

**PREVIOUS BERT HALPERN LECTURERS:**

- 1988 ALAN M. SARGESON (AUSTRALIAN NATIONAL UNIVERSITY)  
1989 HANS C. FREEMAN (UNIVERSITY OF SYDNEY)  
1990 ROBERT BREAKSPERE (UNIVERSITY OF TECHNOLOGY, SYDNEY)  
1991 GRAHAM JOHNSTON (UNIVERSITY OF SYDNEY)  
1992 GRAEME PEARMAN (CSIRO DIVISION OF ATMOSPHERIC RESEARCH)  
1993 ATHEL BECKWITH (AUSTRALIAN NATIONAL UNIVERSITY)  
1994 ANTHONY G WEDD (UNIVERSITY OF MELBOURNE)  
1995 ARTHUR J BIRCH (AUSTRALIAN NATIONAL UNIVERSITY)  
1996 LEN LINDOY (UNIVERSITY OF SYDNEY)  
1997 PETER COLMAN (BIOMOLECULAR RESEARCH INSTITUTE)  
1998 DON NAPPER (UNIVERSITY OF SYDNEY)  
2000 PAUL HADDAD (UNIVERSITY OF TASMANIA)  
2001 JOHN BOWIE (UNIVERSITY OF ADELAIDE)  
2002 GRAEME CLARK (UNIVERSITY OF MELBOURNE)  
2003 DAVID BLACK (UNIVERSITY OF NEW SOUTH WALES)  
2004 BRUCE CORNELL (AMBRI PTY LTD)  
2005 ROGER SUMMONS (MASSACHUSETTS INST. OF TECH., USA)

**ORDER OF PROCEEDINGS:**

**5.30 – 6.00 p.m. Refreshments**  
UniCentre Function Rooms 3 & 4

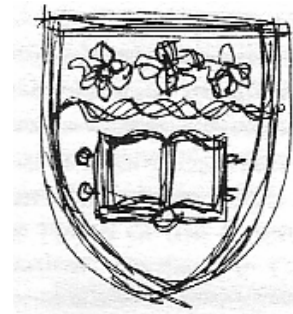
6.00pm *Welcome:* Prof. William Price  
Head, Department of Chemistry

*Introduction:* Prof. Rob Whelan  
Dean, Faculty of Science

Lecture: Prof. Leo Radom

*Vote of thanks:* Prof. Margaret Sheil  
Deputy Vice-Chancellor (Research)

**UNIVERSITY OF WOLLONGONG**  
**DEPARTMENT OF CHEMISTRY**



**THE BERT HALPERN LECTURE - 2006**

**Prof. Leo Radom**  
University of Sydney  
School of Chemistry

**Thursday 16th November, 2006**

Union Function Centre  
5.30pm. for 6.00pm

RSVP Louisa Willdin (by 13<sup>TH</sup> November, 2006)  
Phone: (02) 42 213509  
Email: [louisa@uow.edu.au](mailto:louisa@uow.edu.au)

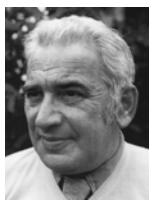
## THE BERT HALPERN LECTURE

The Bert Halpern Lecture is a public lecture presented annually at The University of Wollongong by a distinguished visiting scientist on a subject in chemistry or biochemistry.

It honours the memory of Bert Halpern, the Professor of Chemistry at the University of Wollongong from 1970-1980. Professor Halpern's pioneering studies in amino acid, peptide and protein chemistry impacted across the fields of medicine, biochemistry, chemistry and geochemistry. Among his notable achievements was the development of novel techniques for the diagnosis and study of metabolic disorders and genetic defects. In recognition of his contributions to Science, he was elected a Fellow of the Australian Academy of Science in 1978.

The Department of Chemistry is pleased to announce that the *Bert Halpern Lecturer* for 2006 is **Prof. Leo Radom**.

*The late Professor Bert Halpern*



## THE BERT HALPERN LECTURER 2006

### PROF LEO RADOM

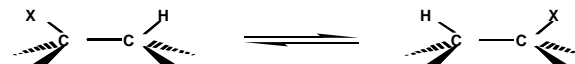
Leo Radom was educated at the University of Sydney where he graduated with First Class Honours and the University Medal in 1965, and subsequently a PhD in 1969 with R.J.W. Le Fèvre. Leo then turned to theory through a 3.5 year postdoctoral period with John Pople at Carnegie-Mellon University in Pittsburgh. He returned to Australia in 1972 to the Research School of Chemistry of the Australian National University, and moved to the University of Sydney in 2003. He has been a visiting faculty member at the University of California, Irvine and Berkeley, the Ben Gurion University, Beer Sheva, the Institute of Molecular Science, Okazaki, the National University of Singapore, and the Autonoma University of Madrid. Leo's main research interests are concerned with the study of the structures and stabilities of molecules and the mechanisms of reactions in which they are involved by use of computational quantum chemistry procedures. He is the co-author of the classic text in the field and about 450 research papers. Leo's achievements have been recognized through the award of the Rennie Medal, the H.G. Smith Medal and the Archibald Olle Prize of the RACI, the Schrödinger Medal of WATOC, the Maccoll Lectureship of the BSMS, the Mulliken Lectureship of the University of Georgia, the Marchon Lectureship at the University of Newcastle upon Tyne, the BBV Foundation Chair at the Autonoma University of Madrid, the Stranks Lectureship of the University of Melbourne, the Lise-Meitner Lectureship of the Hebrew University Jerusalem, the Raymond Lemieux Lectureship of the University of Ottawa, and the 2006 Fukui Medal of the APATCC, and through election to the Australian Academy of Science and the International Academy of Quantum Molecular Science.



### Abstract

#### THE MECHANISM OF ACTION OF COENZYME B<sub>12</sub>: A COMPUTATIONAL APPROACH

In the presence of the appropriate enzyme, coenzyme B<sub>12</sub> mediates reactions that have a remarkably simple form, namely the formal interchange of a group of X and a hydrogen on adjacent atoms:



Despite this simplicity, these reactions have proved difficult to resolve mechanistically. It is generally accepted that radicals are involved but the precise nature and details of the rearrangement has yet to be established definitively.

We have used high-level computational quantum chemistry calculations to study a selection of such reactions and this has provided valuable insights into the mechanism. Some of our theoretical predictions are amendable to experimental testing.

This presentation will begin with a brief discussion of the use of computational procedures to study chemistry, followed by highlights from our recent research on coenzyme-B<sub>12</sub>-mediated reactions.