

INTRODUCTORY REMARKS
(A brief description of the participating institutions
in the Seminar and scientific activities)

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The first Seminar on the Structure and Physical Properties of Crystals held in Barcelona (28 May to 1 June 1990) is a result of the agreement established between the Institut d'Estudis Catalans (IEC) and the Institute of Crystallography (Moscow) of the USSR Academy of Sciences (ICM), signed in Moscow in July 1989.

This specific collaboration agreement established the exchange of information and research work in the field of the structural analysis of crystals and the physical, biological and technical properties of crystalline materials; it also provided for the interchange of scientific staff working in crystallography; and the commitment to organize an annual seminar, one year in Catalonia and the following in the USSR, dealing strictly with problems of methods and results in the structural research carried out as part of this agreement, to be held at a high level of specialization and restricted to ten persons from each party.

The Seminar was organized by the Institut d'Estudis Catalans and Institute of Crystallography of Moscow with the help of different Centers of Barcelona which gave access to their laboratories and collaborated with some research papers. The addresses of all these Institutions are as follows:

Institut d'Estudis Catalans,

Carme 47, 08001 Barcelona; tel. (34-3) 318 55 16.

Institute of Crystallography, USSR Academy of Sciences,

Leninsky Prosp. 59, Moscow 117333; tel (7-095) 135 64 00.

Universitat de Barcelona,

- a) Departament de Cristal·lografia, Mineralogia i Dipòsits Minerals, Martí i Franquès s/n, 08028 Barcelona; (34-3) 402 13 43.
- b) Facultat de Física, Departament de Física Fundamental, Diagonal 647, 08028 Barcelona; tel. (34-3) 402 11 57.

Universitat Politècnica de Catalunya,

- a) Departament d'Enginyeria Química, ETSEIB, and Grup de Macromolècules, CSIC, Diagonal 647, 08028 Barcelona; tel. (34-3) 401 66 88.

Consejo Superior de Investigaciones Científicas,

- a) Institut de Ciència de Materials de Barcelona, Campus Universitari 1AB, Universitat Autònoma de Barcelona, 08193 Cerdanyola (Bellaterra); tel. (34-3) 580 18 53.

As this was the first institutional contact between most of the scientists of the centers concerned, some of the lectures were dedicated to explaining the composition, equipment and type of work of the Institutions. Professors Simonov, Solans and Subirana gave short lectures on the problems they have to obtain good research results with a normally limited budget which, in general, is a problem faced by all the research centers in the world. Effort and devotion on the part of scientists is the way to overcome the deficiencies of public support, and to obtain good results and new conclusions in the complicated problems of Science.

Professor B. K. Vainshtein, director of the Institute of Crystallography of Moscow and academician of the USSR Academy of Sciences, and Professor B. P. Sobolev, gave a lecture on their specific topics, proteins and the non-stoichiometry of fluorites.

The lectures and research papers offered at the Seminar were divided in three groups in accordance with their field: structure of crystals, methods and applications; non-stoichiometry and phases in fluorites and the crystal properties of superionic conductors; and macromolecules.

The first group (structure of crystals, methods and applications) started with the lecture by Professor V. I. Simonov, Assistant Director of the Institute of Crystallography of Moscow, on "Atomic structure and physical properties of crystals", in this he explained their advances in the techniques of accurate crystal structure analysis make it possible to establish regular correlations between the atomic structure and physical properties of crystalline materials; modern diffraction methods ensure not only a high accuracy of the determination of atomic coordinates but also provide

reliable data on atomic thermal motion, with allowance for both anharmonic and deviations from the harmonic law; structural analysis yields atomic mechanisms of phase transitions in crystals, as well as qualitative characteristics of isomorphous replacements in samples and the degree of structure perfection of a particular single crystal. During the lecture some results of structural studies of high-temperature superconductors, crystals with high ionic conductivity, ferroelectrics and some other crystalline materials were presented. This was a highly interesting lecture which was followed with great attention by those present, who asked the lecturer special questions at the end.

The following speakers were Professor X. Solans, Director of the Department of Crystallography, Mineralogy and Mineral Deposits, together with Professor M. Font-Altaba, who explained the situation of X-ray diffraction in our University in a lecture entitled "X-ray Diffraction and Crystal Structure at the University of Barcelona". The lecture included some problems arising in research and the complementary techniques used in laboratories, such as goniometry, optical crystallography and electron microscopy. It listed the journals in which papers have been published and the average number of publications per year.

Four research papers were presented orally: structure investigation of twinned crystals, integration of Patterson function in direct methods, the atomic structure of sillenites and retamine bromide.

