MERCURY PHOTOSENSITIZATION OF TOLUENE VAPOR AND AEROSOL FORMATION

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PREFACE

The triplet-mercury photosensitized decomposition of toluene vapor was performed at room temperature in a large recirculating photochemical reactor, using the 253.7 nm Hg resonance line. The products were identified by GC and the major product, bibenzyl, further characterized by GC/MS, FT-IR and NMR spectroscopy. Kinetics for product formation was determined using both the flow reactor and a static reactor. Aerosols, formed as a result of irradiation were attributed to bibenzyl. The aerosols were visible when a He-Ne laser beam was passed through the reaction vessel, this enabled the rates of aerosol formation and deposition to be determined in a laser light extinction spectrometer.

Finally, ab initio quantum mechanical calculations were done at the 3-21G level with almost full optimization for ground state toluene, triplet state toluene and the benzyl radical, which forms bibenzyl.

I wish to express my gratitude to the Chemistry Department faculty and staff who made my studies here worthwhile. I am especially indebted to my major adviser, Prof. Gilbert J. Mains for his unyielding support, constant guidance and parental advice.

I am also thankful to the other members of my committee, Prof. Anthony L. Hines, Prof. J. Paul Devlin and Prof. Edmund J. Eisenbraun for their advice, especially to the last who provided authentic hydrocarbon samples for my research.

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LIST OF SYMBOLS

a	- Projected area of particle
a_i	- Proton hyperfine coupling constants
a_i'	- Calculated proton hyperfine coupling constants
CHT	- Cycloheptatriene
C.I.	- Configuration Interaction
CNDO/2	- Complete neglect of differential overlap method (2nd version)
e	- Electron contribution from ring substituent to aromatic ring
E	- Total Mie scattering coefficient
E_a	- Activation energy
E_{abs}	- Absorption efficiency
EPA	- Ether-isopentane-ethyl alcohol matrix
E_{scat}	- Scattering efficiency
E_y'	- Total Mie scattering coefficient at a position of maximum of order y
E_y''	- Total Mie scattering coefficient at a position of minimum of order y
FT	- Fourier transform
g	- Acceleration due to gravity
3-21G	- Split-valence basis set
4-21G	- "
6-31G	- "
3-21G*	- Polarization basis set

List of Symbols (cont'd)

6-31G* - Polarization basis set

6-31G** - "

GC - Gas chromatograph

h - Height a particle falls through in the light beam

HF - Hartree-Fock method

HMO - Huckel molecular orbital method

I/I_o - Transmittance

INDO - Intermediate neglect of differential overlap method

IP - Ionization potential

IR - Infrared

k - Constant, defined in equation 13

k_q - Bi-molecular quenching rate constant

l - Length of reaction vessel

m - Refractive index

M - Parameter calculated from the Lorentz-Lorentz equation (11)

2-MDPM - 2-Methyldiphenylmethane

3-MDPM - 3-Methyldiphenylmethane

4-MDPM - 4-Methyldiphenylmethane

m/e - Mass to charge ratio

MINDO/3 - Modified INDO method (3rd version)

MO - Molecular orbital

MS - Mass spectrometer

n - Particle number, number of particles per unit volume

NMR - Nuclear magnetic resonance

p - Normalized size parameter

p(r) - Particle radius distribution function

List of Symbols (cont'd)

p_y - Position of extrema of order y for the total Mie scattering coefficient

p_y' - Position of a maximum of order y for the total Mie scattering coefficient

p_y'' - Position of a minimum of order y for the total Mie scattering coefficient

Q - Constant for calculating proton hyperfine coupling constants, equation 16

r - Particle radius

R - Rydberg constant

RHF - Closed shell restricted Hartree-Fock method

RIC - Reconstructed ion chromatogram

RT - Product of the gas constant and absolute temperature

SCF - Self-consistent-field method

SEM - Scanning electron microscopy

STO-3G - Minimal basis set

t - Time

T - Transmittance

UHF - Open shell unrestricted Hartree-Fock method

UV - Ultra-violet

VIS - Visible

x - Particle size parameter

y - Order of extrema

ε - Molar extinction coefficient

ε_{max} - Molar extinction coefficient at wavelength of maximum absorption

List of Symbols (cont'd)

