. A third special session will be devoted to the usage of X-rays techniques in forensic medicine. 16) Nobel laureates, such as Karl, Hauptman, Huber, Michel, Deisenhofer and others, will be invited for a session where young people meet the founders of modern crystallography (tentative title: Inspiration for the future from the lessons of the past).

Finally, to testify the inter-sectorial character of crystallography, there will be a large industrial exhibition, not only devoted to highly sophisticated and new scientific instrumentation, but also to illustrate the potential applications of crystallography in everyday life. Near to the congress, two satellite meetings will be hosted in renowned University towns of Tuscany (Siena and Pisa), one of which on computational crystallography and the other on powder diffraction. These schools, by exploiting the attraction of the congress, will offer another chance to young people to learn about frontier areas of crystallography and, more in general, of science. Packages to facilitate the participation to all of the subsequent events will be offered.

B2. QUALITY OF THE RESEARCH TRAINING *(MAXIMUM THREE A4 PAGES)*

Crystallography is multidisciplinary by all means and, since its birth in 1946, IUCr pursues the dissemination of the crystallographic knowledge worldwide. Mastering the art of determining the 3D structures is a decisive step for understanding the properties of any materials and foreseeing their applications in disparate fields. On the other hand, teaching crystallography is not a trivial task. It requires that a delight for the usage of the method is inspired to the student together with the awareness of the potential applications which are relevant in many fields of science and technology. The training aspects have always been highly emphasized at IUCr congresses. In general, any scientific conference provides some spin-off for older and younger researchers but this is particularly true for crystallography, given its multidisciplinary and inter-sectorial character. In a single event, the participant has the unique opportunity of gaining a broad overview of many different frontier areas of science and, in particular, the young researcher has a chance to orient himself for his future commitments. At the congress, he can make direct comparisons between different branches of science under the unifying light of the crystallographic structural approach. Moreover, the contacts with the numerous representatives of industry attending the meeting can prompt careers other than the academic one. As a matter of fact, IUCr conferences traditionally host large exhibitions of the most modern apparatuses. Normally, several dozens of companies present their products and provide detailed and personal explanations to any interested person. The latter is a non-secondary aspect of training, as the direct evaluation of new technological performances is very inspiring. Back home, the congress attendees can orient the future acquisitions of scientific apparatuses by their own institutions. For all the above reasons, IUCr encourages the presence of young people by bestowing considerable funds to cover their expenses. Also, the Florentine organizers are strongly committed to find additional resources for a higher number of travel and staying scholarships. The present, as well as other applications to national and international institutions, shall favour the participation of PhD students and postdoctors who could hardly obtain any other support.

Here, we wish to illustrate how the educational aspects are privileged by IUCr under the coordination of the *Commission on Crystallographic Teaching.* IUCr journals, since 1946, have published many seminal papers which have opened new trends in research. Also the number of books published by IUCr is impressive. Above all, we mention the fundamental International Tables of X-ray Crystallography, which are the crystallographer’s bible for their highly specialized contents of symmetry theories, mathematics, physics,

chemistry, etc. Moreover, many textbooks for chemistry, physics, biology, etc. dedicate entire chapters to the relevance of the structural methodologies. IUCr is also very sensitive to the modern dissemination tool, represented by the web. Its and other crystallographic websites are of the highest quality and are intensively consulted especially by students and young researchers. Over the years, there has been also a flourishing of meetings with educational aims, workshops and schools on crystallography worldwide (amongst the latter, the famous schools in Erice). Beside such a seminal activity, the Congress is the top appointment promoted by the Union, not only for encouraging the exchange of ideas but also for promoting the diffusion of crystallography. Since the first Congress at Harward (310 participants), the registrations have grown dramatically (up to 3000 in Moscow, 1966), in particular those of the young attendees.

