

REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0188		
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1. REPORT DATE (DD-MM-YYYY) 28-06-2007		2. REPORT TYPE FINAL TECHNICAL REPORT		3. DATES COVERED (From - To) 01-01-04 to 31-12-06	
4. TITLE AND SUBTITLE Theoretical Studies of Gas Phase Elementary Reactions			5a. CONTRACT NUMBER		
			5b. GRANT NUMBER FA9550-04-1-0080		
			5c. PROGRAM ELEMENT NUMBER		
6. AUTHOR(S) Keiji Morokuma			5d. PROJECT NUMBER		
			5e. TASK NUMBER		
			5f		
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Department of Chemistry, Emory University, 1515 Dickey Dr., Atlanta, GA 30322			8. PERFORMING ORGANIZATION REPORT		
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) Air Force Office of Scientific Research 875 North Randolph Street Suite 325, Room 3112 Arlington, Virginia 22203 C/o Dr. Mike Berman, Theo. Chem.			10. SPONSOR/MONITOR'S ACRONYM(S)		
			11. SPONSOR/MONITOR'S REPORT		
			12. DISTRIBUTION / AVAILABILITY STATEMENT Approved for public release. distribution unlimited		
13. SUPPLEMENTARY NOTES					
14. ABSTRACT This final technical report begins with the objective the project, followed by summary reports on new accomplishments and findings obtained in the project. They are presented in four sections: A. Potential Energy Surfaces of Ion-Molecule Reactions and Ionic Species, B. Potential Energy Surfaces for Elementary Reactions of Atmospheric Importance, C. Potential Energy Surfaces for Electronic Spectroscopy, Photochemical Reactions and Nonadiabatic Processes. D. Interaction of Oxygen and Other Small Molecules with Electron and Other Molecules..					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			19b. TELEPHONE NUMBER (include area code)

AFRL-SR-AR-TR-07-0215

1. Objectives.

Elementary gas phase reactions are simple and can provide detailed information concerning their mechanism, kinetics and dynamics toward better understanding of chemical reactions, one of the ultimate goals of chemistry. Some gas phase elementary reactions are very important also in practical applications. For instance, the chemistry in the ionosphere is controlled mainly by ion-molecule reactions. Detailed understanding of ion-molecule reaction dynamics is essential for understanding plasma dynamics effects and some of the optical radiation associated with the spacecraft-atmosphere interactions. For instance, we have studied the mechanism of reactions of N^+ and N_3^+ with O_2 molecule, and provided mechanistic insight into the reaction pathways of these reactions. In another aspect, the reaction of upper excited electronic states of the oxygen molecule has not been studied carefully.

The present research of carrying out high-level ab initio potential energy surface (PES) and some dynamics calculations on gas phase elementary reactions had dual goals. The first was to provide, based on ab initio calculations, information concerning the PESs that govern the mechanism and dynamics of elementary reactions. We mostly chose reactions relevant to upper atmospheric chemistry and atmospheric photochemistry. This kind of theoretical information, otherwise hard to obtain, will allow deeper insight and understanding of experimental findings on reaction mechanism, kinetics and dynamics. The second and practical goal was to help research groups at Air Force Laboratories and university scientists supported by AFOSR grants, who are performing excellent experimental studies in the elementary reaction dynamics and are in need of collaboration with theoreticians who can provide information concerning the PESs and dynamics to interpret and understand their experiments.

2. Accomplishments and New Findings.

A. Potential Energy Surfaces of Ion-Molecule Reactions and Ionic Species

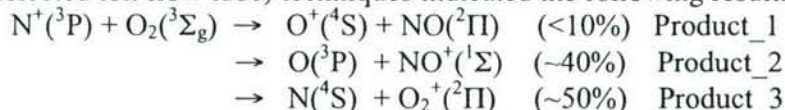
a. The reactivities of NOO^+ ion.