η - Viscosity

λ - Wavelength

ν - Frequency

ν_{max} - Frequency corresponding to wavelength of maximum absorption

$\nu-\nu_o$ - Difference between a frequency and the 0,0 frequency

ρ - Density of particles

ρ_i - Π-electron spin densities

ρ_m - Density of medium

σ^2 - Effective collisional cross section

CHAPTER I

INTRODUCTION

Photochemically generated aerosols were first studied by Tyndall (1) in 1869. On directing a beam of light through a mixture of air, butyl nitrate vapor and hydrogen chloride, he observed a light induced chemical reaction resulting in the formation of aerosols. Other techniques have subsequently been used to produce aerosols by ultra-violet light (2) (3). The irradiation of many vapors should yield high molecular weight products which quickly produce a supersaturated state, by virtue of their low vapor pressures. The supersaturated vapors then condense to form particles capable of coalescing into larger aggregates which scatter light.

In the last two decades, there have been numerous studies of light-scattering aerosols produced by the interaction of ultra-violet light from the sun with atmospheric pollutants (4) (5). These reactions have been simulated in photochemical smog-chambers using hydrocarbons and oxides of nitrogen and sulfur which are present in the parts-per-million to parts-per-billion range of concentrations as pertains in the atmosphere (6). The importance of toluene as an atmospheric pollutant cannot be overlooked, as it is one of the major components of gasoline and widely used as a solvent in the manufacturing industry. Recently, Dumdei et al. (7) have identified as many as twenty-seven atmospheric degradation products of toluene using triple

quadrupole mass spectrometry (MS/MS). Their products were obtained by oxidizing toluene vapor using hydroxyl radicals produced photochemically with simulated sunlight.

In conventional photochemical methods, it is impossible to observe the aerosols if they are formed, unless a high intensity beam from say, a laser is directed through the reaction vessel. Porter and Wright (8) reported the detection of particles during the flash photolysis of toluene vapor. A few milliseconds after the flash, they recorded the formation of a continuous band in the absorption spectrum which reached a maximum after 10^{-1} sec and then decayed over a period of several minutes. Aside from reports like this there has been no attempt to characterize the aerosols so formed.

CHAPTER II

LITERATURE REVIEW

Mercury Photosensitization

When a chemical reaction does not proceed appreciably under the influence of a given wavelength of light, it can sometimes be initiated by the addition of a sensitizer which absorbs the light and transfers its energy to the substrate in a collision of the second kind. Cario and Frank (9) performed the first mercury photosensitized reaction using hydrogen with the 253.7 nm Hg resonance line. Since then, mercury photosensitization has been used extensively as an important photochemical technique in the study of free radical reaction kinetics (10) (11).

Mercury vapor is often the choice as a sensitizer because (a) it possesses a high vapor pressure at room temperature, (b) it has a large absorption coefficient for its resonance line, and (c) the excited mercury atom, on collision, transfers sufficient energy (113 Kcal/mol) to effect the rupture of most chemical bonds.

Energies of the lower excited states and some observed transitions of the mercury atom are shown on the simplified Grotrian energy-level diagram in Figure 1 (12). The two transitions originating from the ground state are shown. The first involves a transition of $Hg(^1S_0)$ to $Hg(^3P_1)$ at 253.7 nm. This transition, called resonance phosphorescence, is spin forbidden but, nevertheless, occurs because of spin-orbit coupling in heavy atoms like mercury. The forbidden nature

