Development of Many-Body Methods for Flame Chemistry and Large Molecule Applications

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Ab initio MBPT and coupled cluster (CC) gradient methods have been developed for studies of potential energy surfaces for molecules. Example calculations include NH_3, SiC_2, B_2H_6, and BH_3 and nucleic acid bases among others. Detailed first principle correlated predictions of IR spectra, frequencies and intensities are reported. These methods are used to search for the unknown N_3H moleculle. It is found that it should exist in three stable forms. Detailed IR spectra are provided to aid in its identification. The same methods demonstrate that the currently accepted experimental spectra of the
20. Abstract (continued...)

transient BH$_3$ molecule is misinterpreted.

Additional work focused on the development and use of MBPT/CC methods in large molecule studies. Methods are developed based upon localized orbitals that should make it possible to study much larger molecules than is currently possible.

Other MBPT/CC results are reported for the relative stabilities of nucleic acid bases, particularly cytosine. Such tautomers are important in the theory of point mutations that can lead to tumor formation. It is demonstrated that the effects of electron correlation are crucial in determining accurate energy differences.
DEVELOPMENT OF MANY-BODY METHODS FOR FLAME CHEMISTRY
AND LARGE MOLECULE APPLICATIONS

FINAL REPORT

3/1/84 - 2/28/87

Rodney J. Bartlett

U.S. ARMY RESEARCH OFFICE

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Gainesville, FL 32611

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I. STATEMENT OF THE PROBLEM

There have been three primary objectives of our recent contract to ARO:

- The development of analytical derivative methods for coupled-cluster (CC) and many-body perturbation theory (MBPT) wavefunctions. Such methods are essential in the location of minima and transition states on potential energy surfaces, and in the first-principle prediction of vibrational spectra.
- Applications of the CC/MBPT methods and associated analytical derivative methods to transient molecules, such as those present in the combustion of rocket fuels, in interstellar space, or occur as reaction intermediates.
- The development of CC/MBPT methods for large molecule applications.

We have made a number of achievements in these three areas. The following highlights several of them.

II. SUMMARY OF SOME IMPORTANT RESULTS

A. During the course of this contract we presented the first report of MBPT(3) and D-MBPT(4) (i.e. fourth-order MBPT limited to double excitations) analytical gradients [B1].* These were illustrated in calculations on H₂O and CH₄. In our earlier work for ARO [1-4]+ the D-MBPT(4) method subject to finite nuclear displacement was found to be quite accurate in structure determinations for flame species like HCO, H₂CO, H₃CO, CH₂N, among others. Hence, the analytical equivalent should be an inexpensive but quite useful level of approximation (see E below).

*B references refer to the bibliography of papers supported by ARO on page 20.
+Other references are listed on page 24.
B. We also reported the first CCD (coupled-cluster double) analytical gradients [B3], and illustrated this method to H₂CO. CC/MBPT methods scale correctly with molecular size but are non-variational. Consequently, the simplifications that occur for variational methods cannot be used, requiring that some rather different methods be developed than in SCF, MCSCF and CI.

C. The above application of CC/MBPT theory employed a procedure that would require roughly the equivalent of a CC or MBPT calculation for each distinct vibrational-rotational degree of freedom. This is not a practical way to solve the analytical CC/MBPT problem, so we presented a very general formulation that demonstrates that all energy derivatives with respect to 3N nuclear displacements may be computed with only about twice the effort required by the CC/MBPT energy calculation [B4]. Only this simplification makes it possible to use the very accurate CC/MBPT methods for searching energy surfaces for molecules with several degrees of freedom.

D. Building upon this development, we presented a paper with detailed equations for any level of CC theory and extracted the full fourth-order (i.e. SDTQ-MBPT(4)) gradient formula as a special case [B8].