Specific actions are planned by the Florentine organizers to increase the impact of training at the congress. Beside a scientific program of absolute excellence, many initiatives will be devoted to attract the interest of students and young researchers and to enhance their role as participants. For instance, each of the 98 micro-symposia will consist of five speeches. Each chair and co-chair will invite four renowned scientists while a fifth one will be selected between the submitters of the abstracts. The latter will be recommended to be a young promising researcher. Also, the poster session is expected to be quite large with up to 2500 contributions. Prizes will be awarded to the best presentations and there will be extra bonuses for the younger people. Moreover, a series of informal workshops and demonstrations will be held during the Congress. For instance, it is well known that successful crystallographic research requires an exceptional computing power, both in terms of hardware and software resources. The authors of the most famous software packages will be available to make demonstrations in hands-on sessions, held in rooms equipped with computers and workstations suitable to the purpose. Analogous training sessions will be held by many manufacturers of crystallographic equipment at the exhibition stands. Also relevant for training are the satellite meetings (Siena, Pisa) on crystallographic computing and powder diffraction, immediately before or after the Congress. Young researchers will be encouraged to attend more events with the offer of special packages. Another intended feature of the XX IUCr Congress, will be an unprecedented convention of Nobel laureates. A special session is planned to favour the meeting between these scientific authorities and an audience made mainly by young people. These will ask questions about a successful research and its best

approach. Together with the keynote lectures, this special event will have a "virtual" access through the web. Also remotely located researchers will be able to forward their questions interactively.

Under the 6th Framework Program, the European Commission plans to support with financial contributions both Series of Event and Large Conferences. In spite of the smaller budget reserved to the latter action, the present initiative deserves full support. In fact, the nature of the IUCr Congress is unique for bringing together scientists, who preferentially participate in highly specialized meetings, but share on this occasion their interests with a much broader community. The Congress meets all the requirements to be considered one of the most relevant Large Conferences organized in Europe for size, scientific quality, multidisciplinar and inter-sectorial characters. Moreover, the event has real international dimensions, since crystallography is a science cultivated even in less favoured countries. In this respect, applications from members of the latter (especially the younger ones) will be given special attention.

The variety of disciplines on stage will help the career orientations of young participants. For instance, the invited speakers, expert in one specific discipline, will be asked to outline the important connections between neighbouring areas of research to give an important added value to the young listener. On the other side, the presence of industrial companies with their research personnel will enhance the inter-sectorial character and will stimulate commercial promotions and recruitment possibilities. The chances to contact new and interesting people at the congress are countless and new collaborations may start. To favour the latter, the poster, lunch and exhibition spaces will be adjacent, thus allowing continuous interaction, discussion and exchange of ideas between the senior and younger participants. Quite often in the past congresses, young researchers established a direct contact with firms producing crystallographic apparatus and could start an industrial or management career. Indeed, most of the researchers working in the crystallography related industries come from academic schools, where they were trained by renowned crystallographers.

B3. QUALITY OF THE HOST(S) (MAXIMUM ONE A4 PAGE PER PARTICIPANT)

Dr. Carlo Mealli is Research Director at ICCOM-CNR of Florence. In 35 years of career, he has published 200 publications in international journals mainly dealing with the relations between structure and chemical properties of inorganic and organometallic compounds. Also, he has been involved in many professional activities being in the boards of Associazione Italiana di Cristallografia (AIC) and of Italian Chemical Society. He has organized schools and conferences at national and international levels. In Florence (1994), he chaired the international Symposium on “Reaction Mechanisms Involving Transition Metals” (with 300 participants and a top quality scientific program). C.M. was a member of the Program Committee of the XXXIII ICCC (Cordination Chemistry, Florence, 1998) with about 1800 participants. In Parma, 2001, he chaired the national AIC congress. In San Feliu (Spain 2002), C.M. was vice-chair of the Euresco Conference in Inorganic Chemistry and he is appointed as the chair of the next event, later this year. C.M. has organized series of bilateral meetings such as the Italian-Israeli on crystallography (1987, 1992 and 1995) and the Italian-Korean on Inorganic Chemistry (1998, 2000 and 2003).

C.M. pursues the organization of the XX IUCr Congress since 1996 and, in Glasgow (1999), he obtained the nomination of Florence after competition with Nagoya (Japan). In his presentation, C.M. focused, not only on the appropriate competences for hosting such a major event but also on the unique tourist attractions of the town. A team of local organizers (about 15, about 50% women) is formed by expert crystallographers of CNR and the Universities of Florence and Siena. Important charges are taken by Paola Paoli (chair of the committee), Patrizia Rossi (secretary) and Annalisa Guerri (responsible for fund raising). A company (Newtours), which boasts long experience in organizing large conferences, has been engaged. The support of all the Italian crystallographers is assured for important tasks, such as processing of the abstracts and other issues. Some Italian colleagues have important charges in IUCr (Davide Viterbo, member of the Exec.Committee), Giuseppe Filippini, (secretary of the European Crystallographic Association) and Paola Spadon (president of AIC and permanent secretary of the International School on Crystallography in Erice). In the year 2003, Dr. Mealli has nominated a committee of 22 international experts in all areas of crystallography to set up the scientific program of IUCr-XX. The program will be discussed next June in Erice and later submitted for the Executive Committee approval (August 2004).