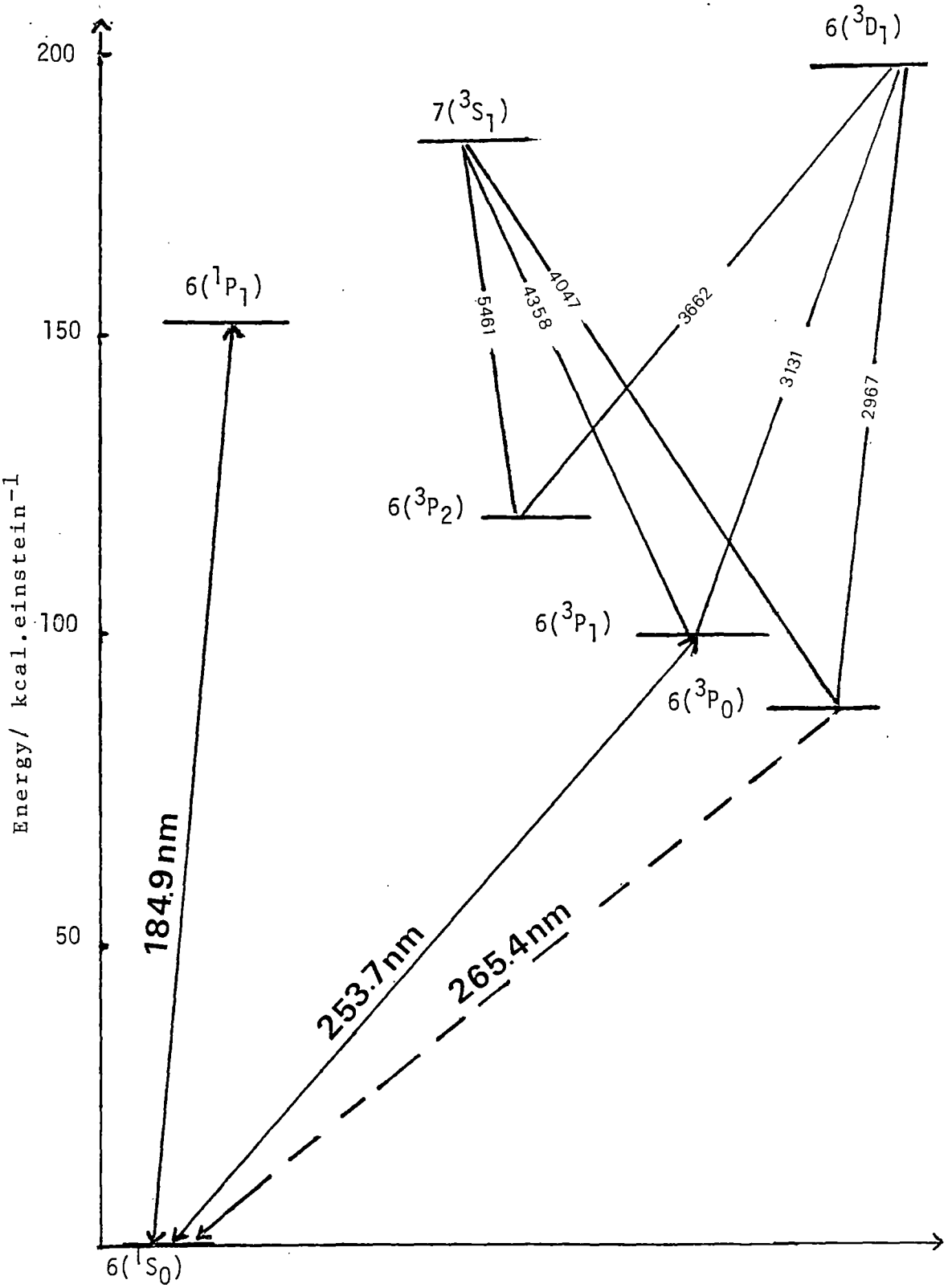


Figure 1. Grotrian Energy-Level Diagram for Mercury

of this transition is reflected in the relatively long life of the triplet state, 110 nsec, compared to 1.3 nsec for the singlet state (13). The transition from $Hg(^1S_0)$ to $Hg(^1P_1)$ occurs at 184.9 nm (resonance fluorescence), giving rise to an absorption coefficient so high that effects due to imprisonment of radiation are impossible to eliminate, and hence relatively little work has been done with this line (14).

