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MOLECULAR INTERACTIONS WITH MANY-BODY METHODS(U)
FLORIDA UNIV GAINESVILLE R J BARTLETT 04 MAR 88
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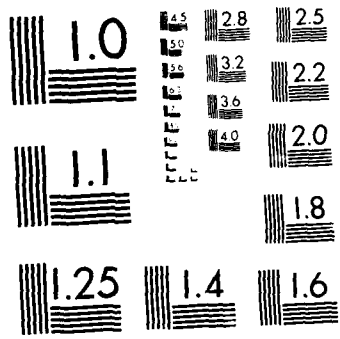
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<p>This report summarized publications and invited presentations supported by our AFOSR grant on "Molecular Interactions with Many-Body Methods." In this effort new many-body methods have been developed to treat open-shell molecules; to apply to properties like moments, polarizabilities, hyperpolarizabilities, spin-densities and spin-spin coupling constants; infra-red spectra; and a variety of applications to interesting molecules including the unknown metastable $N_3H_3^+$ system. The latter molecule, though isoelectronic with ozone and cyclopropane is not known experimentally. However, we find that it should exist in three stable structures. Furthermore, we have predicted its IR spectra to aid in its experimental identification, which should be possible in matrix isolation. Other applications work has focused on the accurate, numerical orbital treatment of anions. (mjm)</p>			
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I. PUBLICATIONS AND PRESENTATIONS SUPPORTED BY AFOSR (1986-present)

- L. Adamowicz and R.J. Bartlett, "Very Accurate Coupled Cluster Calculations for Diatomic Systems with Numerical Orbitals," Nobel Laureate Symposium on Applied Quantum Chemistry, ed. V.H. Smith, H.F. Schaefer III, and K. Morokumo, Reidel, Dordrecht, The Netherlands, pg. 111 (1986).
- S. Kucharski and R.J. Bartlett, "Fifth-Order Many-Body Perturbation and Its Relationship to Various Coupled Cluster Approaches," in Advances in Quantum Chemistry, 18, 281 (1986).
- G.W. Trucks and R.J. Bartlett, "Isomers of Si_2C_2 : An MBPT Study," Mulliken Issue, J. Mol. Structure (Theochem) 135, 423 (1986).
- H. Sekino and R.J. Bartlett, "Hyperpolarizabilities of the Hydrogen Fluoride Molecule: A Discrepancy Between Theory and Experiment?" J. Chem. Phys. 84, 2726 (1986).
- D.H. Magers, R.J. Harrison and R.J. Bartlett, "Isomers and Excitation Energies of C_4 ," J. Chem. Phys. 84, 3284 (1986).
- L. Adamowicz and R.J. Bartlett, "Numerical Coupled Hartree-Fock Study of the Total Electronic and Nuclear Parallel Polarizability and Hyperpolarizabilities for FH, H_2^+ , HD^+ , and D_2^+ Molecules," J. Chem. Phys. 84, 4988 (1986).
- L. Adamowicz and R.J. Bartlett, "Accurate Numerical Orbital MBPT/CC Study of the Electron Affinity of Fluorine and the Dissociation Energy of Hydrogen Fluoride," J. Chem. Phys. 84, 6837 (1986).
- H. Sekino and R.J. Bartlett, "Frequency Dependent Non-linear Optical Properties of Molecules," J. Chem. Phys. 85, 976 (1986).
- L. Adamowicz and R.J. Bartlett, "Coupled-Cluster Calculations of Electron Affinities of LiF," Chem. Phys. Lett. 129, 159 (1986).
- H. Sekino and R.J. Bartlett, "Nuclear Spin-Spin Coupling Constants Evaluated Using Many-Body Methods," J. Chem. Phys. 85, 3945 (1986).
- L. Adamowicz and R.J. Bartlett, "Direct Coupled Cluster Calculations of Excited States," Int. J. Quantum Chem. Symp. 19, 217 (1986).
- E.A. Salter, L. Adamowicz, and R.J. Bartlett, "Comment on MBPT/CC Nickel Calculations," Chem. Phys. Lett. 130, 152 (1986).
- S.J. Cole and R.J. Bartlett, "Comparison of MBPT and Coupled-Cluster Methods with Full CI. II. Polarized Basis Sets," J. Chem. Phys. 86, 873 (1987).
- J. Noga, R.J. Bartlett and M. Urban, "Towards a Full CCSDT Model for Electron Correlation II. CCSDT-n Models," Chem. Phys. Lett. 134, 126 (1987).
- L. Adamowicz and R.J. Bartlett, "MBPT and Coupled-Cluster Calculation on the Neon Atom with Numerical Orbitals," Int. J. Quantum Chem. 31, 173 (1987).

E.A. Salter, H. Sekino and R.J. Bartlett, "Orbital Relaxation and Property Evaluation by Coupled-Cluster Methods," J. Chem. Phys. 87, 502 (1987).

J. Noga and R.J. Bartlett, "The Full CCSDT Model for Molecular Electronic Structure," J. Chem. Phys. 86, 7041 (1987).

M. Rittby and R.J. Bartlett, "An Open-Shell Restricted Coupled-Cluster Method: Application to Ionization Potentials in N₂," J. Phys. Chem., in press.