E. This formulation is very different than our original analytical gradient method, and it requires substantial computational effort to implement. Just recently, we have achieved its implementation at the MBPT(3) and D-MBPT(4) levels [B14]. Since both are recognized as a very high level of correlated theory for molecular structures and transition states, computer codes we have written should be extensively applicable to a wide range of chemically interesting problems.
F. In another totally new development, we developed the first methods for the analytical evaluation of MBPT(2) second derivatives [B5,B6]. No routinely applicable correlated second derivative method was available prior to this work. Initial illustrations were to \( \text{H}_2\text{CO} \) [B5] and \( \text{N}_2\text{H}_2 \) [B6].

G. In a serious application of our analytical MBPT(2) second derivative methods to a large basis set study of the interstellar species \( \text{SiC}_2 \), we showed that the triangular form of this molecule, observed experimentally by Smalley, was indeed a minimum on the MBPT(2) energy surface [B7]. This conclusion differs from that of Grey and Schaefer [5] who found the triangular form to correspond to a transition state at the SCF or GVB level, but they assumed that a higher level of theory would find the triangular structure as a minimum, once substantial amounts of correlation were included. Via MBPT(2), we find the triangular form to be a true minimum. We also predict the experimental vibrational frequencies. These are found to be in excellent agreement with an experiment [6] which we found after our results had appeared (See Table 1).

H. Since analytical energy second derivatives with respect to nuclear displacement (i.e. \( \frac{\partial^2 E}{\partial x_{\alpha} \partial y_{\beta}} \)) provides the harmonic force constants for molecules, a generalization to the mixed second derivatives relative to a nuclear displacement and an electric field, (i.e. \( \frac{\partial^2 E}{\partial x_{\alpha} \partial F_z} \)) provide the dipole derivatives required to obtain the intensity of a vibrational transition. We have recently added these terms to provide MBPT(2) level
Table 1
SiC$_2$ DZ+P $^1$A$_1$ RING STRUCTURE

<table>
<thead>
<tr>
<th></th>
<th>SCF$^{(a)}$</th>
<th>GVB$^{(a)}$</th>
<th>MBPT(2)$^{(b)}$</th>
<th>Expt.$^c$</th>
<th>Expt.$^d$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(C-C)</td>
<td>1.256</td>
<td>1.267</td>
<td>1.294</td>
<td>1.268</td>
<td>1.250</td>
</tr>
<tr>
<td>R(Si-C)</td>
<td>1.835</td>
<td>1.821</td>
<td>1.835</td>
<td>1.837</td>
<td>1.812</td>
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<tr>
<td>C-Si-C</td>
<td>40.0</td>
<td>40.7</td>
<td>41.3</td>
<td>40.4</td>
<td>40.4</td>
</tr>
<tr>
<td>C-C str.</td>
<td>1976</td>
<td>1892</td>
<td>1720</td>
<td>1742$^e$</td>
<td></td>
</tr>
<tr>
<td>Si-C A$_1$ str.</td>
<td>851</td>
<td>873</td>
<td>839</td>
<td>852$^e$</td>
<td></td>
</tr>
<tr>
<td>Ring Open.</td>
<td>3281</td>
<td>1711</td>
<td>183</td>
<td></td>
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IR intensities as well [B12]. These techniques make it possible to routinely predict IR spectra for molecules while including much of the essential electron correlation effects.