Low pressure Hg lamps emit both the 253.7 nm and 184.9 nm resonance lines. With appropriate filters, the latter can be removed. Both lines are termed resonance lines because both direct absorption and emission occur at these wavelengths. However, 265.4 nm radiation from the $Hg(^3P_0)$ state is simply called phosphorescence since direct absorption from the ground state does not occur to that state (15).

A mercury atom in the $^3P_1$ energy state has acquired 113 Kcal or 4.86 eV of electronic energy, and in addition to phosphorescence it can undergo the following deactivation steps:

(a) Quenching to the ground ($^1S_0$) state through a collision of the second kind, in which 113 Kcal of energy is transferred to a quencher. The efficiency of this quenching reaction is expressed as k_q, the bi-molecular quenching rate constant, or σ^2, the effective collisional cross section (15).

(b) Quenching to the metastable $^3P_0$ state (partial quenching), with a loss of 5 Kcal of energy. This state being a doubly forbidden state has a long lifetime and has been found to be important only in molecules like nitrogen, water and carbon monoxide, which have vibrational spacing in the ground state close to 5 Kcal (16).

(c) Activation to the $^3P_2$ state through collision with the acquisition

of 13 Kcal of energy. At room temperature, only one collision in about 10^{10} is capable of effecting this transition (13). Hence it can conveniently be neglected in most photochemical studies.

Gunning and Strausz (17) have reviewed the factors which affect the intensity of Hg resonance lines, ie., natural broadening, Doppler broadening, Lorentz broadening, Holtzmark broadening, Stark broadening and self-absorption. The last, which is the most significant, occurs when radiation from the hot-central portion of the emitting light source passes through an outer cooler-layer of the same vapor. The atoms in the cooler layer are capable of absorbing the radiation, resulting in partial or total absence of the central region of the line. Serious self-absorption will produce a reversed resonance line where the light intensity is distributed with a maximum on either side of the center line and a minimum at the center, as depicted by the broken line in Figure 2.

During mercury photosensitization a higher light intensity is attained if the exciting line is not reversed and broadening kept to a minimum. It has been shown that this can best be achieved by use of a well-cooled electrodeless-discharge low pressure Hg lamp, operating at the minimum power level which is consistent with a steady radiation output (18).

Toluene Photolysis

Over the years, several workers have studied the photochemistry of toluene in the gas phase and at different temperatures (19)-(24). Among the range of products identified were, hydrogen, methane, ethane, benzene, o-, p-, m-xylenes, ethylbenzene, bibenzyl, other dimeric