CURRICULUM VITAE AND PROFESSIONAL ACTIVITIES OF DR**. CARLO MEALLI**

Personal Data: Birth Date: June 11, 1946. Married, two children.

Education and Career: Doctor degree in Chemistry at Università di Firenze (1969). 1972 (July) → present: Researcher of CNR and, since 1991, *Dirigente di Ricerca (Research Director).*

Experience: C.M. made numerous training stages abroad: 1) University of Washington, (1970, with E. C. Lingafelter). 2) Northwestern University (1974 with J.A. Ibers). 3) Cornell University (1980, 83, 85 with R. Hoffmann, Nobel Laureate). 4) Universities of Osaka (1985), Deakin (Australia, 1991), Northwestern (1992), Leipzig (1995 and 2001), UNS (Argentina, 2001), Sevilla (2001), Strasbourg (2003). In the latter and in Italian universities, he has taught monographic courses on the relations between structure and bonding. He has lectured in prestigious universities and has been plenary and section lecturer at international meetings. C.M. has been the leader of research units in national and international projects and cooperates with research groups in Italy and around the world (Germany, Portugal, Spain, Mexico, USA, Argentina, etc.).

Professional Activities: Elected member in various boards of Italian Chemical Society, AIC, ECA, etc.. Representative of CNR at IUCr. C.M. has organized numerous conferences and schools (see previous section). Since 1997, C.M. acts as an evaluator of the European Commission (INTAS, Marie Curie, INCO programs). C.M. acts often as referee for renowned international journals of chemistry and crystallography.

Field of Scientific Interest: Structural and theoretical studies on chemical bonding and reactivity of inorganic and organometallic compounds. The two following approaches are pursued: i) Experimental structure determination by crystallographic techniques, ii) Theoretical quantum-mechanical MO Calculations (ehmo, *ab-initio, DFT*). C.M. is the author of the package CACAO for the theoretical analysis of bonding and reactivity. The package is freely distributed and used worldwide.

Five Recent Publications: 1) Baratta ; Mealli; Herdtweck; Ienco; Mason; Rigo. *J. Am. Chem. Soc*. **2004**, *126,* xx-yy. *"* Non Classical *vs*. Classical Metal···H_3C-C Interactions: Accurate Characterization of a 14-Electron Ruthenium(II) System by Neutron Diffraction, Database Analysis, Solution Dynamics and DFT Studies". **2)** Anillo; Díaz; García-Granda; Obeso-Rosete; Galindo; Ienco; Mealli *Organometallics*. **2004**, *23,* 471-481. "Structural and Electronic Rearrangements upon the Oxidation of Binuclear (Ru_2) and Trinuclear ($MoRu_2$) Complexes with Bridging *o*-Phenylenediamido Ligands". **3)** Barbaro; Ienco; Mealli; Scherer; Schmitt; Vizza; Wolmershäuser; Peruzzini *Chem. Eur. J*. **2003**, *9,* 5195-5210. "Activation and Functionalization of White Phosphorus at Rhodium: Experimental and Computational Analysis of the [(triphos)Rh(η^1:η^2-P_4RR')]Y Complexes [triphos = MeC(CH_2PPh_2)$_3$; R = H, alkyl, aryl; R' = 2 electrons, H, Me)". **4)** Grirrane; Pastor; Galindo; Ienco; Mealli; Rosa *Chem. Commun.*, **2003**, 512-513. "First example of a tetra-carboxylate bridged dimanganese species". **5)** Catellani; Mealli; Motti; Paoli; Perez-Carreño; Pregosin *J. Am. Chem. Soc,* **2002**, *124,* 4336-4346. "Palladium-Arene Interactions in

Catalytic Intermediates: an Experimental and Theoretical Investigation of the Soft Rearrangement between η^1 and η^2 Coordination Modes"