L. Adamowicz and R.J. Bartlett, "Excited State Electron Affinities of NaF, LiCl and NaCl," J. Chem. Phys. 88, 313 (1988).

R.J. Bartlett, S.J. Cole, G. D. Purvis, W.C. Ermler, H.C. Hsieh and I. Shavitt, "The Quartic Force Field of H₂O Determined by Many-Body Methods II. Effects of Triple Excitations," J. Chem. Phys. 87, 6579 (1987).

D.H. Magers, E.A. Salter, R.J. Bartlett, C. Salter, B.A. Hess and L.J. Schaad, "Do Stable Isomers of N₃H₃ Exist?," J. Am. Chem. Soc., in press.

T. Pluta, A.J. Sadlej and R.J. Bartlett, "Polarizability of OH⁻," Chem. Phys. Lett. 143, 91 (1988).

G.D. Purvis III, H. Sekino and R.J. Bartlett, "Multiplicity of Many-Body Wavefunctions Using Unrestricted Hartree-Fock Reference Functions," Coll. of Czechoslovak Chem. Comm., in press.

M. Urban and R.J. Bartlett, "MBPT and Coupled-Cluster Investigation of Isomerization Reactions: HCN•HNC, BH₃CH⁻•BH₃NC⁻ and HCNBH₃•HNCBH₃," J. Am. Chem. Soc., submitted.

G.W. Trucks, J. Noga and R.J. Bartlett, "Convergence of Coupled Cluster Singles, Doubles and Triples Method," Chem. Phys. Lett., in press.

INVITED PRESENTATIONS (1986 - present)

Sept.	1988	ACS Conference on Analytical Derivatives and Molecular Properties, Los Angeles, CA.
Aug.	1988	Sixth International Congress on Quantum Chemistry, Jerusalem, Israel.
June	1988	Workshop on Quantum Chemistry, Basic Aspects, Actual Trends, Girona, Spain.
Feb.	1988	Workshop and Symposium on Aspects of Many-Body Effects in Molecules and Extended Systems, Calcutta, India.
Sept.	1987	National ACS Meeting, Symposium on Bound and Temporary Anions in Chemical Systems, New Orleans, LA.
July	1987	American Conference on Theoretical Chemistry, Gull Lake, MN.
June	1987	The Ninth Annual West Coast Theoretical Chemistry Conference, Berkeley, CA.
May	1987	Fifth School of Advanced Methods of Quantum Chemistry, "Frontiers of Atomic and Molecular Structure Theory," Bachotek, Poland.
April	1987	National ACS Meeting, Symposium on Applications of New Methods for Correlated <u>Ab Initio</u> Studies of Large Molecules, Denver, CO.

April 1987 National APS Meeting, Division of Atomic Molecular and Optical Physics, Symposium on Many-Body Physics, Crystal City, VA.
 March 1987 Parr/Eliel Symposium, Chapel Hill, NC.
 June 1986 Canadian Symposium on Theoretical Chemistry, Toronto, Ontario, Canada
 April 1986 Workshop on Interface between Electronic Structure and Dynamics, Snowbird, Utah.

III. Non-refereed Papers - None

IV. Honors

Rodney J. Bartlett has been promoted from Professor to Graduate Research Professor of Chemistry and Physics. The latter rank, which is the highest offered by the University of Florida, is held by only 2% of the faculty.

Three of Dr. Bartlett's papers (published 1978-1981) and supported by AFOSR have recently been designated as Science Citations Classics. Classics are determined by frequency of citation by other scientists and must be among the most cited papers in their respective journals. His paper in Physica Scripta 21, 255 (1980), "Molecular Applications of Coupled-Cluster and Many-Body Perturbation Methods," in the Proceedings of Nobel Symposium Issue, is the third most cited paper in the history of that journal, being cited over 160 times. His paper from the International Journal of Quantum Chemistry 14, 561 (1978), "Many-Body Perturbation Theory, Coupled Pair Many Electron Theory, and the Importance of Quadruple Excitations for the Correlation Problem," has been cited over 200 times, and is the eighth most cited paper in that journal's history. His review in Annual reviews of Physical Chemistry 32, 359 (1981), "Studies of Electron Correlation in Molecules with Many-Body Perturbation Theory and Coupled Cluster Methods," has also been cited over 200 times, and is the twelfth most cited paper in that review series.

V. Patent Requests - None

VI. Patents Granted - None

VII. Students Supported by Grant

D. Bernholdt
 D. Magers
 S. Zarrabian
 E.A. Salter
 G. Trucks
 T. Pluta

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VIII. Postdoctoral Associates Supported by Grant

S. Pal
M. Rittby
G. Fitzgerald
L. Adamowicz
C. Sosa
J. Watts
R.E. Brown (visiting research associate)
S. Kucharski (visiting research associate)

IX. Students Under AFOSR Support Graduated

S. Zarrabian - Convergence to the Solution of the Eigenvalue Problem by
Perturbative Methods (December, 1987)

E.A. Salter - Analytical One-Electron Response Properties, Molecular
Gradients and Force Constants in Many-Body Methods
(May, 1988)

END

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