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CENTRE FOR RESEARCH IN MOLECULAR MODELING
and the
DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY**

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**Computational Chemistry as
a Complementary Tool for the Study of Biological Radicals**

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The tremendous advances in the development of computational quantum chemistry have established theory as a viable partner to experiment in chemical research. Quantum chemical methods are especially helpful for the study of biological radicals for which there is a paucity of experimental information on the identity of the radicals and even less on the mechanisms by which they affect the physiology of living systems. Many bioradicals are formed by exposure of living matter to ionizing radiation. For example, radiation causes damage to DNA, the primary products being base or sugar radicals that subsequently lead to strand breaks and DNA-DNA or DNA-protein cross-links. An overview of our current research on radicals formed in radiation damage to amino acids and DNA components, including cross-linking between a DNA base and an amino acid, will be presented. Other aspects of our recent research, including the use of nucleobases as catalysts and the mechanism by which the antitumor drug tirapazamine cleaves DNA will be discussed briefly.

Russell Boyd graduated in 1967 from the University of British Columbia with Honours in Chemistry and the Lefevre Gold Medal. He then went east to pursue his PhD in Theoretical Chemistry at McGill University, and to Oxford University as a National Research Council Postdoctoral Fellow at the Mathematical Institute. He returned to the University of British Columbia where he held a Killam Postdoctoral Fellowship in the Department of Chemistry from 1973 to 1975. Dr. Boyd joined Dalhousie University in 1975, rose through the ranks to become a Professor in 1985, and has served as Chair of Chemistry since 1992. He was named a Faculty of Science Killam Professor in 1997 and became the seventh holder of the Alexander McLeod Chair of Chemistry in 2001. Dr. Boyd is a Fellow of the Chemical Institute of Canada, a member of the College of Reviewers of the Canada Research Chairs, and a member of the Analytical and Physical Chemistry Grant Selection Committee of the Natural Sciences and Engineering Research Council of Canada. He has served on many boards, including the Canadian Society for Chemistry, the Canadian Journal of Chemistry, and the Dalhousie University Foundation. Dr. Boyd has published nearly 200 peer-reviewed papers in computational and theoretical chemistry, and has trained a number of excellent young scientists who now hold academic positions in Canada, the USA and Europe.