B4. MANAGEMENT AND FEASIBILITY *(MAXIMUM THREE A4 PAGES)*

B4.1 Organisational Management

The organization of the XX IUCr Congress is in progress since 1996. After a significant preparative work, the candidacy of Florence was presented at the General Assembly (Glasgow, 1999) on behalf of CNR, the University of Florence and AIC. Italian authorities (Major of Florence, University Rector, CNR president and the Ministers of Education and Foreign Affairs) signed letter of support. The proposal was convincing since the town won the competition with Nagoya (Japan). The main income for such an event will come from registration fees, the charges paid by the exhibitors and the sponsorships of various institutions. The overall cost is high; mainly due to the fees paid for renting the Congress Center. This structure, with a theatre for 2500 people and rooms for seven parallel sessions (the capacity ranging from 200 to 700 people) is adequate. Moreover, there is a number of smaller rooms for meetings, scientific demonstrations, internet-café, etc., while a large space will host the commercial exhibition (see more details below). Other major expenses are for travelling and accommodation of invited speakers, personnel, promotional activities, services, technological equipment, published materials, web site and facilities for on-line registration and submission of abstracts, etc. Moreover, important social events are planned (*e.g.* welcome party and banquet). It is estimated that the total of income/expenditure for all of the previous items will be about one million euros (based on a minimum of 2000 participants). Another important commitment of the organizers is to raise funds to favour participation of third country nationals. Although IUCr itself devotes $50.000 to the purpose, the budget is insufficient to support the expected large number of applicants. Thus, applications are made to national and international institutions (governments, research agencies, foundations, European Commission, etc.), including the present one. If the latter is granted, the funds will be distributed according to the MC LCF criteria, by privileging early stage researchers and by respecting the 30% ceiling for the third country citizens. Already, the participation of students is favoured by halved registration fees and other forms of support are reserved to third country participants. The organizing machine is already working at full stretch, with duties being equally subdivided between the Florentine organizers. The chairs of the scientific and local organizing committees (C. Mealli and P. Paoli, respectively) are assisted by an efficient secretariat (A. Ienco, P. Rossi), while A. Guerri is in charge for fund raising. The list of the local organizing committee members (about 15) may be found at http://www.iucr2005.it/. The congress web page has been created by

professionals and it is being constantly updated with practical and scientific information. Given the size of the event, the professional company Newtours SpA has been engaged. This boasts 20-year experience in managing large conferences in Italy and abroad and guarantees high level services also because, being on the spot, it can easily solve logistic and bureaucratic problems. The firm will manage hotel booking activities. Rooms for up to 4000 guests are reserved in hotels of various categories, at different prices. Importantly, more than 500 rooms have been reserved in the student dormitories of the University of Florence at a reasonably low cost (about 20€ per night). The preparation of the scientific program is already in an advanced stage. A Program Committee, with 22 international experts (see the names in the web page), will select keynote speakers and the topics for about 100 microsymposia (see the presentation in section B1). The program, set up by June 2004, will be finalized after the deadline for abstracts (March 31st, 2005). An important promotional activity is to reach potential sponsors and/or exhibitors with information about the congress. Promotional booklets have been sent to the firms which develop equipments, software, publications related to crystallography. Additionally, non-profit foundations have been contacted in Italy and abroad, to illustrate the role of crystallography in science and in everyday life and to stimulate their interest. Continuous contacts are maintained with IUCr and its President (Prof. W. Duax). Beside scientific sessions, the social events shall encourage reciprocal knowledge and promote new collaborations. Thus, joint refreshments and lunches during the working days will be set up. A welcome party will take place immediately after the opening ceremony, while a banquet will be organized in one of the last days. Also, some evening concerts are programmed. Since Florence has most renowned artistic and historical sites, guided tours to the important museums are planned. The congress site is Fortezza da Basso, an ancient military fortress. In the heart of downtown and next to the train station, the site is surrounded by hotels. Its capabilities are enormous, as confirmed by the size of the previously hosted events (e.g., the world conferences on AIDS and geology with 12 and 8 thousand participants, respectively). All spaces (about 60,000 m^2) are modular and rooms, poster areas, offices, etc. can be easily arranged depending on the needs. The facilities satisfy IUCr standards, as confirmed by its President. Feasibility and success of the Congress are guaranteed by a unique mixture of factors such as scientific quality, fame of speakers, multidisciplinary and inter-sectorial character of crystallography, focus on training aspects, facilities for younger participants, attractiveness of Florentine culture, high level tourist facilities, intensive social program, etc.