The kinetics for the reactions of NOO^+ ions with neutral molecules having ionization potentials from 9.27 to 15.58 eV were measured in a selected ion flow tube (SIFT) at 298 K. The NOO^+ ions are produced from the reaction of $N_3^+ + O_2$ and have been reacted with the following: NO, C_6F_6 , CS_2 , CF_3I , C_3F_6 , OCS, C_2H_6 , Xe, SO_2 , O_3 , N_2O , CO_2 , Kr, CO, D_2 and N_2 . Numerous types of reactions were observed with the various neutral reagents, including production of NO^+ (which may involve loss of an O from the ion or addition of O to the neutral reactant, although the two channels could not be distinguished here), charge transfer, isomerization of NOO^+ to ONO^+ , and hydride abstraction. High level theoretical calculations of the structures and energetics of the various isomers, electronic states, and transition states of NOO and NOO^+ were performed to better understand the observed reactivity. All neutral species with an IP ≤ 11.18 eV were observed to react with NOO^+ in part by charge transfer. Detailed calculations showed that the recommended adiabatic and vertical IP's of NOO are 10.4 and 11.7 eV, respectively, at the MRCISD(Q)/AVQZ level of theory. The observed experimental limit for charge transfer of 11.18 eV agreed well with the energetics of the final products obtained from theory if dissociation of the neutral metastable product occurred, i.e., the products were $X^+ + [O(^3P) + NO(^2\Pi)]$, where $[O(^3P) + NO(^2\Pi)]$ formed via dissociation of metastable NOO. Charge exchange with neutral reagent X would, therefore, be exothermic if $IP(X) < (IP^{ad}(NOO) - \Delta E_{(O+NO)-NOO}) \approx 11.1$ eV, where $IP^{ad}(NOO)$ is the adiabatic IP. The potential energy surface for the reaction of NOO^+ with C_2H_6 was also calculated, indicating that two pathways for formation of $HNO_2 + C_2H_5^+$ exist. This work was published as paper 6 of the Publication List.

b. The mechanism of the ion-molecule reaction of $N^+(^3P) + O_2(^3\Sigma_g^-)$

The reaction of oxygen molecule with nitrogen cation has been recently studied by Air Force Research Laboratory at Hanscom AFB. It is one of the important reactions in controlling electron

density in the ionosphere. Recent experiments using HTFA (high temperature flowing afterglow) and SIFT (selected ion flow tube) techniques indicated the following results:

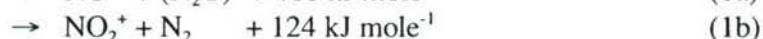


None of the channels have strong energy dependence. But at high energy, drift tube measurements showed that the charge transfer and O^+ production became increasingly important. Since none of the products can correlate to the reactants based on the dominant electron configuration argument, non-adiabatic transition must occur in the reaction. The goal of present study is theoretically to clarify the reaction mechanism, calculate the rate constants and explain the experimental observations, such as the temperature dependence of charge transfer and O^+ products. In the present study, we have performed MRCISD(Q) and CASPT2 methods to map out the potential energy surfaces that involve in the reaction. Qualitatively, we explained the observed the reaction product and their branching ratio. The results were published as paper 9 of the publication List

c. The mechanism of the ion-molecule reaction: $\text{N}_3^+ + \text{O}_2$

Air plasmas at elevated pressures are currently the subject of intensive study for a variety of applications. Typical non-equilibrium plasmas have heavy particle temperatures below 1000 K and average electron energies on the order of a few eV. These conditions are favorable for associative ionization processes and the presence of polyatomic nitrogen ions such as N_3^+ and N_4^+ are expected. However, temperature dependent data even for the relatively simple cases involving reactions of these ions with major species are insufficient or nonexistent.

In light of these issues, the kinetics of the reaction of N_3^+ with O_2 has been studied in more detail. The reaction has two observed product channels:



The calculated singlet PES shows that two products are produced, namely NO_2^+ and NO_4^+ . The former is favored at low temperature due to small reaction barrier. The triplet PES might also involve in the NO^+ formation through a one-step but three-body fragmentation TS. The NO_2^+ produced in the reaction is shown to be a peroxide form, $\text{NOO}^+(\text{}^1\Sigma^+)$. MRCISD(Q) calculations confirm that this is a stable isomer, with a barrier to dissociation of about 0.9 eV both in the adiabatic and non-adiabatic processes. The energy of this isomer is 4.5 eV above that of the most stable isomer, linear ONO^+ . The reactivity of $\text{NOO}^+(\text{}^1\Sigma^+)$ is further investigated in the charge transfer reaction with NO and H abstraction reaction with ethane (C_2H_6). Calculations show that the charge transfer reaction occurs in the vicinity of $\text{NOO}^+(\text{}^1\Sigma^+)$ minimum and a charge transfer barrier will be formed with the increase of the ionization potential of the other reactant. The negative reaction barrier relative to the reactant will lead to quick H abstraction in the reaction with C_2H_6 . The work was published as paper 12 of the Publication List.

