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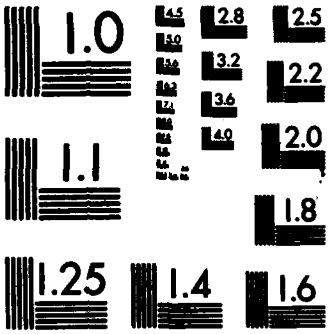

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19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

coupled-cluster; many-body perturbation theory (MBPT); ab initio; quantum chemistry; gradients; transient molecules; flame chemistry; molecular structure; molecular spectra; N_3H_3; SiC_2; B_2H_6; BH_3; infra-red spectra; vibrational intensities; vibrational frequencies.

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Ab initio MBPT and coupled cluster (CC) gradient methods have been developed for studies of potential energy surfaces for molecules. Example calculations include N_2H_2, 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_3 molecule. 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

ove

20. Abstract (continued...)

contd

transient BH_3^{η} 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.

ARO 21033.12-PH

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

CONTRACT NUMBER: #DAAG29-84-K-0025

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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 H_2O and CH_2. 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, H_2CO, H_3CO, CH_2N, among others. Hence, the analytical equivalent should be an inexpensive but quite useful level of approximation (see E below).

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*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 H_2CO. 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 H_2CO [B5] and N_2H_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 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 Grev 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 <u>predict</u> 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. $\partial^2 E/\partial X_\alpha \partial Y_\beta$) 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. $\partial^2 E/\partial X_\alpha \partial F_z$) 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 $^1A_1$ RING STRUCTURE

	SCF[a]	GVB[a]	MBPT(2)[b]	Expt.[c]	Expt.[d]
(C-C)	1.256	1.267	1.294	1.268	1.250
R(Si-C)	1.835	1.821	1.835	1.837	1.812
C-Si-C	40.0	40.7	41.3	40.4	40.4
C-C str.	1976	1892	1720	1742[e]	
Si-C A_1 str.	851	873	839	852[e]	
Ring Open.	328i	171i	183	---	

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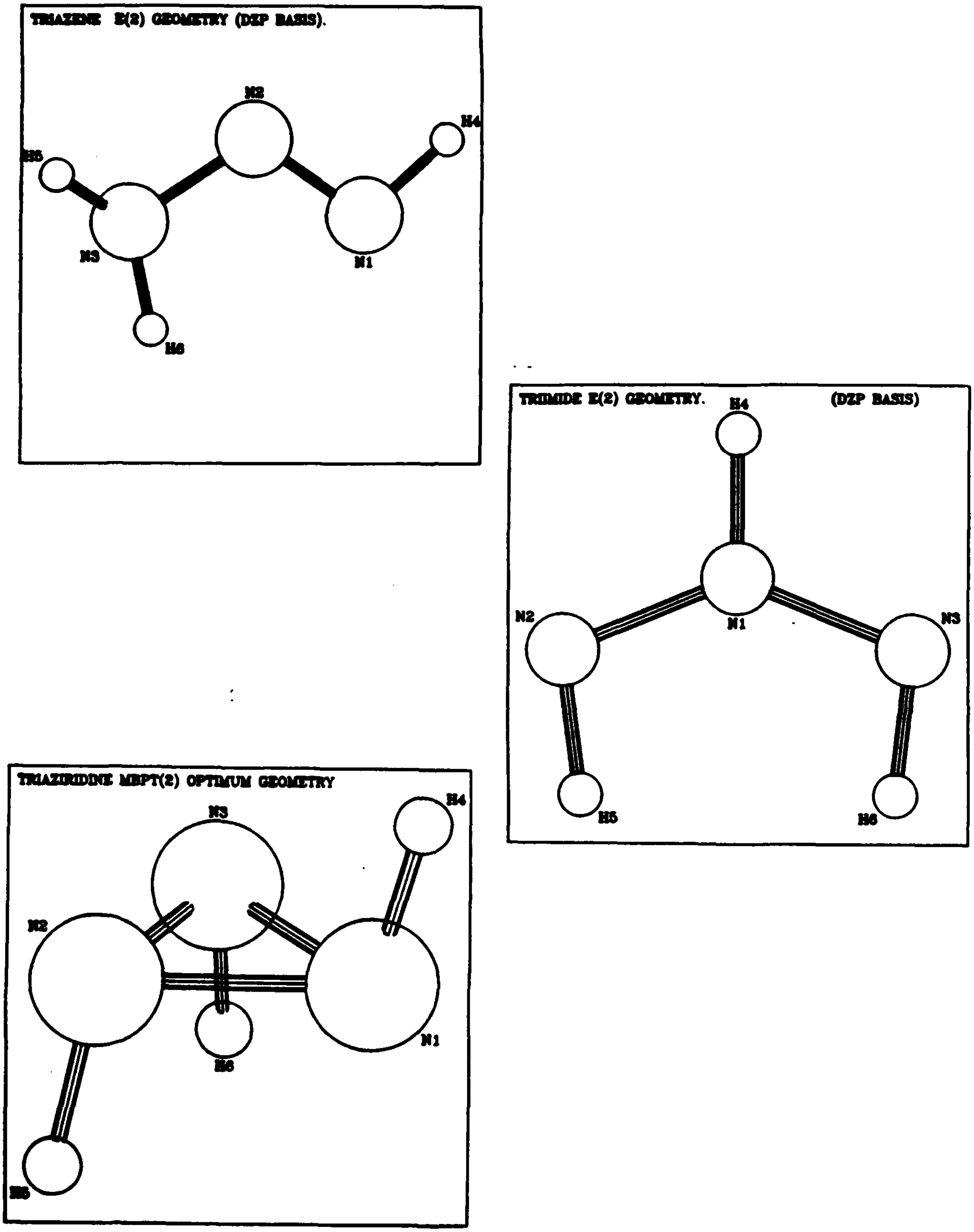
IR intensities as well [B12]. These techniques make it possible to routinely predict IR spectra for molecules while including much of the essential electron correlation effects.