B4.2 Publicity and Selection

The Conference will be advertised by any possible mean (press, circulars, web site, *ad-personam* e-mail messages etc.). The Congress web site, created by professionals, is being constantly updated. Members of the organising committee are always present at all the international meetings of relevance. In Italy, the press and TV networks are properly informed and journalists will be invited to attend important sessions, especially those attractive for a wider audience (e.g., connections between crystallography and art, cultural heritage, forensic science, drug design, etc.). No selection of the participants will be made on the basis of gender, ethnic and religious origins, according to the regulations of the International Council for Science (ICSU). The availability of grants will be advertised in IUCr Newsletters (with a mailing list of about 15,000 scientists) and in many scientific journals. During the on-line registration and submission of the abstract, the eligible applicant can apply for a grant. The final selection will be elaborated by an international committee.

B4.3 Dissemination

The congress proceedings will be published in a book edited by the organizers and also as a supplement of Acta Crystallographica, edited by the IUCr. The abstracts will be available on the web site, two weeks before the event. A CD-ROM with a digital copy of the proceedings will be in the bag of any registered participant. Acknowledgments to all of the sponsors and supporting institutions (hopefully, to Marie Curie LCF), will appear in all Congress documents and boards. During the event, press conferences will be organized with the participation of the most prominent lecturers, especially the Nobel laureates. Such an action, opened to the wider public, will highlight the importance of crystallography and its impact on the everyday life.

B4.4 Financial Management

To favour a numerous participation of eligible researchers, the organizers plan to use the EU contribution mainly to cover their registration fee. For students, this is fixed at 270 euros and includes lunches and two main social events, one of which is a dining banquet. The corresponding regular fee (applicable to eligible experienced researchers) is 520 euros. By considering that the possible EU grant amounts to 50000 euros, the sum will be sufficient to support 130 early stage researchers and 28 experienced ones. In exceptional cases, the organizers could use the funds also to pay living and/or travel allowances for some eligible researcher. These costs will be properly justified and the total budget will be adjusted to the purpose. Consider, in this respect, that the lodging of one person at the student dormitory is about 20 euros per night.

B5. RELEVANCE TO THE OBJECTIVES OF THE ACTION *(MAXIMUM ONE A4 PAGE)*

Crystallography has wide interests across sciences and the IUCr Congress attracts scientists of different extraction and from all over the world. This appointment presents an unique overview of science. Topics in physics, chemistry, biology, material science, etc. are scattered in the program. Moreover, there is much interest from industry for the development of either the most sophisticated instrumentation (e.g. radiation sources such as synchrotron, new generation diffractometers, electron microscopes, etc.) or application tools (diagnosis of materials, drug design, etc.). These multi-disciplinary and inter-sectorial characters are rare for a single scientific event. Moreover, this cannot be hosted in Europe more than once in a decade, due to the round robin between different continents. Europe boasts an excellent tradition in crystallography as it has witnessed many seminal discoveries. Its crystallographers continue to be faithful participants of the IUCr congresses as, in the two most events, about 40% of the audience belonged to EU and Associated States. New European generations keep cultivating the discipline with enthusiasm and the congress will be a persuasive action in this respect. In fact, Europe will be at the centre of the attention, in particular of the many extra-european participants who will have the first chance of visiting Europe and establishing new contacts with its scientific community. An event of this size and relevance is an evident burden for the organizers, hopefully with some important benefit derived from the experience. Contacts with prominent scientists, industry representatives, managers of public and commercial institutions, European Union headquarters, etc. take place routinely. Since all the organizers belong essentially to the academic and research world, these new tasks are opening new broad horizons and enhance their managerial attitudes. The experience will be particularly precious for the younger members of the organizing committee (which includes about 50% of women) and it may be transmitted to any colleague who will assume similar responsibilities in the future. The dedication of the organisers may be rewarded also for other aspects. By becoming a reference point for hundreds of colleagues from all over the world, they will certainly gain a wide overview of the hottest scientific themes and of their best interpreters. These contacts may be fruitful also for the scientific activity especially of the younger persons in the committee. Thanks to this kind of activity, they will not only become familiar with the management of scientific events but also they will be trained as potential group leaders. Given the intention of the European Commission to assemble groups of scientific and managerial excellence, the latter educational aspects are of evident importance.