The second group (non-stoichiometry and phases in fluorites and crystal properties of superionic conductors) began with the lecture of Professor B. P. Sobolev on "Non-stoichiometry in inorganic fluorides and phases with fluorite structure" in which he offered the results of the program of investigations carried out of over 200 phase diagrams of the MF_m-RF_n type systems, comprising fluorides of 27 metals, such as Na, K, Sc, Y, La and lanthanides, Zr, Hf, Th, U. Numerous non-stoichiometric phases (heterovalent solid solutions) with a specific, partially disordered structure, are formed in them. These phases crystallize mostly in two structural types: CaF_2 (49%) and LaF_3 (25%), retaining their single-crystalline form upon cooling. Fluoride non-stoichiometric phases, formed in MF_2-RF_3 and $MF-RF_3$ systems, are of special interest as they are a new family of inorganic fluoride materials with controlled defect structure and physical characteristics variable over a wide range. The main, at present and most promising directions for the practical application of fluorite grossly non-stoichiometric phases for technological purposes were considered.

Four research papers on X-ray and neutron diffraction studies, the association of point defects and the preparation of single crystals of multi-component fluoride materials and non-stoichiometry fluorite phases were

expounded orally and discussed. Another three papers on molecular dynamics simulation, structural features and intrinsic and impurity-induced structure disorder of superionic conductors were also orally presented and discussed.

Professor B. K. Vainshtein presented a very interesting lecture in the Institut d'Estudis Catalans on "Modern State and Perspectives of X-ray Crystallography of Proteins". He considered the aims and principal possibilities of the X-ray analysis of proteins; he gave a detailed description of the structure of *Lupinus Luteus leghemoglobin* and the mechanism of oxygen binding by this protein. Analysis of the structure of inorganic yeast pyro-phosphatase (*Saccharomyces cerevisiae*) has been carried out. High resolution structure study of five proteins in the family of specific microbial and fungal ribonucleases has been made. A description was given of the structure determination of complex proteins-catalases from various sources: *Penicillium vitale* (m. w. 290 kDa), *Micrococcus lysodeikticus* (m. w. 240 kDa), *Thermus thermophilus* (m. w. 210 kDa). The results obtained allow the mechanism of enzymatic reactions catalysed by these proteins to be explained. The lecture was attended by a large number of people who asked the lecturer questions concerning different points of his talk.

The third group (macromolecules) started with a lecture by Professor J. A. Subirana on "Research at the Macromolecular Chemistry Group in Barcelona" in which he established that the Macro-molecular Chemistry Group was created in the Department of Chemical Engineering of the Polytechnic University of Catalonia about twenty years ago as a joint venture with the Consejo Superior de Investigaciones Científicas, which has supported the group at various levels during this time. In this period about 230 publications have been produced and 41 students have obtained a PhD in the group. About 80% of them are now in academic positions. The group concentrates on structural studies such as electron microscopy, infrared spectroscopy, calorimetry and, more specifically, on X-ray diffraction. Several generations of collaborators have been access to pinhole and low angle cameras only available. The most recent acquisition is a GX-21 rotating anode generator provided with a Enraft CAD4 automatic diffractometer. The main lines of activity are: nuclear proteins, peptide models and their complexes with DNA; to improve knowledge of basic proteins it was decided to investigate several basic peptides in a systematic way, since very few of them had been previously studied; oligonucleotides, generally in fiber form, to understand nucleic acid structures; they have recently started with the determination of protein structures by X-ray diffraction; and several years ago studied the structure of polyamides which might have an intermediate conformation between classical nylons, which form sheet structures, and proteins, which often have helical structures.

He referred to the wholehearted dedication of his many colleagues, without whom the work carried out would not have been possible.

Five research papers were presented in this group, introducing the evaluation of "free energy" for non-covalent interactions in protein studies; crystallization and structure determination of an antibody; molecular structure of a dipeptide; oligonucleotide-protein complexes; and molecular and crystalline structures by X-ray diffraction with stereochemical restriction.

The organizing commission hopes that scientists found this Seminar interesting, and hope to meet the same interest at the II Seminar to be held in the USSR next year.

ABSTRACT

The Seminar was organized by the Institut d'Estudis Catalans and the Institute of Crystallography of Moscow. The Centres of Barcelona which gave access to their laboratories and collaborated with some research papers were: Department of Crystallography, Mineralogy and Mineral Deposits, and Department of Fundamental Physics of the Barcelona University; Department of Chemical Engineering and Group of Macromolecular Structures of Polytechnic University of Catalonia; Material Sciences Institute of Consejo Superior de Investigaciones Científicas (CSIC).

The lectures and research papers offered at the seminar were divided in three groups in accordance with their field: structure of crystals, methods and applications; non-stoichiometry and phases in fluorites and the crystal properties of superionic conductors; and macromolecules.

Professors B. K. Vainshtein and B. V. Sobolev gave a lecture on their specific topics, proteins and the non-stoichiometry of fluorites. Professors V. I. Simonov, X. Solans and J. A. Subirana gave a short lecture on the problems to obtain good results and new conclusions in their Institutes.