PROJECT REPORT

Project Title: **Theoretical Studies on Radiation-Induced Transformations in Nucleic Acid Bases**

Project No.: **DE-FG03-93ER61605**

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The work funded by the Department of Energy, Project No. DE-FG03-93ER61605, represents efforts in method development application studies in the area of *ab-initio* quantum chemistry. The following publications resulted:

1) H. Rostkowska, M.J. Nowak, L. Lapinski, M. Bretner, T. Kulikowski, A. Leś and L. Adamowicz, Infrared Spectra of 2-Thiocytosine and 5-Fluoro-2-Thiocytosine; Experimental and *Ab-Initio* Studies, *Spectrochim. Acta*, **49A**(4), 551 (1993).

2) H. Rostkowska, M.J. Nowak, L. Lapinski, M. Bretner, T. Kulikowski, A. Leś and L. Adamowicz, Theoretical and Matrix-Isolation Experimental Studies on 2-Thiocytosine and 5-Flouro-2-Thiocytosine, *Biochimica et Biophysica Acta* **1172**, 239 (1993).

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4) Z. Slanina, A. Leś and L. Adamowicz, The Effects of Temperature on the Relative Stabilities of Five Complexes of 4-Hydroxypyridine and Water, *Thermochimica Acta* **224**, 13 (1993).

5) Z. Slanina, A. Leś and L. Adamowicz, Complexes of 2-Aminopyrimidine, 2-Hydroxy-pyrimidine and Their Tautomers With Water: Relative Thermodynamic Stabilities, *Thermochimica Acta* **228**, 1 (1993).

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DISCLAIMER

10) L. Lapinski, M.J. Nowak, A. Leś and L. Adamowicz, *Ab Initio* Calculations of IR Spectra in Identification of Products of Matrix Isolation Photochemistry: Dewar Form of 4(3*H*)-Pyrimidinones, *J. Am. Chem. Soc.* **116**, 1461 (1994).

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Papers Submitted for Publication:

1. K.B. Ghose, L. Adamowicz and S. Pal, The State Selective Multireference Coupled-Cluster Method. Some Recent Developments, *J. Chem. Phys.*, submitted.

Progress Report, DOE Grant DEFG0393ER61605, Theoretical Studies on Radiation-Induced Transformations in Nucleic Acid Bases.

Period Covered: May 1, 1994 - April 30, 1995 (All funds allocated for this budget period will be spent by April 30, 1995).

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Since I submitted my last report at the end of January, 1993, our research effort funded by the above-mentioned grant has resulted in twenty-one [1-21] papers, ten of them already published or accepted for publication and eleven currently under review by the journals. Part of the funding was used to purchase an IBM RISC 6000 590 workstation, which has been very instrumental in performing some of the large scale *ab-initio* calculations relevant to the project. The following research developments have been accomplished:

1. UV-induced transformations of a number of nucleic base molecules and their analogues have been investigated. Of interest to us has been both of the internal structural transformations induced by promoting the molecules to excited electronic states and the excited state proton transfer reactions. The phenomenon of the proton migration induced by the UV-radiation has been studied in isolated base molecules and in complexes with water and in the base dimers. Attempts have been made to describe the dynamics of the proton transfer reactions on the excited state potential energy surfaces. This work has been described in Refs. 5,6,8,9 and 17.

2. Free electron release and its attachment to nucleic acid bases is one of the primary effects taking place in irradiated genetic material. It has been long believed that electron affinities of the nucleic acid bases are negative. Our calculations on thymine, uracil, guanine and adenine have demonstrated that due to sizable dipole moments of some of the base tautomers, excess electrons can attach to the bases forming stable dipole-bound states. The formation of these states, which is more effective for some tautomers than for the others, leads to significant shifts in the tautomeric equilibria and, in some cases, for example, adenine, to the appearance of noticeable amounts of rare tautomers in the mixture. The work on molecular anions has also covered investigations of some smaller model systems where the formation of the dipole-bond anionic states compete with formation of conventional "valence" anions. In order to verify our theoretical predictions regarding the electron affinities of nucleic acid bases, we have established a collaboration with the experimental group of Professor Schermann from the University of Paris, France. With the use of photoelectron

spectroscopy, this group recently measured the electron affinities of uracil and thymine and the results agree very well with our computed values. The work on the anions has been described in Refs. 1, 2, 11, 13, 15, 16, 20 and 21.