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 CC 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



TRIAZENE E(2) GEOMETRY (DZP BASIS).

TRIIMIDE E(2) GEOMETRY. (DZP BASIS)

TRIAZIRIDINE MBPT(2) OPTIMUM GEOMETRY

Fig. 1

TABLE 2

RELATIVE ENERGIES OF N_3H_3 ISOMERS AT MBPT(2) OPTIMUM GEOMETRIES

Isomer	Relative Energy in kcal				
	MBPT(2)	SDQ–MBPT(4)	SDTQ–MBPT(4)	CCSD	CCSD+T(CCSD)
Triaziridine	40.96	41.21	41.43	40.84	41.24
Triimide	13.48	20.01	15.64	20.58	17.30
Triazene	0.00	0.00	0.00	0.00	0.00

All above calculations used a DZP basis set.

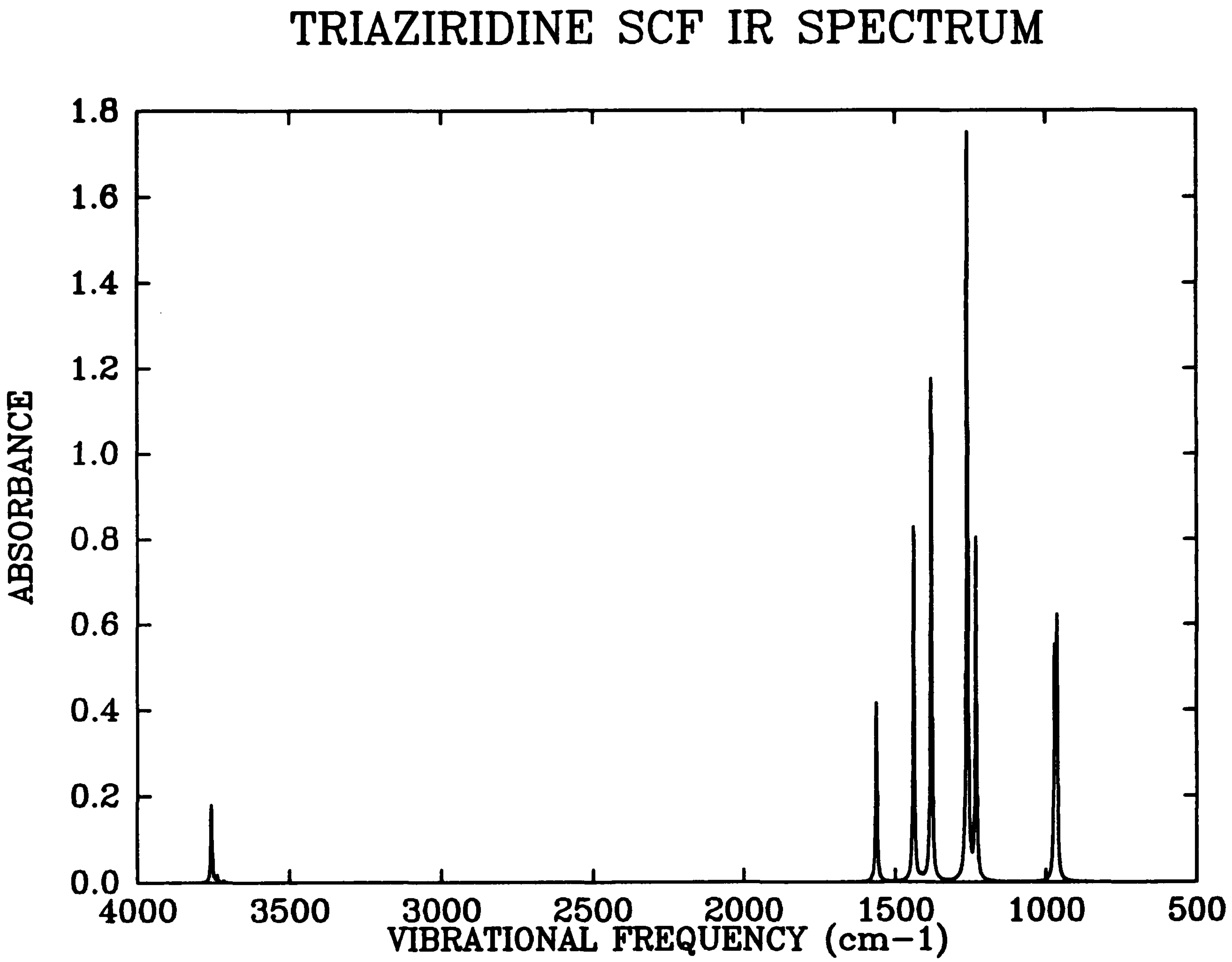

TRIAZIRIDINE SCF IR SPECTRUM

Fig. 2

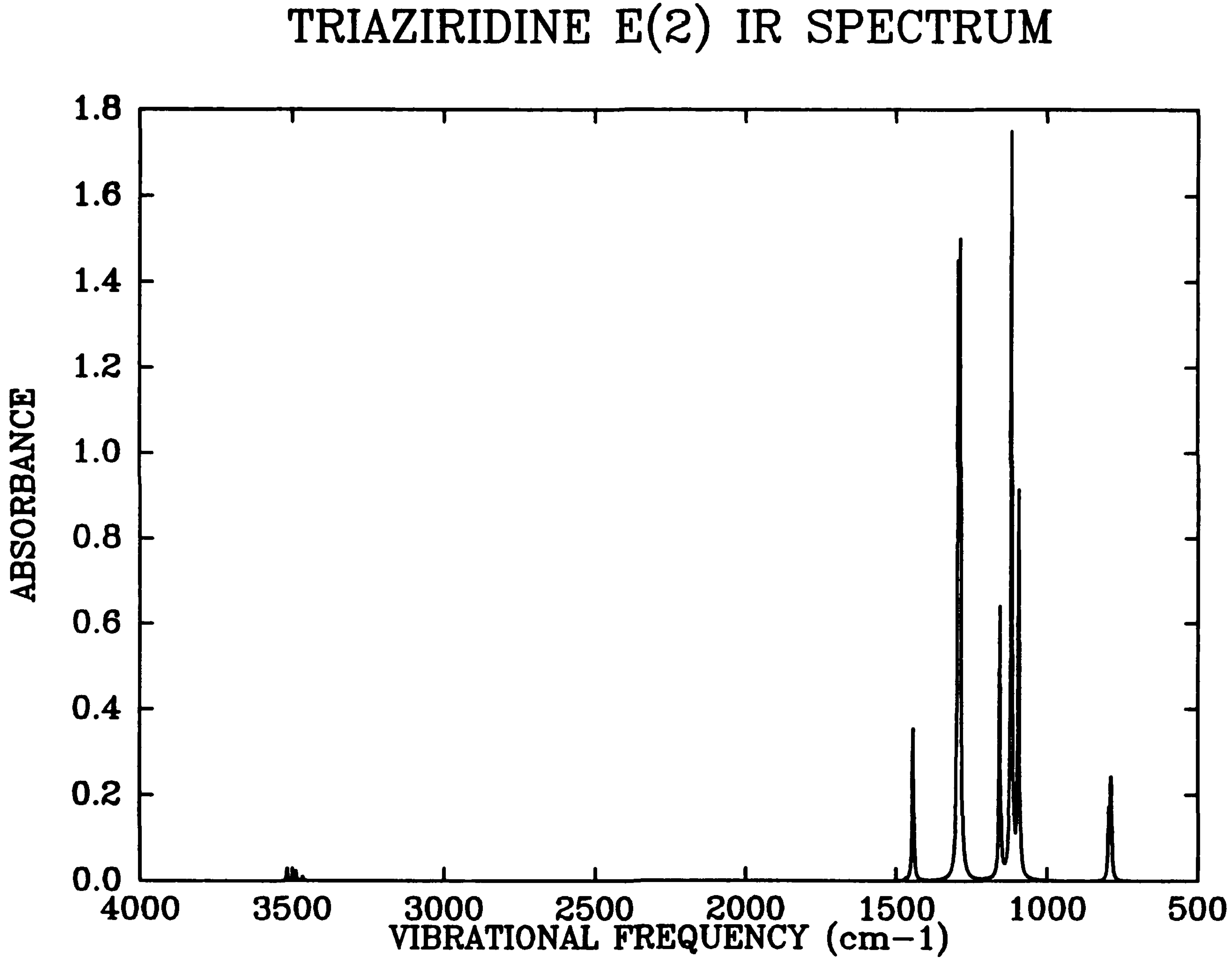
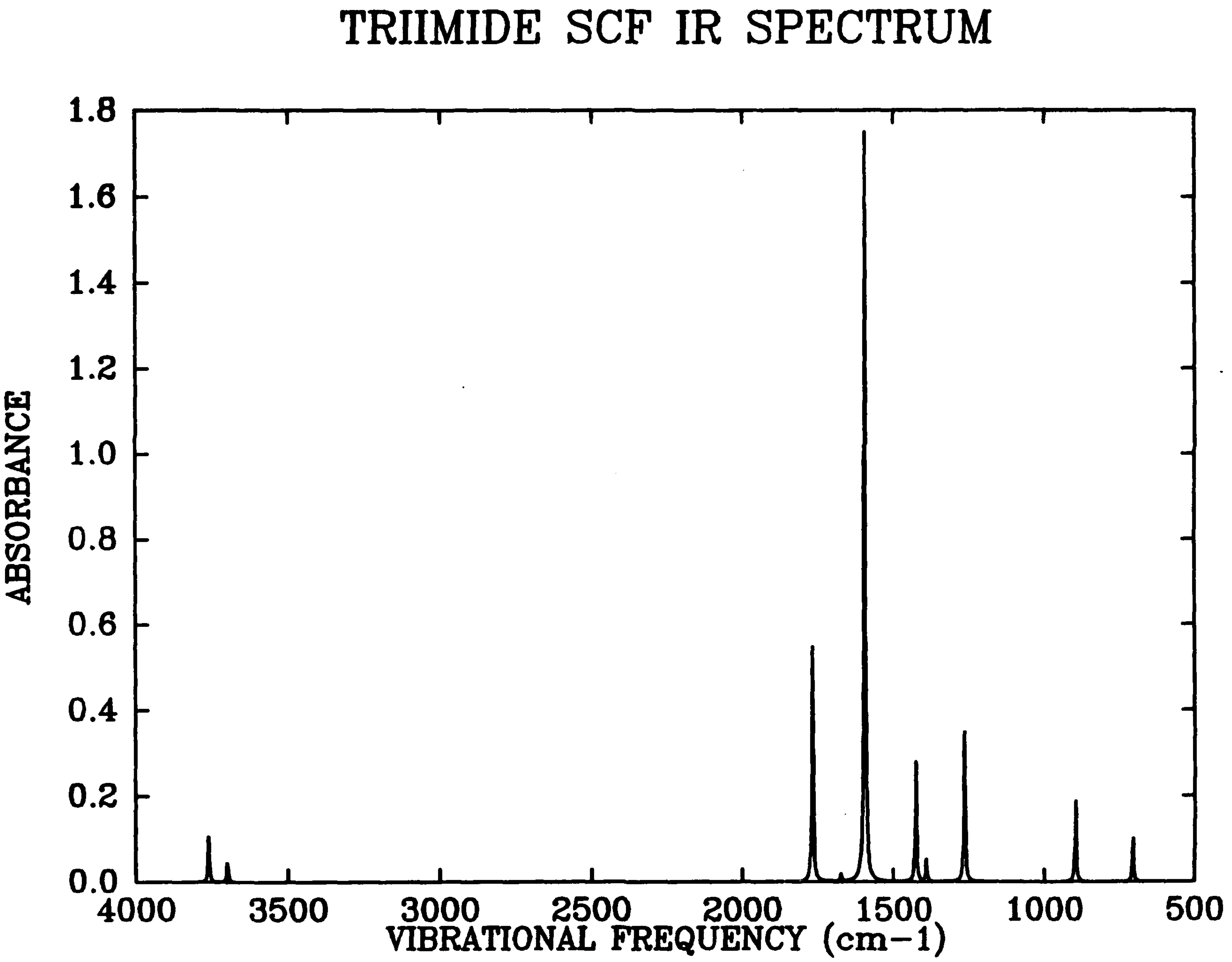