d. Geometries, energetics, electronic structure and vibrational structures of SF_6^- and CO_3^-

In collaboration with experimental groups (Viggiano at AFRL & Johnson at Yale), geometries, energetics, electronic structure and vibrational structures of SF_6^- and CO_3^- were studied theoretically and compared with ongoing experiments when available. The $\text{CO}_3^- \rightarrow \text{CO}_2 + \text{O}^-$ dissociation was predicted to be barrierless. Theory predicts that CO_3^- has D_{3h} symmetry, but with a very flat potential for C_{2v} distortion. SF_6^- has O_h symmetry, and accurate calculation of vibrational frequencies and intensities is in progress. SF_6 and SF_5 structures, energetics and electron affinities were also calculated. The work is being written up and will be submitted in the renewal period of the present grant.

e. Potential energy curves and Xe_2^+

The calculated potential energy curves were calculated for g and u states, respectively. The current project is a collaboration with Dr. R. Dressler of AFRL at Hanscom and a joint paper is in preparation.

B. Potential Energy Surfaces for Elementary Reactions of Atmospheric Importance

A new mechanism for the production of highly vibrationally excited OH in the mesosphere. An ab initio study of the reactions of $\text{O}_2 (A^3\Sigma_u^+ \text{ and } A'^3\Delta_u) + \text{H}$,

In an attempt to explain the observed nightglow emission from OH ($v=10$) in the mesosphere that has the energy greater than the exothermicity of the $\text{H} + \text{O}_3$ reaction, potential energy surfaces were calculated for reactions of high lying electronic states of $\text{O}_2 (A^3\Sigma_u^+ \text{ and } A'^3\Delta_u)$ with atomic hydrogen $\text{H}(^2\text{S})$ to produce the ground state products $\text{OH}(^2\Pi) + \text{O}(^3\text{P})$. From collinear two-dimensional scans, several adiabatic and non-adiabatic pathways have been identified. MRSDCI (multi-configurational single and double excitation configuration interaction) calculations show that the adiabatic pathways on a $^4\Delta$ potential surface from $\text{O}_2(A'^3\Delta) + \text{H}$ and a $^4\Sigma^+$ potential surface from $\text{O}_2(A^3\Sigma_u^+) + \text{H}$ are the most favorable, with the zero-point corrected barrier heights of as low as 0.191 eV and 0.182 eV, respectively, and the reaction are fast. The transition states for these pathways are collinear and early, and the reaction coordinate suggests that the potential energy release of ca. 3.8 eV (larger than the energy required to excite OH to $v=10$) is likely to favor high vibrational excitation. The paper 9 has been published based on the work.

C. Potential Energy Surfaces for Electronic Spectroscopy, Photochemical Reactions and Nonadiabatic Processes.

a. Photodissociation of cyclic N_3

Nitrogen cluster have received considerable attention as good candidate for high-energy density materials (HEDM). Their natural tendency to decompose to N_2 also makes them high on the list of environmentally friendly explosives and propellants. Cyclic N_3 is the smallest cluster of these species and is the only precursor to tetrahedral N_4 cluster. So study of this kind of system is obviously very important. Recently, Wodtke's group found strong evidence of photochemical production of cyclic N_3 in the velocity map imaging results on ClN_3 photochemistry.[N Hansen and A.M. Wodtke, private communication] However, there is no experiment concerning the means for photochemical formation of cyclic N_3 ; Also, there is no experiment, which could directly detect the cyclic N_3 . Therefore, theoretical study would be very helpful in providing important information in experimental design and gaining much deeper insights into its photodissociation dynamics. We have applied MRCISD(Q)(15e/12o)/aug-cc-pVTZ method for geometry optimization of the equilibrium, transition states, products for both doublet (D) and quintet (Q) states and seam of crossings between those corresponding states. We studied the non-adiabatic dissociation mechanism on the ground state surface. Five MSXs (minimum of seam of crossing) between Double and Quartet states have been identified on the dissociation and isomerization reaction coordinates. Energetically, all these MSXs are lower in energy than the corresponding TS. One-dimensional Landau-Zener calculations indicate that the spin-forbidden processes will not be appreciated unless the kinetic energy is approaching to zero around the MSX regions; and correspondingly, the lifetime of cyclic N_3 is estimated to be at ps level and could be longer if it has less internal energy. The work was published as paper 11.

