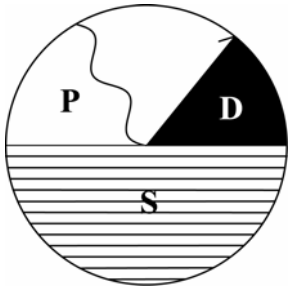

The 63rd Annual Pittsburgh Diffraction Conference

Argonne National Laboratory
Intense Pulsed Neutron Source - Building 360
Argonne, IL 60439

November 3-5, 2005

Program and Abstracts

Symposia to Honor
Prof. L.E. Alexander
Prof. M. Sundaralingam

Additional Symposia
Frontiers in Neutron Scattering
Advances in Chemical Biology

On the occasion of the 63rd Pittsburgh Diffraction Conference, colleagues, collaborators and friends from around the world meet to celebrate the scientific careers of Leroy E. Alexander and of Muttaiya Sundaralingam.

Leroy E. Alexander (1910-2004)

In June, L. E. Alexander passed away in his 94th year. Leroy retired in 1976 from the Mellon Institute of Carnegie-Mellon University in Pittsburgh, Pennsylvania, as Professor of Chemistry and Senior Fellow. To obtain his academic education he had a difficult road to follow. After high school he obtained his teacher's certificate and was teaching in one-room rural schools by the age of eighteen. By alternating teaching and college studies, he was able to earn a bachelor's degree at the State Teacher's College in River Falls, Wisconsin in 1937. During his teaching years, he organized a school band and taught the students how to play all the instruments. He supported himself during graduate school by playing clarinet and saxophone in dance bands, and was awarded a Ph.D. in physical chemistry from the University of Minnesota in 1943. After working at the General Electric Laboratories in Pittsfield, Massachusetts, Leroy was offered a position in the Department of Chemical Physics at the Mellon Institute of Industrial Research in Pittsburgh. He headed up the x-ray diffraction section and became an authority in this field. Together with Harold P. Klug he wrote the classic "X-ray Diffraction Procedures" (Wiley, 1954). This book can still be found in many x-ray diffraction laboratories throughout the world, because it is written in a clear and instructive way. With Gordon S. Smith, he published a number of influential papers on the geometry of single-crystal x-ray diffractometry. His second book "X-ray Diffraction Methods in Polymer Science" (Wiley, 1969), was also a success, and for quite some years was the only book on this subject. He was ACA secretary 1958 to1960.

In the early sixties Leroy was on sabbatical at the Delft University of Technology in The Netherlands, where he worked with his long time friend the late Peter de Wolff. While at Delft he collected material for his book on diffraction methods in polymer science. Those fifteen months in the Netherlands were a wonderful time for the Alexanders. While he was working on his second book, Leroy started a project to study chain folding in polymers, in particular of polyamides. This subject was a source of controversy and played an important role in the phenomenological description of the deformation of polymers. The study resulted in a series of papers on the structural determination of nylon cyclic oligomers. Together with Roger Pettersen and Earl Baker he worked on the synthesis and the structures of chlorophyll-related compounds.

With his great knowledge of x-ray diffraction and talent for writing well-styled and clearly formulated texts, he was a source of inspiration for all those who had the privilege to work with him. Leroy was a great friend and colleague to many people from different countries and backgrounds. He had a broad range of interests; playing music was one of his greatest pleasures. He was an optimistic and religious man, respected as well as admired by those who knew him. In his work he was strongly supported by his beloved wife Eleanor, who for many years transcribed books into Braille. She died several years ago. Leroy is survived by his daughters Kathryn and Karen and two grandchildren.

Maurits Northolt
(from the ACA Newsletter, Winter 2004)

X-ray crystallographers at the Mellon Institute, 1966

Front, from left: Harold Klug, Leroy Alexander.
Behind, from left: Wayne Orr, Bob Stewart, Sid Pollack, Maurits Northolt, Maureen Sullivan.

Absent: Gordon Smith, Roger Pettersen, Gardner Sumner, Patricia Brown, John Beres.
Note: The biologist Roy Worthington had a separate small-angle X-ray facility.

Leroy Alexander and the Pittsburgh Diffraction Conference

Leroy Alexander joined the staff of the Mellon Institute in Pittsburgh in January 1946. His involvement with the Pittsburgh Diffraction Conference began with the fourth Conference which was held in December, 1946. Thereafter, he was active in the affairs of this annual Conference until his retirement from the Mellon Institute of Carnegie-Mellon University in 1976. Throughout these thirty years he took part in the Conference in two different ways. First he became a regular among the Conference organizers. Second, he joined in the presentation of research that came from a growing X-ray group at the Mellon Institute of whom Harold Klug and Leroy Alexander were the leaders.

Now that the Pittsburgh Diffraction Conference is in its 63rd year, with a history older than that of the ACA, it is important to recognize the work of Leroy Alexander in gathering and preserving records that go back continuously to the first Pittsburgh Diffraction Conference. This took place at the University of Pittsburgh in 1943 (during the siege of Leningrad; now St Petersburg). Leroy made use of his archival material in his account of *"Surhain Sidhu and the Early Pittsburgh Diffraction Conferences"* which appears in abbreviated form in the ACA Newsletter, December 1992 and in full on the website, www.pittdifsoc.org. Leroy includes his own stories of those early years. His article points out that the early Pittsburgh Diffraction Conferences drew an audience of hundreds and were attended by leading figures including Sir Lawrence Bragg, Isadore Fankuchen, Charles Barrett and David Harker.