TRIAZIRIDINE E(2) IR SPECTRUM
ABSORBANCE
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
4000
3500
3000
2500
2000
1500
1000
500
VIBRATIONAL FREQUENCY (cm−1)

Fig. 3


TRIIMIDE SCF IR SPECTRUM
ABSORBANCE
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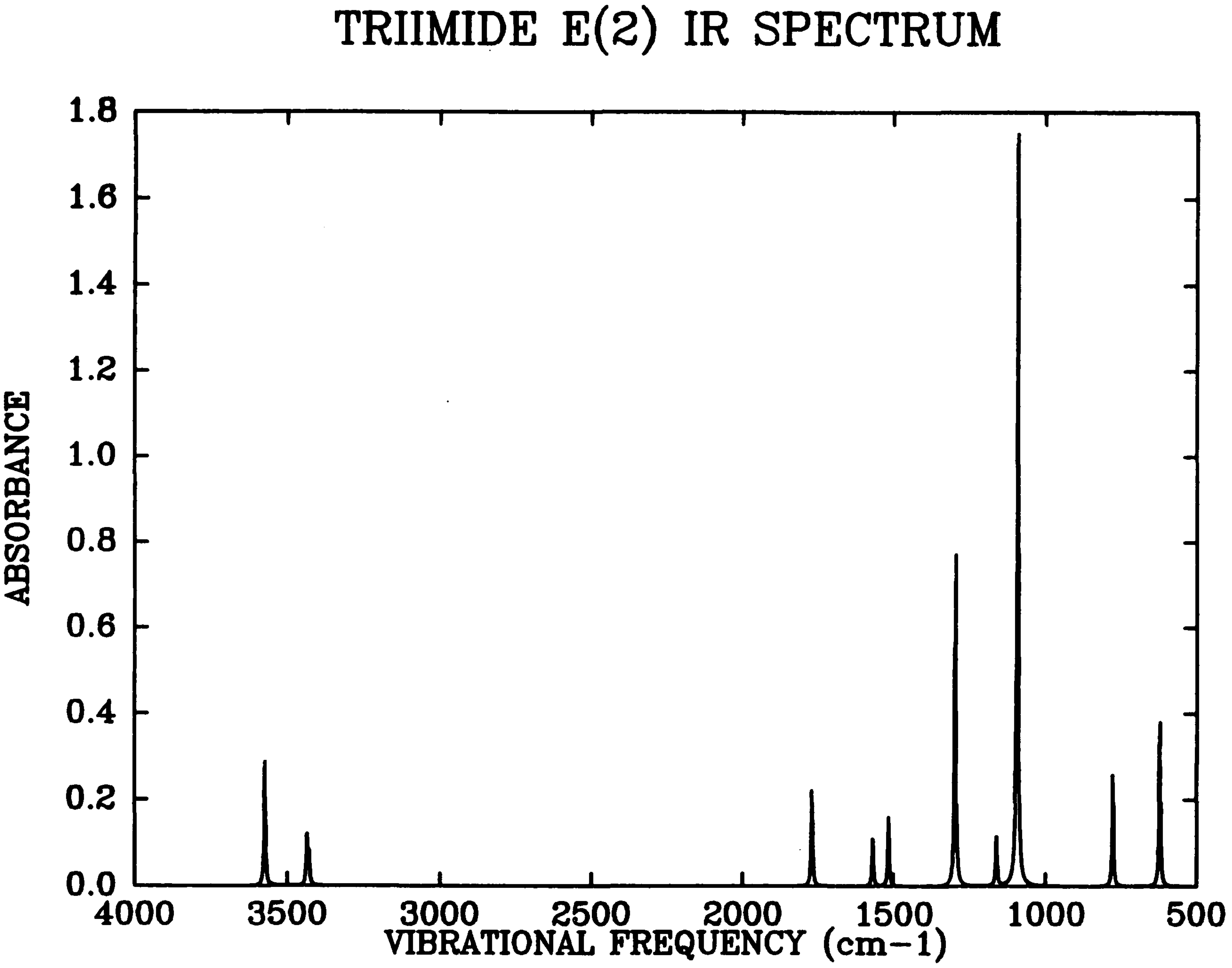
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
4000
3500
3000
2500
2000
1500
1000
500
VIBRATIONAL FREQUENCY (cm−1)

Fig. 4


TRIIMIDE E(2) IR SPECTRUM
ABSORBANCE
1.8
1.6
1.4
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0.8
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0.2
0.0
4000
3500
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VIBRATIONAL FREQUENCY (cm-1)