An extension of the present work to higher excited states of N_3 has been initiated. Here the emphasis is finding a pathway to generate cyclic N_3 in excited state. The study will continue and will be completed with the renewal grant of the present grant.

b. Cyclic-N₃. Accurate potential energy surfaces and dynamics.

I. An accurate potential energy surface for the ground doublet electronic state up to the energy of the ²A₂/²B₁ conical intersection.

A sophisticated adiabatic ground electronic state potential energy surface for a pure nitrogen ring (cyclic-N₃) molecule is constructed based on extensive high level *ab initio* calculations and accurate three-dimensional spline representation. Most of the important features of the PES are presented using various reduced dimensionality slices in internal hyperspherical coordinates as well as full dimensional iso-energy surfaces. Very significant geometric phase effects are predicted in the spectra of rotational-vibrational states of cyclic N₃. This was published as paper 13.

II. Significant geometric phase effects in the vibrational spectra. All vibrational states are analyzed and assigned in terms of the normal vibration mode quantum numbers. The comparison between these two calculations showed that the standard, BO results, where the geometric phase is totally neglected, are not even qualitatively correct in the case of cyclic-N₃. The shifts of the vibrational eigenvalues (due to the geometric phase effect) are unusually large and exceed 600 cm⁻¹ for several states. Since even the ground vibrational states of the cyclic-N₃ are formed at energies well above the pseudorotation barriers, the geometric phase affects these states too, especially the lowest energy of A₂ symmetry where the shift due to the geometric phase is as large as 286 cm⁻¹. Significant changes have been observed not only in the position, but also in the order of the vibrational states and in the ordering of the fundamental frequencies. Such adverse changes should clearly be seen in the experimental spectra and the comparison with experiment is anticipated. This result has been published as Paper 10.

c. Photodissociation of vinyl radical, ketyl radical and formaldehyde

Potential energy surfaces and dynamics of photodissociation of radical species, vinyl and ketyl radicals, as well as those of the triplet state of formaldehyde have been studied with accurate *ab initio* quantum chemical methods. The work is essentially complete but has not been written up yet. Papers will be prepared and published in the renewal project of the present grant.

d. Photodissociation of HN₃

For nitrogen unlike most elements, the energy of an N–N single bond is substantially less than one-third, and the energy of an N=N double bond is substantially less than two-thirds of an N≡N triple bond. Consequently, all-nitrogen species that form rings at the expense of multiple bonds are subject to a strong chemical driving force toward dissociation to N₂. Not surprisingly, the ability of nitrogen to form cyclic structures has been difficult to observe, directly or indirectly. Several experiments have led to the postulate of a cyclic poly-nitrogen species; but, these have either remained unconfirmed or later been disproved. Therefore, to further explain the interesting experimental observation and as our continuous interests in the theoretical study of the high energy and density materials, we systematically examined the potential energy surfaces of HN₃ and their associated photodissociation processes.

On both of the ground (S₀) and excited (S₁ and T₁) states, non-planar minima featured with cyclic N₃ fragment were identified. The ring closure TS on the S₁ state was calculated to be ~130.2 kcal/mol above the ground state, which agrees with energy threshold (~5.6 eV) for the slow channel observed in Wodtke's experiment. The competitive H migration pathway is only 4.5 kcal/mol higher in energy, but the absence of the HNN bending excitation makes this pathway less important. The dissociation TS leading to the cyclic N₃ product was discovered and about ~5 kcal/mol above the ring closure TS. A brief account of the findings has been published as paper 5 of the publication list.

An extension of the work to cover photodissociation involving higher excited states of HN₃ is in progress but has not been completed. The full account of the PESs of HN₃ will be completed and published in the renewal period of the present grant.

e. Heat of formation of chlorine-isocyanate and the relative stability of isoelectronic molecules.