I. The unknown, transient molecule $N_3H_3$, occupies an essential place in the understanding of the chemical bond and as a reaction intermediate, since it is isoelectronic with ozone ($O_3$), cyclopropane and propene ($C_3H_6$). It may exist in three forms, a cyclic ring, triaziridine; an open form, triimide, and a triazene structure (see Fig. 1). None have ever been observed. Using our MBPT(2) first and second derivatives we have determined that all three forms of $N_3H_3$ are local minima on the potential energy surface and defined this detailed structure. Using high-level MBPT(4) and CCSD+T(CCSD) methods we predict that the triazene isomer is the lowest in energy, being more stable than the triimide form by 17.30 and triaziridine by 41.24 (see Table 2). Furthermore, we have predicted the IR spectra of the three $N_3H_3$ isomers (see Figs. 2-7) at the SCF and the correlated MBPT(2) level. Note the dramatic differences between the SCF and the correlated MBPT(2) predictions, particularly for triaziridine and triimide. The differences pertain to the intensities and the frequencies. Since we know the error in the frequencies at the MBPT(2) level is typically less than 5% compared to 10-20% for SCF predictions (see Table 3), we believe the MBPT(2) results to be sufficiently accurate to be used as a guide to experimental spectroscopists to identify $N_3H_3$ in interstellar space or in matrix isolation.

J. In two other studies [B9,B11] we have used our MBPT(2) analytical second derivative methods and high level $C^r$ calculations to further characterize the decomposition of $B_2H_6 \rightarrow 2BH_3$. A particularly interesting conclusion from this study is that the accepted experimental IR spectra [7] of the
<table>
<thead>
<tr>
<th>Isomer</th>
<th>MBPT(2)</th>
<th>MBPT(4)</th>
<th>CCSD</th>
<th>CCSD+</th>
<th>T(CCSD)</th>
</tr>
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<tbody>
<tr>
<td>Triaziridine</td>
<td>40.96</td>
<td>41.43</td>
<td>40.84</td>
<td>41.24</td>
<td>17.30</td>
</tr>
<tr>
<td>Triimide</td>
<td>13.48</td>
<td>20.01</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>Triazene</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
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</tbody>
</table>

All above calculations used a DZP basis set.
TRIAZIRIDINE E(2) IR SPECTRUM

VIBRATIONAL FREQUENCY (cm⁻¹)
TRIIMIDE SCF IR SPECTRUM

VIBRATIONAL FREQUENCY (cm\(^{-1}\))

ABSORBANCE
TRIMIDE E(2) IR SPECTRUM

Fig. 5

ABSORBANCE

VIBRATIONAL FREQUENCY (cm⁻¹)

1.8 1.8 1.4 1.2 1.0 0.8 0.6 0.4 0.2 0.0

3500 3000 2500 2000 1500 1000 500
TRIAZENE SCF IR SPECTRUM

VIBRATIONAL FREQUENCY (cm$^{-1}$)

ABSORBANCE

Fig. 6
### Table 3

**AVERAGE PERCENTAGE ERROR FOR VIBRATIONAL FREQUENCIES RELATIVE TO EXPERIMENT (ANHARMONIC)**

*(DZP BASIS SETS)*

<table>
<thead>
<tr>
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<th>SCF</th>
<th>MBPT(2)</th>
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<tr>
<td>HNO</td>
<td>20.5</td>
<td>4.7</td>
</tr>
<tr>
<td>CF₂</td>
<td>13.5</td>
<td>3.1</td>
</tr>
<tr>
<td>N₂H₂</td>
<td>15.5</td>
<td>4.2</td>
</tr>
<tr>
<td>SiC₂</td>
<td>6.7</td>
<td>1.3</td>
</tr>
<tr>
<td>CH₃NO₂</td>
<td>12.9</td>
<td>4.9</td>
</tr>
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transient BH$_3$ molecule is erroneous! Since BH$_3$ can only be made by
dissociation, the experiment produced BH$_3$ from the decomposition of
BH$_3$CO. After subtracting all peaks associated with CO, B$_2$H$_6$, and various
impurities, one strong peak and three weak IR peaks remained. These were
ascribed to BH$_3$. Our calculation for BH$_3$ (Table 4) gives good agreement
in terms of intensities and frequencies with three of the peaks, but the
strong peak occurs at an incorrect frequency compared to our calculation.
Furthermore, our prediction of its intensity shows that it would be less
than one-tenth as intense as the weak peaks, meaning it could not have
been observed in the experiment. This study attests to the power of
modern-day ab initio methods to offer a reliable voice in resolving
experimental discrepancies. In Table 5 are presented MBPT(2) frequencies
and intensities for B$_2$H$_6$ and B$_2$D$_6$, showing the exceptional agreement we
achieve.