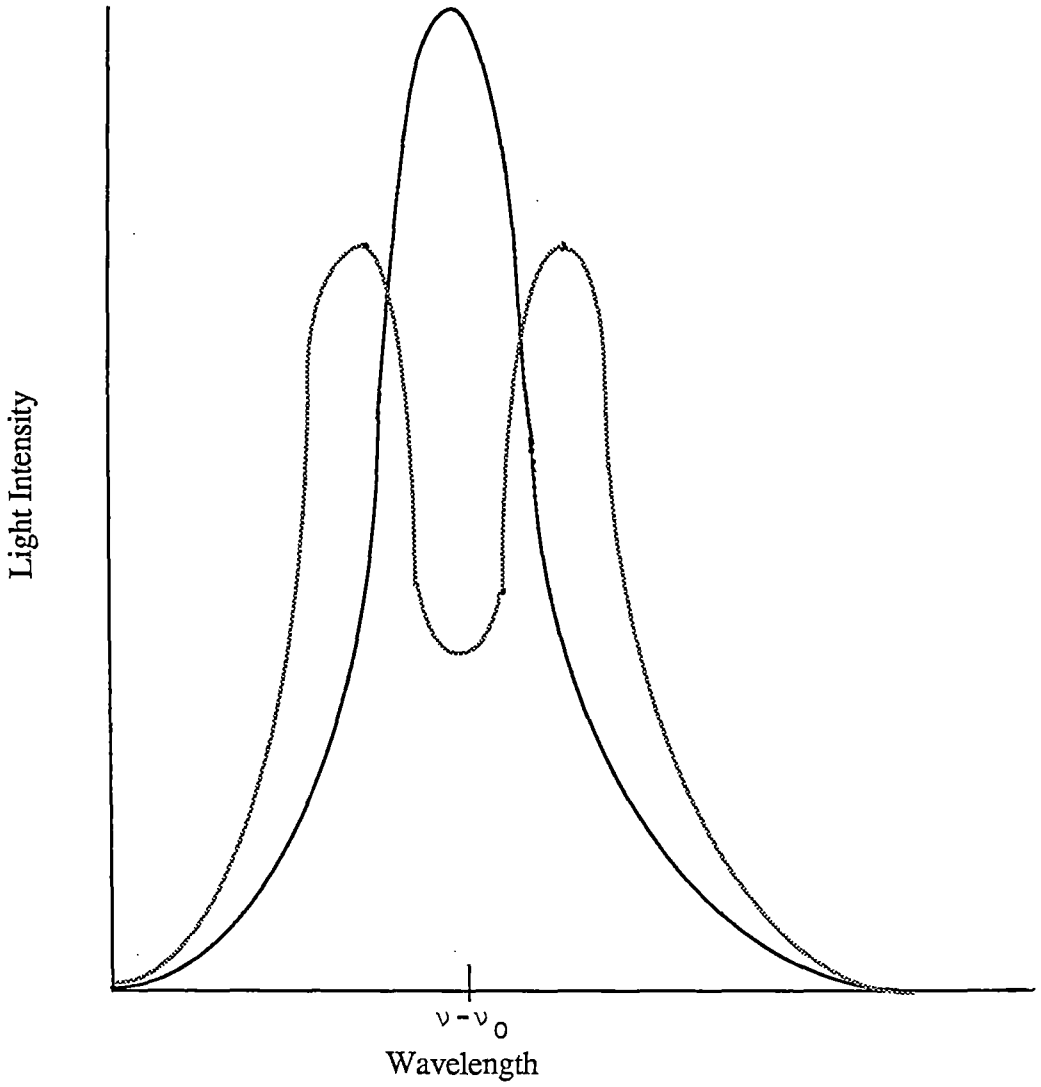


Figure 2. Effect of Self-Absorption

products and a polymer.

Burton and Noyes (20) failed to obtain any aromatic or dimeric products at room temperature or even elevated temperatures during the direct photolysis at 266.8 nm and 248.0 nm. Photolysis at room temperature and wavelengths of 200.0 nm and 184.9 nm by Pitts et al. (21) produced only methane, ethane and an unidentified product. However, Wilzbach and Kaplan (22) identified all the products listed above, after direct photolysis at 35 ^{o}C and 250.0 nm using a high pressure Hg lamp. They found the major product to be the polymer and the rest present in low yields.

The mercury photosensitized reactions also produced low yields. After 48 hrs of irradiation in the presence of mercury, Sehon and Darwent (23) obtained no products at room temperature, but identified hydrogen, methane and ethane at temperatures between 150 ^{o}C and 400 ^{o}C. The quantum yield of hydrogen, their major product, was 5×10^{-4} at 150 ^{o}C. The whole range of products was also obtained by Yamamoto et al. (24) at 25 ^{o}C. Their products were identified on a gas chromatograph, among other things they reported bibenzyl as their major product and identified the methyldiphenylmethanes among the products.

The disparity in results can be attributed to different methods of product analysis. Use of a gas chromatograph or a mass spectrometer enabled more of the products to be identified (22) (24). Also, at room temperature, mercury photosensitized reactions yield relatively more products than direct photolysis. It has been pointed out that irradiation of a mixture of toluene and mercury vapors may result in competitive absorptions by toluene molecules and mercury atoms for the 253.7 nm resonance radiation, resulting in both direct photolysis and

mercury sensitized reactions (23). Referral to the absorption spectrum of toluene vapor in Figure 3 (obtained from reference 25), however, depicts only a broad weak band at 253.7 nm (26). Thus contributions from direct photolysis at that wavelength will be minimal and there are some doubts as to the purity of light used in studies where reactions have been observed (27). Additionally, the complete elimination of mercury vapor from a reaction vessel is an almost impossible task.