Calculations show that the difference in energetics between azides (XNNN) and isoelectronic isocyanates (XNCO), X=H, Cl, is due to the weakening of the N-NN bond relative to the N-CO bond, because of the less favored electrostatic and orbital interactions in the former, while the predicted Cl-NCO bond dissociation energy agrees with new experiments. The work has been published as paper 4 of the Publication List.

D. Interaction of Oxygen and Other Small Molecules with Electron and Other Molecules.

This series of studies was mainly supported by another AFOSR grant: Closed-Cycle ElectricOIL Technology AFOSR Contract No. F49620-02-1-0357, but was in part supported by the present grant.

a. Nonadiabatic collision between oxygen molecules.

Potential energy surfaces for interactions of $O_2(X^3\Sigma_g^-, a^1\Delta_g, b^1\Sigma_g^+) + O_2(X^3\Sigma_g^-, a^1\Delta_g, b^1\Sigma_g^+)$ have been calculate with accurate ab initio methods and a mechanism of quenching of excited $O_2(a^1\Delta_g)$ has been proposed. The work has been published as paper 8 of the Publication List. Wave packet quantum dynamics calculation for the $O_2(X^3\Sigma_g^-, a^1\Delta_g, b^1\Sigma_g^+) + O_2(X^3\Sigma_g^-, a^1\Delta_g, b^1\Sigma_g^+)$ collision are in progress and will be continued and completed in the renewal of the present grant.

b. Low energy electron collisions and electronic excitation/de-excitation of oxygen and other diatomic molecules.

R-matrix theory and code have been developed for calculation of integrated and differential cross sections for electronic excitation/de-excitation in low energy electron collisions. The studies on the integrated and differential cross sections for oxygen molecules have been published as paper 2 and 3 of the Publication List, and those for nitrogen molecule as paper 1. Work is continuing for cross sections with polarized electrons as well as those for polyatomic molecules, and will be completed in the renewal of the present grant.

3. Personnel.

Dr. Ioannis Kerkenis, postdoctoral fellow, Department of Chemistry

Zhi Wang, graduate student, Department of Chemistry

Dr. Motomichi Tahsiro, postdoctoral fellow, Department of Chemistry

Dr. Petia Bobadova-Parvanova, postdoctoral fellow, Department of Chemistry

Dr. Stephan Irle, Associate Scientist and Systems Manager, Emerson Center for Scientific Computation

Dr. Jianjun Liu, postdoctoral fellow, Department of Chemistry

Peng Zhang, graduate student, Department of Chemistry (has defended his PhD thesis on August 19, 2005)

Qingfang Wang, graduate student, Department of Chemistry

Martin McCullagh, undergraduate student, Department of Chemistry

4. Publications.

1. M. Tashiro and K. Morokuma, R-matrix calculation of integral and differential cross sections for low-energy electron impact excitations of N_2 molecules, Phys. Rev. A, 75, 012720/1-10 (2007).

