

First Indo–U.S. Workshop on Mathematical Chemistry with Applications in Molecular Design and Hazard Assessment of Chemicals

During January 9–13, 1998 at Visva-Bharati University, Santiniketan, West Bengal, India, was held the first Indo–U.S. Workshop on Mathematical Chemistry. In this issue of the *Journal of Chemical Information and Computer Science* are included a selection of scientific papers presented at the Workshop.

The idea for this meeting originated with Dr. Subhash Basak, a native of Bengal, senior scientist at the Natural Resources Research Institute (NRRI) of University of Minnesota, Duluth. This idea found a welcome reception by Dr. Dilip K. Sinha, Vice-Chancellor of Visva-Bharati University, who mobilized local support and together with S. C. Basak chartered the meeting. Santiniketan, which is about 200 km northwest of Calcutta, offered a pleasant environment for the conference attended by about 100 scientists, one-third of whom came from United States, Australia, Japan, Russia, and other European countries and two-thirds came from India. Lectures covered a wide territory encompassing the present day Mathematical Chemistry, including novel results on graph invariants and their physicochemical significance, the inverse problem of QSAR, 3-D QSAR, chirality, drug discovery, similarity analysis, analysis of very large data sets, computer-assisted toxicity evaluation, fullerenes, among others. Selection of the presented papers are included here.

Santiniketan was the place of birth of Rabbindranath Tagore where several houses, his place of living on the present part of the university campus, have been converted to a museum. Tagore was the first person from Asia to receive a Nobel Prize (in 1913) and was highly respected by his contemporaries, which included Albert Einstein and Berthrand Russell, both of whom corresponded with and visited him.

This meeting was possible due to the generous support and understanding of NRRI of the University of Minnesota and the director Dr. Michael J. Lalich, in particular. Additional financial support was obtained from CSIR, New Dehli, DST, Government of India, and last, but not least, the Visva-Bharati University. The fact that two-thirds of the participants (and speakers) came from different parts of India indicates not only the strength of the Mathematical Chemistry in India, the host country of the Workshop, but also the necessity to continue this kind of bilateral meetings which are open to participants from any country on this globe.

Subhash C. Basak,
George W. A. Milne,
Milan Randić,
Dilip K. Sinha

CI9904822