Main bond scissions that are known to occur during the direct photolysis and mercury sensitized reactions of toluene at 253.7 nm, are at the C-H bond α to the ring and at the C-C bond β to the ring, resulting in the following primary photochemical steps:

$$C_6H_5CH_3 \quad \text{----hv, Hg----}> \quad C_6H_5CH_3^* \qquad \text{(I)}$$

$$C_6H_5CH_3^* \quad \text{---------->} \quad C_6H_5CH_2\cdot + H\cdot \qquad \text{(II)}$$

$$C_6H_5CH_3^* \quad \text{---------->} \quad C_6H_5\cdot + CH_3\cdot \qquad \text{(III)}$$

The strength of the bond broken in reaction II, has been estimated to be 78 Kcal/mol and that in reaction III in the range of 85 - 90 Kcal/mol (19) (28). In principle, a 253.7 nm photon would put 113 Kcal/mol into the π-electrons of the aromatic ring during direct photolysis or nearly that much transferred by a $(^3P_1)$Hg atom on collision.

Stable product formation can be represented by the following steps:

$$R\cdot + C_6H_5CH_3 \quad \text{---------->} \quad RH + C_6H_5CH_2\cdot \qquad \text{(IV)}$$

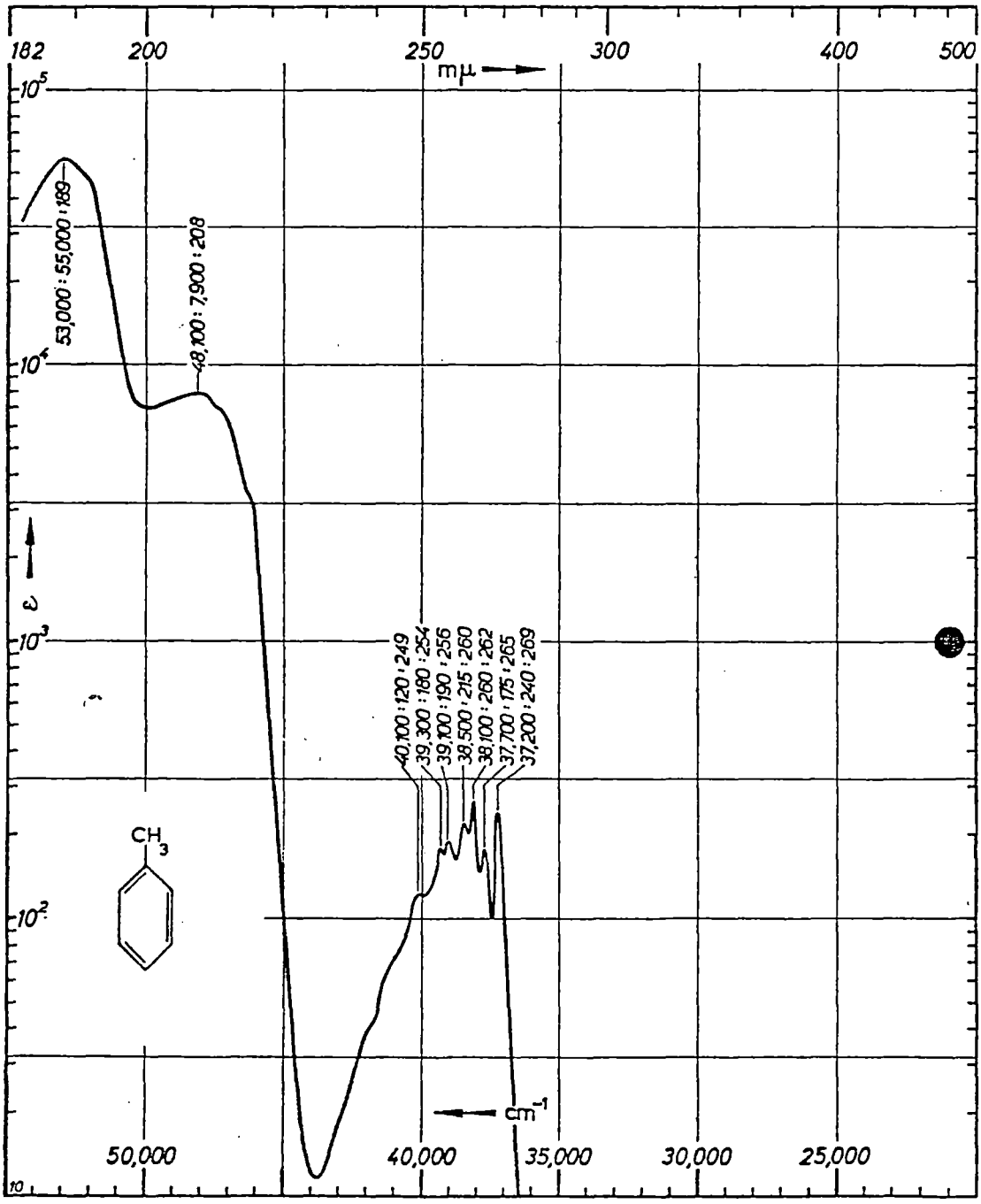


Figure 3. Absorption Spectrum of Toluene

$$R\cdot + R\cdot \longrightarrow R\text{-}R \qquad (V)$$

Here, R is any radical produced in the primary steps or by hydrogen atom abstraction from a toluene molecule in reaction IV.

Sehon and Darwent's (23) plot of the rate of hydrogen formation as a function of toluene pressure passes through a maximum, which they suggest is consistent with the postulation of excited species formation. However, they also propose that more than one type of excited species is produced in reaction I: one type forms the methyl and phenyl radicals while the other forms the benzyl radical. Their suggestion is supported by Yamamoto et al. (24) who have shown that the benzyl radical concentration has a different pressure dependency from the phenyl and methyl radicals. The concentration dependencies of the latter two were equivalent and unlike that of the benzyl radical, tended to decrease with increasing toluene pressure. The approximate steady-state radical concentrations were estimated from product yields.