2. M. Tashiro, K. Morokuma and J. Tennyson, R-matrix calculation of differential cross sections for low-energy electron collisions with ground and electronically excited O₂ molecules, *Phys. Rev. A* 74, 022706/1-8 (2006).
3. M. Tashiro, K. Morokuma, and J. Tennyson, R-matrix calculation of electron collisions with electronically excited O₂ molecules, *Phys. Rev. A*, 73, 052707/1-8 (2006).
4. Y. Ji, P. Bobadova-Parvanova, C. Larson, P. Samartzis, K. Morokuma^c, J. J.-M. Lin, T.-T. Ching, C. Chadhuri, S.-H. Lee and A. M. Wodtke, The heat of formation of chlorine-isocyanate and the relative stability of isoelectronic molecules: an experimental and theoretical study. *J. Chem. Phys.*, 124, 241106/1-5 (2006).
5. J. Zhang, P. Zhang, Y. Chen, K. Yuan, S. A. Harich, X. Wang, Z. Wang, X. Yang, K. Morokuma, A. M. Wodtke, An experimental and theoretical study of ring closing dynamics in HN₃, *Phys. Chem. Chem. Phys.* 8, 1690-1696 (2006).
6. A. J. Midey, A. I. Fernandez, A. A. Viggiano, P. Zhang and K. Morokuma, Ion Chemistry of NOO⁺, *J. Chem. Phys.* 124, 114313/1-8 (2006).
7. A. J. Midey, A. A. Viggiano, P. Zhang, S. Irle and K. Morokuma, A study of the reaction of N⁺ with O₂: Experimental quantification of NO⁺ (a ³Σ⁺) produced (298-500 K) and computational study of the overall reaction pathways, *J. Phys. Chem. A*, 110, 3080-3086 (2006).
8. J. Liu and K. Morokuma, Ab initio potential energy surfaces of O₂(X³Σ_g⁻, a¹Δ_g, b¹Σ_g⁺) + O₂(X³Σ_g⁻, a¹Δ_g, b¹Σ_g⁺): Mechanism of quenching of O₂ (a¹Δ_g). *J. Chem. Phys.* 123, 204319/1-10 (2005)
9. Liu, P. Zhang, K. Morokuma, and R. D. Sharma, A new mechanism for the production of highly vibrationally excited OH in the mesosphere. An ab initio study of the reactions of O₂ (A³Σ_u⁺ and A'³Δ_u) + H, *J. Chem. Phys.*, 122, 104315/1-7 (2005)
10. D. Babikov, B. K. Kendrick, P. Zhang and K. Morokuma, Cyclic-N₃: II. Significant geometric phase effects in the vibrational spectra. *J. Chem. Phys.*, 122, 044315/1-20 (2005)
11. P. Zhang, K. Morokuma and A. M. Wodtke, High level ab initio studies of unimolecular dissociation of the ground state N₃ radical, *J. Chem. Phys.*, 122, 014106/1-11 (2005).
12. S. Popovic, A. J. Midey, S. Williams, A. Fernandez, A. A. Viggiano, P. Zhang and K. Morokuma, Ion-Molecule Rate Constants and Branching Ratios for the Reaction of N₃⁺ + O₂ from 120 to 1400 K, *J. Chem. Phys.*, 121, 9481-9488 (2004).
13. D. Babikov, P. Zhang and K. Morokuma, Cyclic-N₃: I. An accurate potential energy surface for the ground doublet electronic state up to the energy of the ²A₂/²B₁ conical intersection. *J. Chem. Phys.*, 121, 6743-6749 (2004).
14. K. Fukuzawa, T. Matsushita and K. Morokuma, *Ab initio* Potential Energy Surfaces of the Ion-Molecule Reaction: C₂H₂ + O⁺, *J. Chem. Phys.*, 121, 3117-3129 (2004).
15. S. Williams, W. B. Knighton, A. J. Midey, A. A. Viggiano, S. Irle, Q. Wang and K. Morokuma, Oxidation of Alkyl Ions, C_nH_{2n+1}⁺ (n=1-5), in Reactions with O₂ and O₃ in the Gas Phase, *J. Phys. Chem. A*, 108, 1980-1989 (2004).

5. Interactions/Transactions.

Consultative and advisory functions to other laboratories and agencies, especially Air Force and other DoD laboratories.

We have been in close contact with Dr. Viggiano and Dr. Williams of the Air Force Research Laboratory at the Hanscom Air Force Base concerning the interpretation of their ion-molecule experimental results. We also collaborated with Dr. Sharma of the Air Force Research Laboratory at the Hanscom Air Force Base, and studied computationally the potential energy surface for the reaction

of highly excited states of the oxygen molecule, $O_2(A^3\Sigma_u^+)$ and $O_2(A'^3\Delta_u)$, with a hydrogen atom, as a possible source of highly vibrationally excited state of the OH ($v=10$) species.

6. New inventions and patent disclosures.

None.

7. Honors/Awards.

a. President of the International Academy of Quantum Molecular Science. (This is an organization of about 85 prominent molecular quantum scientists in the world that include five Nobel Prize winners in Chemistry and Physics.) Served for July 2000 – July 2006.

b. Received a Japan Society for Promotion of Sciences Invitation Fellowship for April-June, 2005

e. Received the First Fukui Medal of Asian Pacific Association of Theoretical & Computational Chemists, 2005

c. Listed in top 100 most cited scientists in chemistry for January 1993 - June 30, 2004.
<http://www.in-cites.com/nobel/2004-che-top100.html>