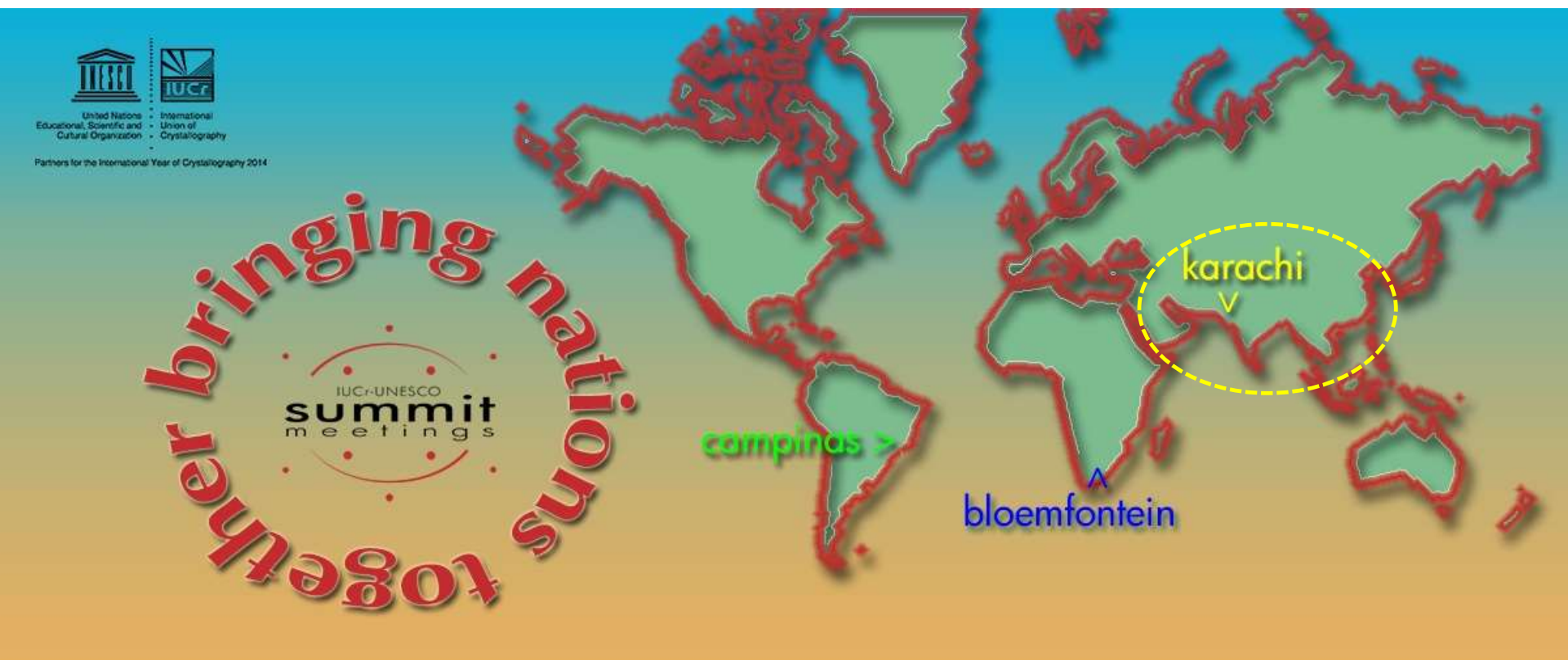




IYCr South Asia Summit Meeting

Vistas in structural chemistry



Dr. Maqsood Ahmed, Pakistan

5 years back....