K. Under this contract we have also devoted substantial effort to approaches
for providing ab initio correlated predictions of energies and properties
for large molecules. Since many-body methods scale properly with
molecular size, unlike CI methods, they offer an appropriate vehicle to
study correlation effects in large molecules. The basic idea of such
large molecule methods is to require some form of electron pair
localization to make most of the molecular integrals involving disjoint
parts of a molecule vanish [B2]. By so doing, the difficulty of an ab
initio calculation scales roughly as the square of the number of bonds
($\sim N^2$), rather than as $-N^6$ where $N\gg M$ is the number of basis functions.
In a series of studies on prototype systems C$_2$H$_6$, C$_2$H$_4$ and C$_2$H$_2$ we have
shown that even very crude selections of localized orbitals could be used
with CC methods to obtain the same accuracy as the conventional choice of
TABLE 4: MBPT(2) harmonic vibrational frequencies, $\omega_c$, and infrared absorption intensities, $I_c$, calculated for $^{11}$BH$_3$ using the 6-31G** basis set. Also included are the observed fundamentals, $\nu_{obs}$, and intensities, $I_{obs}$. Units are the same as in table 4.

<table>
<thead>
<tr>
<th>Mode</th>
<th>Type</th>
<th>$\omega_c$</th>
<th>$\nu_{obs}$</th>
<th>$I_c$</th>
<th>$I_{obs}$</th>
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<tr>
<td>$A_1'$</td>
<td>stretch</td>
<td>2671</td>
<td>2623</td>
<td>b</td>
<td>b</td>
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<tr>
<td>$A_2''$</td>
<td>bend</td>
<td>1207</td>
<td>1125</td>
<td>113</td>
<td>v</td>
</tr>
<tr>
<td>$E'$</td>
<td>stretch</td>
<td>2817</td>
<td>2808</td>
<td>259</td>
<td>v</td>
</tr>
<tr>
<td>$E'$</td>
<td>bend</td>
<td>1273</td>
<td>1604</td>
<td>42</td>
<td>s</td>
</tr>
</tbody>
</table>

a) Taken from ref. [7]. Intensities are given as: v-weak, s-strong.
b) Zero in double-harmonic approximation.
Table 5. Calculated HBPT(2) harmonic frequencies, ω_c, and infrared absorption intensities, I_c, for $^{11}B_2H_6$ and $^{11}B_2D_6$ using the 6-31G** basis set. Also included are frequencies of the observed fundamentals, ω_obs, harmonic frequencies calculated from the experimental quadratic force field, ω'_obs, and observed intensities, I'_obs. Experimental results from ref. [29]. Frequencies in cm$^{-1}$, theoretical intensities in km/mol.