3. We have continued studies on the IR spectral characterizations of analogues and derivatives of the nucleic acid bases. With the use of harmonic frequency analysis and an effective method to account for anharmonicity developed by us, we have studied the spectra 4-pyrimidinone, 2-aminopyrimidine and 2-quinoline-thione. This work has been carried on in collaboration with the matrix-isolation spectroscopy group of Dr. Nowak, of the Institute of Physics, The Polish Academy of Sciences. One aspect of this work which is particularly relevant to this project is UV-irradiation of the studied molecules and alternating the tautomeric equilibria. This effect was very instrumental in the identifying the spectra of different tautomers. The work has been described in Refs. 4, 12 and 18.

4. The dimerization of the nucleic bases constitutes an essential mechanism for the duplication of the genetic information. Our goal is to eventually study how the radiation affects the structure of the dimers. The complexity of this problem requires, however, that we study smaller model systems first before we turn to dimers. In the course of this study, extensive *ab-initio* calculations have been performed to determine isomeric structures of singly- and double-bonded complexes involving nucleic acid molecules and water molecules. We considered the following systems: 2-OH-pyridine and 2-OH-pyrimidine; 4-OH-pyridine and 4-OH-pyrimidine; 2-NH_2-pyridine and 2-NH_2-pyrimidine; 3-OH-pyridine and 3-OH-pyrimidine; adenine; 1-methyl-adenine; 3-methyl-adenine; 7-methyl-adenine and 9-methyl-adenine. The purpose of the calculations was to determine the relative thermodynamic stability of the complexes formed by the base molecules with water molecules attached at different H-bonding sides. The water complexation with the rare tautomers of the basis was also considered. Our theoretical work has been carried in collaboration with the IR matrix-isolation studies by the group of Professor G. Maes from the Catholic University of Leuven, Belgium. This work representing the first step in subsequent theoretical and spectral characterization of the base pair complexes has been described in Refs. 10 and 19.

5. We have continued our work on developing new *ab-initio* methodology to study electron excitations and molecular fragmentation processes. This work was centered on the theoretical formulation and numerical implementation of the state-selective multi-reference coupled-cluster method. The work has been described in Refs. 3 and 7.

6. Lastly, we wrote a review article entitled, "*Ab-Initio* Calculations of Biomolecules," which will be published in Proceedings of the CAM'94 Physics Meeting in Cancun, Mexico.

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7. V. Alexandrov. P. Piecuch and L. Adamowicz, State-Selective Multi-Reference Coupled-Cluster Theory Employing the Single-Reference Formalism: Application to Excited States of H_8, *J. Chem. Phys.*, accepted for publication.

8. A. Sobolewski and L. Adamowicz, Theoretical Investigations of the Excited-State Intra-molecular Proton Transfer Reaction in N-substituted-3-hydroxypyridinones, *Chem. Phys.*, accepted for publication.

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13. G. Gutsev, A. Sobolewski and L. Adamowicz, Theoretical Study on the Structure of Acetonitrile (CH_3CH) and its Anion (CH_3CH^-), *J. Chem. Phys.*, submitted.

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15. G.L. Gutsev and L. Adamowicz, Relationship Between the Dipole Moments and the Electron Affinities for Some Polar Organic Molecules, *Chem. Phys. Lett.*, submitted.

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19. F. Buyl, J. Smets, G. Maes and L. Adamowicz, Matrix-isolation FT-IR Studies and *Ab-Initio* Calculations of Hydrogen-bonded Complexes of Molecules Modeling Cytosine and Isocytosine Tautomers. 3. Complexes of 4-OH-Pyridine and 3-OH-Pyridine with H_2O in Ar Matrices, *J. Phys. Chem.*, submitted.

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