2014

international year of
crystallography

IUCr-UNESCO

Karachi, 28-30 Apr 2014

summit
meetings

Vistas in structural chemistry



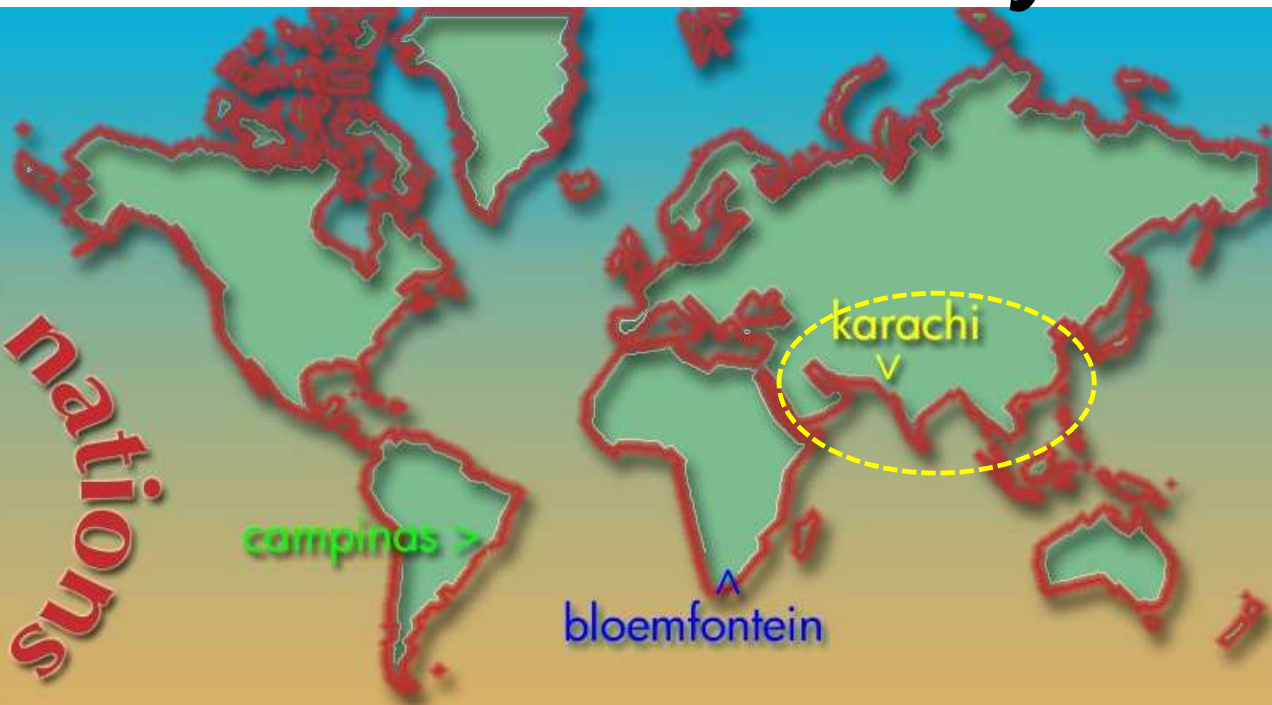
United Nations
Educational, Scientific and
Cultural Organization



International
Union of
Crystallography

Partners for the International Year of Crystallography 2014

together bringing nations
IUCr-UNESCO
summit
meetings



THE SOUTH ASIA REGION

- Internal strife and conflicts
- Baggage of history and geo-political compulsions
- Limited free trade and commerce
- Rivalry rather than healthy competition

Yet,

- Endowed with immense natural wealth and enviable human resources

Hope : In less than a decade this region will be home to over a billion people who would have been born after 1990 Who will carry no memory or baggage of the past



International Center for Chemical and Biological Sciences (ICCBS), University of Karachi, Pakistan



Jointly organized by



Ministry of Science and Technology (MoST), Government of Pakistan



Pakistan Academy of Sciences (PAS)



Chinese Academy of Sciences (CAS)



Indian National Science Academy (INSA)



Commission on Science and Technology for Sustainable Development in the South (COMSATS)

Objectives

The proposed event had the following objectives:

- To address issues and challenges relevant to the research in chemical crystallography, structural chemistry and pharmaceutical sciences.
- To provide a platform to the young researchers to interact with the leading scientists and crystallographers.
- To establish a bridge between the researchers and the related pharmaceutical industries
- To identify areas of common interest and to plan for a meaningful and vigorous practical collaboration between the researchers and centers.