<table>
<thead>
<tr>
<th>Fundamental</th>
<th>$ω_c$</th>
<th>$ω'_obs$</th>
<th>$ω'_obs$</th>
<th>$ω_c/ω'_obs$</th>
<th>$I_c$</th>
<th>$I'_obs$</th>
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<tr>
<td>$B_2H_6$</td>
<td>2150</td>
<td>1906</td>
<td>2622</td>
<td>2089</td>
<td>1.041</td>
<td>1.044</td>
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<tr>
<td>$B_2D_6$</td>
<td>2270</td>
<td>1620</td>
<td>2133</td>
<td>2088</td>
<td>1.059</td>
<td>1.059</td>
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<tr>
<td>$B_2H_6$</td>
<td>1260</td>
<td>969</td>
<td>1207</td>
<td>911</td>
<td>1.044</td>
<td>1.044</td>
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<tr>
<td>$B_2D_6$</td>
<td>849</td>
<td>753</td>
<td>796</td>
<td>717</td>
<td>1.059</td>
<td>1.059</td>
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<tr>
<td>$B_2H_6$</td>
<td>870</td>
<td>652</td>
<td>850</td>
<td>602</td>
<td>1.034</td>
<td>1.033</td>
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<tr>
<td>$B_2D_6$</td>
<td>1976</td>
<td>1419</td>
<td>1814</td>
<td>1309</td>
<td>1.088</td>
<td>1.084</td>
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<tr>
<td>$B_2H_6$</td>
<td>901</td>
<td>720</td>
<td>870</td>
<td>712</td>
<td>1.026</td>
<td>1.027</td>
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<tr>
<td>$B_2D_6$</td>
<td>2030</td>
<td>1121</td>
<td>2703</td>
<td>2031</td>
<td>1.067</td>
<td>1.064</td>
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<tr>
<td>$B_2H_6$</td>
<td>1609</td>
<td>746</td>
<td>968</td>
<td>716</td>
<td>1.042</td>
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<td>$B_2D_6$</td>
<td>378</td>
<td>266</td>
<td>376</td>
<td>263</td>
<td>0.997</td>
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<tr>
<td>$B_2H_6$</td>
<td>2187</td>
<td>2115</td>
<td>2699</td>
<td>2013</td>
<td>1.047</td>
<td>1.051</td>
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<td>$B_2D_6$</td>
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<td>776</td>
<td>934</td>
<td>742</td>
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<td>1.046</td>
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<td>$B_2H_6$</td>
<td>2401</td>
<td>1569</td>
<td>1984</td>
<td>1402</td>
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<td>$B_2D_6$</td>
<td>1023</td>
<td>737</td>
<td>993</td>
<td>733</td>
<td>1.030</td>
<td>1.033</td>
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<tr>
<td>$B_2H_6$</td>
<td>1067</td>
<td>769</td>
<td>1041</td>
<td>741</td>
<td>1.044</td>
<td>1.038</td>
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<tr>
<td>$B_2D_6$</td>
<td>2716</td>
<td>1944</td>
<td>2611</td>
<td>1895</td>
<td>1.040</td>
<td>1.042</td>
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<tr>
<td>$B_2H_6$</td>
<td>1810</td>
<td>1327</td>
<td>1652</td>
<td>1227</td>
<td>1.101</td>
<td>1.081</td>
</tr>
<tr>
<td>$B_2D_6$</td>
<td>1252</td>
<td>927</td>
<td>1196</td>
<td>887</td>
<td>1.047</td>
<td>1.045</td>
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</table>

a) Taken from ref. [28]. Intensities are given as: m-medium, s-strong, vs-very strong.
b) Zero in double-harmonic approximation.
c) Not observed.
SCF orbitals [B2]. Furthermore, various extensions of these techniques can be proposed that will restrict the correlation treatment to certain regions of space. There is the potential for an important development in this area for large molecules that should be pursued in future work.

L. An important problem in the theory of point mutations is the tendency for bases of DNA, like cytosine to tautomerize (see Fig. 8). The cyt form is a rare tautomer of cytosine which will not replicate properly, often leading to tumor formation. Using some of our large molecule methods, we have studied the effects of electron correlation on this tautomerization using models of cytosine, adenine and uracil, as well as cytosine itself [B10]. We find that uniformly, the effects of electron correlation are greater for the amino (cyt) than the imino (cyt*) forms. Similarly, correlation favors lactim forms of uracil over lactam forms. Unlike uracil, the very slight energy differences between the two forms of cytosine prohibit any definitive conclusions about relative stability to be drawn without extensive calculations, but it is apparent that electron correlation which accounts to ~1000 kcal/mol in cytosine will be essential in understanding the frequency of tautomerization. Additional studies are devoted toward predicting IR spectra of such complex molecules.
Tautomeric Pairs of Nucleic Acid Bases of DNA