B6. ADDED VALUE TO THE COMMUNITY *(MAXIMUM ONE A4 PAGE)*

The IUCr Congress is a precious occasion for co-operation between research teams working in different areas and to promote the mobility of people and the exchange of ideas. Since the event will take place in one of the most renowned European cities, a large participation of European crystallographers is predictable also in view of the strong links existing amongst them. In fact, all the national associations are joined, since 22 years, in the European one (ECA) and all adhere to IUCr. The number of Europeans is always high at the IUCr congress (especially when set in Europe) also because the annual ECA congress is not held in the corresponding year. The strength and attractiveness of European crystallography are indicated by the requested incorporation in ECA of some extra-territorial associations (*e.g.,* Israel, South Africa, Morocco, etc.). The IUCr congress of Florence will highlight the quality reached by the crystallographic research in Europe and will be helpful to consolidate joint research programs with intra- and extra-European characters. Any big convention of European citizens is particularly important nowadays, when the political integration is becoming operative and a new constitution is being elaborated. The IUCr Congress will offer a unique opportunity for comparing directly the European scientific know-how with that of the rest of the world and a high degree of cross-fertilization will be enabled. The congress will have great attractiveness for third country researchers and will stimulate their willingness to be trained in Europe. The dissemination of our culture has great perspectives also from the political viewpoint. In fact, any short or long term interaction with our educational system may have a fruitful spin-off after the return home of the third country trainee. If, thanks to the education received, he will take important charges, he will privilege the relations with Europe. This aspect has been successfully pursued by America for many years and much less by Europe.

The attendance of some Nobel laureates, and likely of some future ones, will be adequately advertised in the media. They will be invited to press conferences or interviews to favour the public understanding of the discipline and its impact on every day life. Notice that some microsymposia (beside the highly specialized ones) are aimed to attract the interest of the public and to illustrate the importance of crystallography, not only for science but for the whole culture. As another point, organisers have as a priority that of offering equal opportunities in all respects. For instance, the list of speakers, the distribution of the student bursaries and so on will respect the equal distribution between genders.

B7. PREVIOUS PROPOSALS AND CONTRACTS

The present is a resubmission of a similar proposal (N. 504327, title: XX-IUCR FLORENCE, presented in 2003 to the same LCF action for the Mobility-4 program). The project was not financially supported in spite of a quite good evaluation of the referees (total score 87). Thanks to the useful suggestions of the latter, we think that the proposal has been greatly improved, especially concerning the training of young researchers. Their attendance is now clearly motivated from the intended actions; e.g., special training sessions (for software, instrumentation, etc.), dedicated meetings with the scientists who have made the history of crystallography, explicitly reserved opportunities to present oral speeches, usage of the virtual facilities for disseminating purposes, direct interaction with the world of industry and consequent perspectives for career.

Beside of an introductory part concerning the history and the impact of crystallography, the proposal illustrates the future perspectives in the various fields of science. In particular, the high quality contents of the scientific program will highlight the future developments and applications of this science, which has one of the most multidisciplinary and inter-sectorial characters.

B8. OTHER ISSUES (MAXIMUM TWO A4 PAGES)

There are no ethical or safety issues that may cause controversial matters associated to the contents of the IUCr Congress. As mentioned, IUCr is one of the 24 scientific associates of ICSU, whose basic mission is: *"To identify and address major issues of importance to science and society, by mobilizing the resources and knowledge of the international scientific community; to promote the participation of all scientists, irrespective of race, citizenship, language, political stance or gender in the international scientific endeavour; to facilitate interactions between different scientific disciplines and between scientists from 'Developing' and 'Developed' countries; to stimulate constructive debate by acting as an authoritative independent voice for international science and scientists."*

Although crystallography plays a basic role in biological studies and in the understanding of the molecular mechanisms that govern the processes of life, it must be stressed that it has no direct involvement in the experiments for the reproducibility of the latter. Thus, aside from any ethical consideration, it can be safely stated that no participant at the IUCr congress pursues any of the following goals: *i)* research activity aimed at human cloning for reproductive purposes, *ii)* research activity intended to modify the genetic heritage of human beings which could make such changes heritable; *iii)* research activity intended to create human embryos solely for the purpose of research or for the purpose of stem cell procurement, including by means of somatic cell nuclear transfer; *iv)* research involving the use of human embryos or embryonic stem cells with the exception of banked or isolated human embryonic stem cells in culture.

According to the links of IUCr to the above principles, the organizers and proponents of the present application have no drawback in answering NO to all of the questions raised in the following table that concern ethical aspects of the research involved.

Does the research presented in this proposal raise sensitive ethical questions related to:	**YES**	**NO**
Human beings		NO
Human biological samples		NO
Personal data (whether identified by name or not)		NO
Genetic information		NO
Animals		NO