Participants

380 Participants from 22 Countries

- Prof. Gautum Desiraju, President IUCr
- Prof. Samar Hasnain, Editor in Chief IUCr journals
- Micael H. Dacombe, Executive Secretary, IUCr
- Ahmed Fahmi UNESCO
- Romain Morenzi, TWAS



Topics covered

- Metal-Organic Framework Compounds (MOF)
- Crystal Engineering and Generic Pharmaceuticals
- Chemistry-Biology Interface and Drug Discovery and Designing
- Crystallography and complementary methods
- Regional Development (Dr. Romain Morenzi and Prof. Atta ur Rahman)
- IUCr: Union and Journals

Panel Discussions

THE CHANGING CONTOURS OF SCIENTIFIC ENTERPRISE

- Single investigator and intellectually driven research is under pressure
- Science for science sake is increasingly difficult to sustain
- Solving large societal problems require collaborative efforts; purposeful research becoming multidisciplinary
- Public perception of science is at an all time low ironically at a time when all of us are touched by S&T every day of our lives

Question: How do we balance the best of individually driven science with the societal demands that science address the major problems of the society?



MODES TO PROMOTE CO-OPERATION

- Create special avenues for young scientists to collaborate; ensure project funding covers international travel to neighboring countries
- Directory of young scientists of promise working in structural chemistry, natural products chemistry, chemistry-biology interface across our regions
- Facilitate round tables and platforms for industrial and academic scientists to come together on specific thematic issues and share common thoughts
- Leverage philanthropic funding agencies to create joint research teams from the region for addressing grand challenges
- Leverage more effectively the power of intergovernmental agencies (IuCr, TWAS, UNESCO, Science Academies) to create enabling environments
- Advocacy within nations to ask their respective Governments to create dedicated funding mechanisms for research collaborations

Summit declaration



Appeal

29th April, 2014

Prof. Dr. Gautam R. Desiraju
International Union of Crystallography
UK

Dear President:

We are pleased to report that the IYCr South Asia Summit Meetings on Vistas in Structural Chemistry in Karachi, Pakistan during April 28-30, 2014, has provided us an opportunity to extensively discuss and review the status of education and research in X-ray diffraction sciences in various countries and in the region.

Over 380 senior researchers and young students from some 22 countries have participated in the event. Many of us were engaged in extensive discussions focusing on the promotion of regional and international cooperation in the field of X-ray diffraction/crystallography/drug design and discovery, in line with the objectives of the International Year of Crystallography.

Through this letter, we request the IUCr to initiate actions to promote regional scientific collaboration including joint holding of training workshops, video-based lecturing, encouraging mobility of researchers, promoting joint research projects, leveraging national bodies and institutions for financial support and facilitating regional conferences on the subject of X-ray diffraction and its applications in the South Asian and South East Asian regions.

With very best regards
53 signatories from various countries

The Promise of Science Diplomacy



“Our future must not be hostage to our past. If we can move on cultural exchanges and trade links, why can’t we go ahead with joint efforts in education, science and technology?”

Prof. Atta-ur-Rahman

India-Pakistan science collaboration



“If East and West Germany can unite and if China and India can learn to collaborate, why can’t Pakistan and India overcome their differences?”

“Scientists of India and Pakistan can actually set an agenda and break the ice by taking small collaborative initiatives in scientific research.”

Prof. Gautam Desiraju



Cholesterol oxidase: ultrahigh-resolution crystal structure and multipolar atom model-based analysis

Bartosz Zarychta,^{a,b} Artem Lyubimov,^c Maqsood Ahmed,^{a,d} Parthapratim Munshi,^{a,e} Benoît Guillot,^a Alice Vrielink^f and Christian Jelsch^{a*}

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Examination of protein structure at the subatomic level is required to improve the understanding of enzymatic function. For this purpose, X-ray diffraction data have been collected at 100 K from cholesterol oxidase crystals using synchrotron radiation to an optical resolution of 0.94 Å. After refinement using the spherical atom model, nonmodelled bonding peaks were detected in the Fourier residual electron density on some of the individual bonds. Well defined bond density was observed in the peptide plane after averaging maps on the residues with the lowest thermal motion. The multipolar electron density of the protein–cofactor complex was modelled by transfer of the ELMAM2 charge-density database, and the topology of the intermolecular interactions between the protein and the flavin adenine dinucleotide (FAD) cofactor was subsequently investigated. Taking advantage of the high resolution of the structure, the stereochemistry of main-chain bond lengths and of C=O···H–N hydrogen bonds was analyzed with respect to the different secondary-structure elements.

Thank You!

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