Ura ↔ Ura*  (Thy) ↔ (Thy*)

Gua ↔ Gua*

Cyt ↔ Cyt*

Ade ↔ Ade*

Fig. 8
III. PUBLICATIONS SUPPORTED BY ARO (1984-1987)

BIBLIOGRAPHY


### IV. R.J. BARTLETT INVITED RESEARCH PRESENTATIONS SUPPORTED BY ARO (1984-1987)

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<tr>
<td>April</td>
<td>1987</td>
<td>National ACS Meeting</td>
<td>Denver, CO</td>
<td>&quot;Application of New Methods for Correlated Ab Initio Studies of Large Molecules Using an FPS Scientific Computer.&quot;</td>
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<tr>
<td>April</td>
<td>1986</td>
<td>Workshop on Interface between Electronic Structure and Dynamics</td>
<td>Snowbird, Utah</td>
<td>&quot;Analytical Derivative Methods and Coupled Cluster Theory.&quot;</td>
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<tr>
<td>June</td>
<td>1985</td>
<td>Symposium on Molecular Spectroscopy</td>
<td>Ohio State University</td>
<td>&quot;Many-Body Studies of Molecular Force Constants, Infra-red Intensities, and Polarizabilities.&quot;</td>
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<tr>
<td>April</td>
<td>1985</td>
<td>Fulbright Distinguished Lecturer</td>
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<td>Two lectures.</td>
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<tr>
<td>Dec.</td>
<td>1984</td>
<td>Nobel Laureate Symposium on Applied Quantum Chemistry</td>
<td>Joint Meeting, Pacific Basin Chemical Societies, Honolulu, HI</td>
<td>&quot;Radical Studies with Many-Body Methods.&quot;</td>
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<tr>
<td>Oct.</td>
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<td>NSF Workshop on Future Directions for Supercomputer Use in Chemistry</td>
<td>Evanston, IL</td>
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<td>April</td>
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<tr>
<td>March</td>
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<td>International Symposium on the Quantum Theory of Matter</td>
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The following co-authored papers supported by ARO were presented by members of the Bartlett research group.

**Fifth American Conference on Theoretical Chemistry, June 15-20, 1984**

- **William Laidig**  
  **Analytical Gradients for the Coupled Cluster Method**

**Sanibel Symposia, March 14-23, 1985**

- **Robert Harrison**  
  **Coupled Cluster and MBPT Analytic Energy Second Derivatives**
- **George Fitzgerald**  
  **Gradients of Coupled Cluster Energies**
Sanibel Symposia, March 6-15, 1986

George Fitzgerald  Analytic Energy Gradient Methods for General Coupled Cluster Energies

David Magers  Isomers and Vibrational Spectra of $N_3H_3$

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Ludwik Adamovicz  Coupled Cluster Studies on Excited States of Polar Diatomic Anions

Southeastern Theoretical Chemistry Association (SETCA) Conference
May 22-24, 1986

E.A. Salter  Analytic Evaluation of Infrared Intensities

D. Magers  Structure and Spectra of $N_3H_3$: Does It Exist?

V. PARTICIPATING SCIENTIFIC PERSONNEL

Graduate Students:  David Magers, E. Alan Salter
(Ph.D. degrees expected 1987)

David Bernholdt
(Ph.D. expected 1991)

Postdoctoral Research Associates:  George Fitzgerald, Robert Harrison, Sam Cole, Ludwik Adamovicz
VI. ADDITIONAL REFERENCES


THE VIEW, OPINIONS, AND/OR FINDINGS CONTAINED IN THIS REPORT ARE THOSE OF THE AUTHOR(S) AND SHOULD NOT BE CONSTRUED AS AN OFFICIAL DEPARTMENT OF THE ARMY POSITION, POLICY, OR DECISION, UNLESS SO DESIGNATED BY OTHER DOCUMENTATION.
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