Fig. 5

TRIAZENE SCF IR SPECTRUM

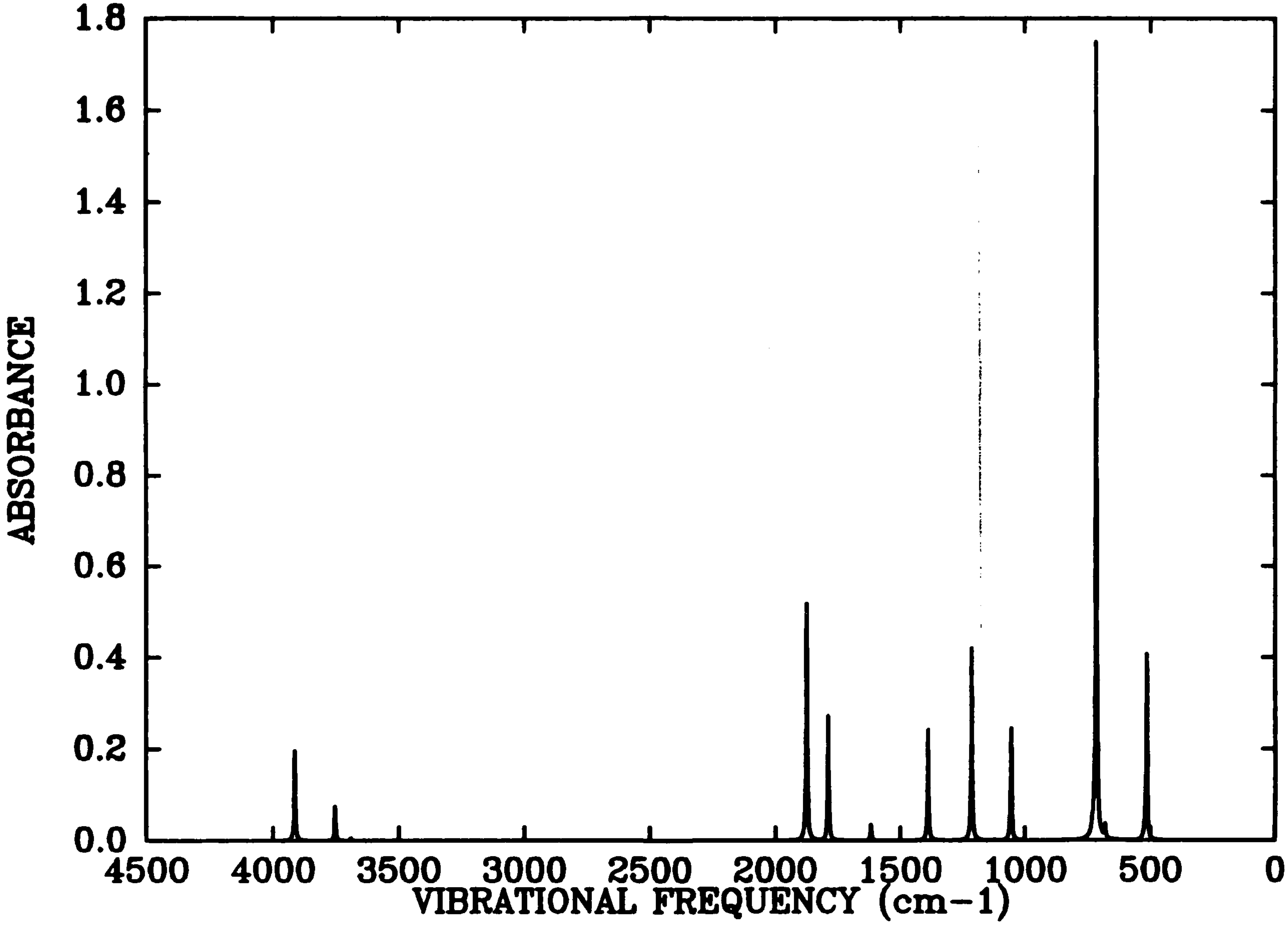


Fig. 6

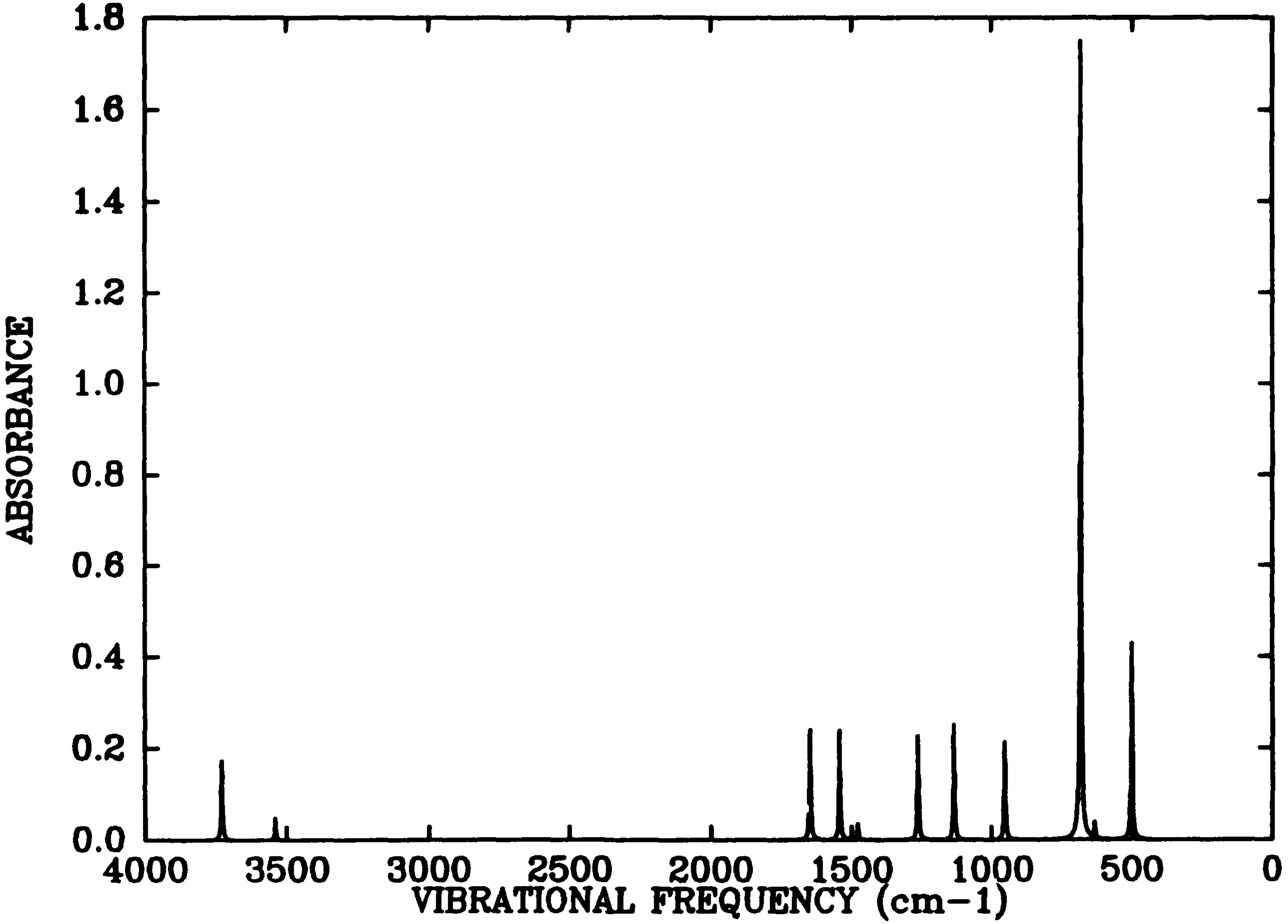

TRIAZENE E(2) IR SPECTRUM

Fig. 7

Table 3

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

(DZP BASIS SETS)