Bryan Craven and Robert Stewart

Muttaiya Sundaralingam (1931-2004)

thoughts of a former student

From a student's perspective, Professor Muttaiya Sundaralingam, universally known as 'Sunda', was a consummate scientist, both rigorously disciplined and highly creative. Following his Ph. D. work with G. A. Jeffrey at the University of Pittsburgh, and a stage of his career at Case Western Reserve University, he moved to the University of Wisconsin, Madison, in 1970 to direct a laboratory focused on the structures of nucleic acids and their components. He was chemical crystallographer in the classical sense, using high resolution crystal structures to deduce principles about the behavior of molecules from their bond distances, angles, torsions, hydrogen bonding, conformation, and crystal packing. He developed this approach through training with George Jeffrey where the focus was often on carbohydrates. Underlying concepts in this research were the value of atomic resolution, the use of crystals to infer chemical interactions, and the need to understand the subtleties and details of hydrogen bonding.

Sunda subsequently employed crystallography in a systematic, virtually exhaustive manner to the components of nucleic acids, the bases, sugars, nucleosides, and nucleotides, of all kinds, and to polynucleotides. This research was inspired by Linus Pauling's analysis of protein structure, and the principle that through precise definition of the building blocks, one could deduce the structure of the biological macromolecule. Sunda's special gift was to visualize and understand stereochemistry, and so he was not afraid to apply the results of his crystal structures to the complicated nucleotide components of nucleic acids. One of his fundamental contributions was to identify the conformational preferences of furanose sugars, in terms of a newly defined pseudorotation angle. Using this analysis, he was able to unravel the observed conformations of nucleosides and nucleotides, and develop the 'rigid nucleotide hypothesis' based on preferred C2′ *endo* and C3′ *endo* sugar puckers. His work further defined favored ranges of torsion angles for all of the sugar and phosphate bonds in the polynucelotide, and the preferred torsion angles about the glycosidic bonds of the bases. In concert with stereochemical analysis from crystal structures, Sunda always built models, and he used the models to infer energy landscapes, especially for helical nucleic acids, through rigorous theoretical calculations. In other words, he extended his

understanding of the repeating units to the macromolecule and its dynamics. Simultaneously, this led him to study crystal structures of transfer RNAs, and RNA and DNA duplexes. It is impossible to imagine a contemporary understanding of nucleic acid structure without Sunda's fundamental insights. He reduced the problem of stereochemical analysis of polynucleotides to simple rules and conformational preferences, much as Ramachandran did for the analysis of protein structure.

The 1999 Pittsburgh Diffraction Conference at Ohio State University was organized to honor Sunda upon his retirement. At that time, a compendium bibliography of Sunda's 330 scientific publications was presented. In his own presentation, entitled 'From Nucleic Acids to Proteins – 40 years of Structural Molecular Biology' he provided an overview of his own career as he focused on the nature of base-base interactions in nucleic acid structures. In his lecture he reviewed many types of base-base hydrogen bonding interactions and their role in RNA tertiary structure and recognition. The lecture was exemplary of Sunda's approach to science: he presented a wide diversity of crystal structures and models, analyzed the complexities seen at high resolution, emphasized the nature of these molecular interactions and hydrogen bonding patterns in folded RNA, and provided a synthesis.

Sunda's life influenced many people, and he had many scientific collaborators. His close colleague of many years, N. Yathindra, has published an excellent and lengthy review of Sunda's life and work in *Acta Cryst.* (vol. D61, pp. 845-849, 2005). As Yathindra points out, 'Sunda attracted a number of bright students and post docs through his charismatic discourse on the unique ability of X-ray diffraction techniques to visualize biological macromolecules'. Personally, I was attracted by exactly such 'charismatic discourse' when as a first year graduate student Sunda enlightened me as to how biochemical molecules could be examined in three dimensions. At that time, in his lab in the 1970s, a number of graduate students were set to work on projects that would influence their careers, especially through a passion for solving structures. Sunda, and other scientists he attracted to his group, in particular S. T. Rao and R. K. McMullan, insisted on and taught crystallographic principles, while the goal was always to solve the next interesting structure. As a mentor, Sunda provided guidance by creating the environment, and generating the energy to ask the interesting questions, but he also left his students to work out the details of the problem on their own. This in turn created an atmosphere that fostered a great deal of interaction and shared learning. Personally, Sunda was a gracious and patient advisor, and fostered the careers of all of his students with care. He and his wife, Indrani, hosted many dinners, picnics and parties, including everyone in his laboratory into his extended family.

This year's special Sunda Symposium at the Pittsburgh Diffraction Conference will include presentations from several of Sunda's students who shared their graduate careers in his laboratory in the period of the 1970s. The aim is to demonstrate that at one time Sunda's lab harbored a special collection of students, who have gone on to do a wide variety of interesting research, all connected in some way to the crystallographic inspiration he provided. This on-going research he inspired, and the careers Sunda mentored, is a testimony to his contribution to crystallography.

Dave Stout