



#### About the Institute

Indian Institute of Technology Kanpur carries out original research of significance and technology development at the cutting edge. It imparts training for students to make them competent, motivated engineers and scientists. The Institute not only celebrates freedom of thought, cultivates vision and encourages growth, but also inculcates human values and concern for the environment and the society.

#### Abstract

Single-molecule magnets (SMMs) are molecules that are magnetized in a magnetic field and show slow relaxation when the magnetic field is removed. The magnetization occurs because there is a large energy barrier between the spin-up and the spin-down states. The magnetic order is within the molecules (single domain). The requirements for SMM behavior are (1) a very high spin state and (2) a large magnetic anisotropy. In contrast to classical nanomagnets obtained by a top-down approach SMMs represent a bottom-up approach. The potential applications of SMMs are vast. These include information processing, data storage, quantum computing, spintronics, biomedical applications (like MRI contrast agents) or magnetic refrigeration. One of the early compounds to have been studied as an SMM is the dodecanuclear mixed-valent manganese cage  $[Mn^{III/IV}_{12}O_{12}(CH_3CO_2)_{16}(H_2O)_4]$ .

This compound has an  $S=10$  ground state and shows slow relaxation of the magnetization. Further, this compound shows hysteresis; evidence of quantum tunneling was also observed. Subsequently, several multinuclear transition metal complexes have been investigated for their SMM behavior. More recently there have been examples of 3d-4f complexes that show SMM behavior.

In this talk we will present our approach for the assembly of SMMs. We have used a phosphorus-supported multi-site coordination ligand to assemble trinuclear heterobimetallic compounds  $\{[L_2Co_2Ln][X]\}$  and  $\{[L_2Ni_2Ln][X]\}$ . The molecular structures of this family of compounds reveal that these are isostructural where all the three metal ions are arranged in a perfectly linear manner and are held together by two trianionic ligands,  $L^{3-}$ . The two transition metal ions are present in the terminal positions and are bridged to the central lanthanide ion by phenolate oxygen ligands. Some members of this new 3d-4f assemblies show SMM behavior at low temperatures. The synthesis, structure and magnetism of this new family of SMMs will be presented in this talk.

#### References

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2. V. Chandrasekhar, B. Murugesapandian, R. Azhakar, J. J. Vittal, R. Clérac. *Inorg. Chem.* 2007, *46*, 5140.
3. V. Chandrasekhar, B. Murugesapandian, R. Boomishankar, A. Steiner, J. J. Vittal, A. Hourri, R. Clérac. *Inorg. Chem.* 2008, *47*, 4918
4. V. Chandrasekhar, B. Murugesapandian, J. J. Vittal, R. Clérac. *Inorg. Chem.* 2009, *48*, 000.

#### Previous Speakers

Year	Name	Title
2008	Manindra Agrawal	The P<=>NP Problem
2007	R. C. Budhani	Low-Dimensional Superconducting and Magnetic Material of Proven Technology Relevance
2006	Kalyanmoy Deb	Evolution Optimization for Problem Solving and Knowledge Discovery
2004	Ashutosh Sharma	Of Small Things and other Stories



## C. N. R. Rao Lecture Series

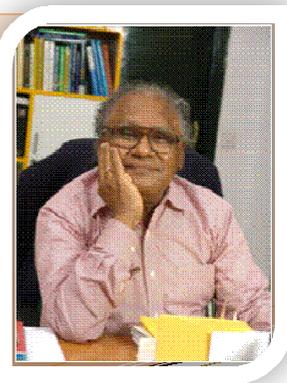
# Single-Molecule Magnets



**V. Chandrasekhar**  
Professor  
Department of Chemistry  
Indian Institute of Technology  
Kanpur

**Friday, 27<sup>th</sup> February, 2009**

**Venue: L-1, Lecture Hall Complex  
Time: 6:00 PM**



## About the Donor

### Professor C. N. R. Rao

**Chintamani Nagesa Ramachandra Rao** was born on June 30, 1934, in Bangalore, India, the son of Hanumantha Nagesa and Nagamma Nagesa Rao. In 1953 he earned a master's degree from Banaras Hindu University; in 1958, a doctor of philosophy degree from Purdue University. In 1958 he became a research chemist at the University of California at Berkeley, returning to India in 1959 to work as a lecturer at the Indian Institute of Science in Bangalore. In 1960 he married Indumati. They have two children, Suchitra and Sanjay.