	SCF	MBPT(2)
HNO	20.5	4.7
CF_2	13.5	3.1
N_2H_2	15.5	4.2
SiC_2	6.7	1.3
CH_3NO_2	12.9	4.9

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_3CO. After subtracting all peaks associated with CO, B_2H_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_2H_6 and B_2D_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 ($\sim M^2$), rather than as $\sim N^6$ where N>>M is the number of basis functions. In a series of studies on prototype systems C_2H_6, C_2H_4 and C_2H_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, ω_c, and infrared absorption intensities, I_c, calculated for $^{11}BH_3$ using the 6-31G** basis set. Also included are the observed fundamentals, ν_{obs}, and intensities, I_{obs}. Units are the same as in table 4.

Mode	Type	ω_c	ν_{obs}	I_c	I_{obs} [a]
A_1'	stretch	2671	2623	b	b
A_2''	bend	1207	1125	113	v
E'	stretch	2817	2808	259	v
E'	bend	1273	1604	42	s

a) Taken from ref. [7]. Intensities are given as: v-weak, s-strong.
b) Zero in double-harmonic approximation.

Table 5. Calculated MBPT(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, ν_{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.

Fundamental	ω_c		ω_{obs}		ν_{obs}		ω_c/ω_{obs}		I_c		I_{obs} [a]	
	B_2H_6	B_2D_6	B_2H_6	B_2D_6	B_2H_6	B_2D_6	B_2H_6	B_2D_6	B_2H_6	B_2D_6	B_2H_6	B_2D_6
1	2730	1988	2622	1904	2530	1855	1.041	1.044	b	b	b	b
2	2279	1620	2153	1530	2088	1497	1.059	1.059	b	b	b	b
3	1260	969	1207	926	1183	911	1.044	1.046	b	b	b	b
4	845	753	798	717	790	711	1.059	1.050	b	b	b	b
5	879	622	850	602	833	593	1.034	1.033	b	b	b	b
6	1974	1419	1814	1309	1760	1280	1.088	1.084	b	b	b	b
7	901	738	878	712	860	700	1.026	1.037	b	b	b	b
8	2830	2121	2703	2031	2609	1977	1.047	1.044	168	97	vs	vs
9	1009	743	968	716	949	705	1.042	1.038	3	1	c	c
10	375	266	376	263	369	260	0.997	1.011	14	7	s	m
11	2817	2115	2690	2013	2596	1960	1.047	1.051	b	b	b	b
12	972	776	934	742	915	730	1.041	1.046	b	b	b	b
13	2101	1569	1984	1482	1925	1449	1.059	1.059	19	14	m	m
14	1023	757	993	733	973	722	1.030	1.033	26	13	s	s
15	1087	769	1041	741	1020	730	1.044	1.038	b	b	b	b
16	2716	1964	2611	1885	2520	1837	1.040	1.042	149	116	vs	vs
17	1819	1327	1652	1227	1603	1199	1.101	1.081	498	280	vs	vs
18	1252	927	1196	887	1172	874	1.047	1.045	82	29	vs	vs

a) Taken from ref. [8]. Intensities are given as: m-medium, s-strong, vs-very strong.

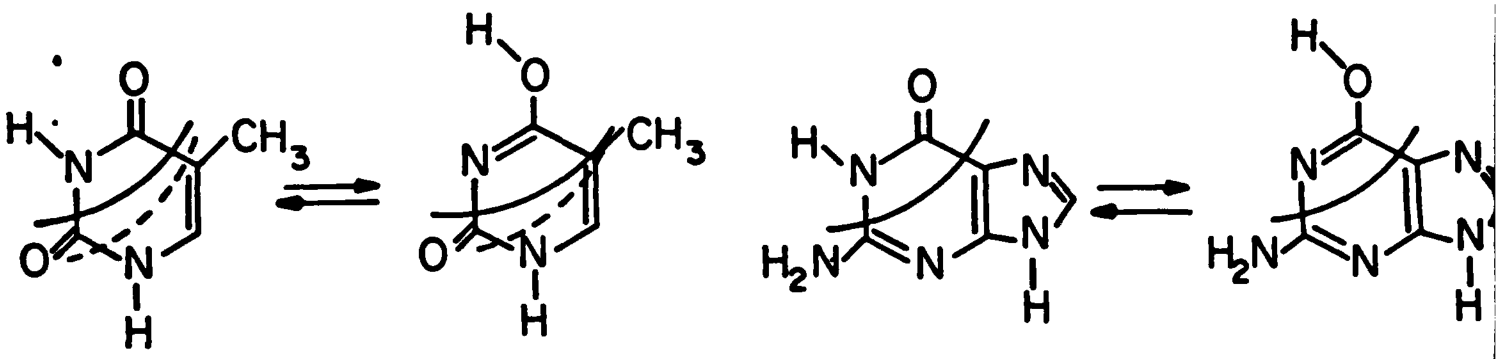
b) Zero in double-harmonic approximation.