From 1963-76, Dr. Rao was a professor of chemistry at the Indian Institute of Technology Kanpur. He served as Head of the chemistry department from 1964 to 1968, and was Dean of Research for three years. He was Chairman of the Solid State and Structural Chemistry Unit and Materials Research Laboratory at the Indian Institute of Science in Bangalore between 1976 and 1984. During 1984-89, Dr. Rao was the Director of the Indian Institute of Science Bangalore. Concurrent with his academic positions in India, Dr Rao was a visiting professor at Purdue University in 1967-68, at Oxford University in 1974-75, and he held a fellowship at King's College of Cambridge University in 1983.

In 1989 three researchers at Princeton University discovered a superconductive material that did not contain copper as part of the alloy. All previous materials were copper-oxide based; the Princeton researchers used nickel oxide, the first time such a compound had been successfully utilized as a superconductor. While initial results of the experiments were still being analyzed, and the crystalline structure of the compound was still a mystery, Professor Rao and co-workers conducted similar tests with nickel oxide

compounds at the Indian Institute of Science and confirmed their superconductivity. His research on the chemical properties of superconductive materials resulted in the publication of three books, *Chemical and Structural Aspects of High Temperature Superconductors*, 1988, *Bismuth and Thallium Cuprate Superconductors*, 1989, and *Chemistry of High Temperature Superconductors*, 1991. During his career Dr. Rao has published more than 25 books and 700 research papers.

Dr. Rao is currently the Research Professor and Honorary President of the Jawaharlal Nehru Centre for Advanced Scientific Research in Bangalore, India. He was appointed Chair of the Scientific Advisory Council to the Indian Prime Minister in January 2005. He was Chairman Board of Governors of IIT Kanpur during 2004-2006.

Dr. Rao was awarded the Hughes Medal by the Royal Society in 2000, and he became the first recipient of the India Science Award. He has won several international prizes and is a foreign member of the US National Academy of Sciences, American Academy of Arts and Sciences and of the Royal Society (London). He was awarded Dan David Prize in 2005, by the Dan David Foundation, Tel Aviv University. He has also been given the high honors of Padma Shri and Padma Bhushan by the Indian Government.

The annual C.N.R. Rao Lecture is supported by a donation received from Professor Rao.



## About the Speaker

### Professor V. Chandrasekhar

**V. Chandrasekhar** was born in Calcutta on sixth November 1958. He went to school at Hyderabad, Sunabeda and Visakhapatnam. He did his B.Sc and M.Sc from Osmania University, Hyderabad. Subsequently he joined the Indian Institute of Science, Bangalore from where he obtained his Ph.D in 1982. After a post-doctoral stint at the University of Massachusetts, Amherst (1983-86), he joined the Indian Petrochemicals Corporation Limited, Vadodara where he worked for an year. Subsequently Dr. Chandrasekhar joined the Department of Chemistry, IITK in July 1987 as an Assistant Professor and has become a full Professor in 1995.

Dr. Chandrasekhar's research interests are in the area of main-group organometallic chemistry. The focus of research in his group is on the synthesis, structure and reactivity of inorganic clusters, rings and polymers. He has also pioneered the chemistry of new inorganic-cored star-burst molecules and polymeric ligands. Currently his group is focusing on the application of these diverse molecules in catalysis, stabilization of nanoparticles and in the assembly of new magnetic and optical materials.

Dr. Chandrasekhar has published over 180 research papers in peer-reviewed international journals. Fifteen students have obtained their Ph. D under his supervision so far. He has authored a book entitled "Inorganic and Organometallic Polymers" which was published by Springer-Verlag in 2005.

Dr. Chandrasekhar's work has been recognized in the form of several national and international awards. Some of the prominent ones are: S. S. Bhatnagar Award (2003) and the Friedrich-Wilhelm-Bessel Research Award of the Alexander von Humboldt Foundation, Germany (2003). He is currently Head and Lalit Kapoor Chair Professor in the Department of Chemistry at IIT Kanpur.