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.

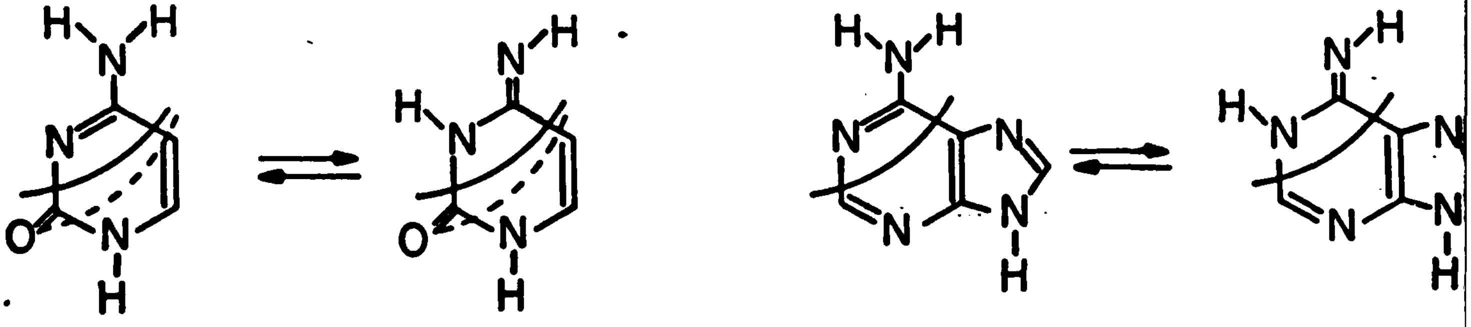
L. An important problem in the theory of point mutations is the tendency for bases of DNA, like cytosine to tautomerize (see Fig. 8). The cyt* form is a rare tautomer of cytosine which will not replicate properly, often leading to tumor formation. Using some of our large molecule methods, we have studied 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 Nuclei Acid Bases of DNA



$\text{Ura} \rightleftharpoons \text{Ura}^*$
(Thy) (Thy*)

$\text{Gua} \rightleftharpoons \text{Gua}^*$



$\text{Cyt} \rightleftharpoons \text{Cyt}^*$

$\text{Ade} \rightleftharpoons \text{Ade}^*$

Fig. 8

III. PUBLICATIONS SUPPORTED BY ARO (1984-1987)

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13. "Coupled-Cluster Evaluation of Geometrical Derivatives of Properties Using Non-relaxed Orbitals," H. Sekino and R.J. Bartlett, Int. J. Quantum Chem. Symp. 21, (1987), in press.

14. "Fast Analytical MBPT(3) Gradients," G. Fitzgerald and R.J. Bartlett, to be published.

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

April	1987	National ACS Meeting, Denver, CO. "Application of New Methods for Correlated Ab Initio Studies of Large Molecules Using an FPS Scientific Computer."
March	1987	Parr/Eliel Symposium, Chapel Hill, NC. "The Correlation Problem: From PPP to Coupled-Cluster Theory."
June	1986	Canadian Symposium on Theoretical Chemistry, Toronto, Ontario, Canada. "Analytical Derivative Methods in Coupled-Cluster Theory.
May	1986	Southeastern Theoretical Chemistry Conference, Tallahassee, FL. "Comparison of Intermolecular Force Theory and Supermolecule Approximations for Nonbonded Interactions."
April	1986	Workshop on Interface between Electronic Structure and Dynamics, Snowbird, Utah. "Analytical Derivative Methods and Coupled Cluster Theory."
June	1985	Symposium on Molecular Spectroscopy, Ohio State University. "Many-Body Studies of Molecular Force Constants, Infra-red Intensities, and Polarizabilities."
April	1985	Fulbright Distinguished Lecturer, University of Arkansas, Fayetteville, AK. Two lectures.
Feb.	1985	Mardi Gras Symposium, New Orleans, LA. "Radical Studies with Many-Body Methods."
Dec.	1984	Nobel Laureate Symposium on Applied Quantum Chemistry, Joint Meeting, Pacific Basin Chemical Societies, Honolulu, HI. "Radical Studies with Many-Body Methods."
Oct.	1984	NSF Workshop on Future Directions for Supercomputer Use in Chemistry, Evanston, IL.
April	1984	West Coast Theoretical Chemistry Conference, Los Alamos, NM.
March	1984	International Symposium on the Quantum Theory of Matter, Palm Coast, FL.

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

Snowbird Conference, April 21-25, 1986

Ludwik Adamowicz	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?

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(Ph.D. expected 1991)

Postdoctoral Research Associates: George Fitzgerald, Robert Harrison,
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VI. ADDITIONAL REFERENCES

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