In the geometrical structure of the toluene molecule, if a methyl hydrogen is constrained in the plane of the ring and the other two hydrogen atoms arranged above and below the plane respectively, then the molecule possesses a C_s symmetry. Its vibrational modes can be classified as $26A' + 13A''$, where A' and A" are symmetric and antisymmetric with respect to the symmetry plane respectively. However, if the effect of the methyl group on the ring is taken as a one atom substitution, the toluene molecule can be assigned a C_{2v} symmetry. Then the 26A' modes decompose into $11A_1 + 10B_1$ ring modes plus five modes of the methyl group and the 13A" modes decompose into $3A_2 + 6B_2$ ring modes, three methyl group modes and one twisting mode (29).

The absorption spectrum of toluene in hexane, depicted in Figure 3, can be divided into three main regions. The first with ν_{max} 38,100 cm^{-1} and ε_{max} 150, is comprised of sharp bands, the second has ν_{max} 48,100 cm^{-1} and ε_{max} 7,000 and the third has ν_{max} 53,000 cm^{-1} and ε_{max} 46,000, the last two are diffuse bands. The bands in the 53,000 cm^{-1} region have been shown by Price and Walsh (30) to fit the Rydberg series:

$$\nu_n = 71,180 - R/(n - 0.50)^2, \qquad n = 4,....,7 \tag{1}$$

$$\nu_n = 71,130 - R/(n - 0.95)^2, \qquad n = 4,....,9 \tag{2}$$

where R is the Rydberg constant and ν is the frequency in cm^{-1}. Both series converge to the first ionization constant limit of 8.77 $\pm$ 0.05 eV. The electronic transition in this band is equivalent to the $^1E_{1u}$ <--- $^1A_{1g}$ transition in benzene. Likewise the 48,000 cm^{-1} band is the equivalence of the $^1B_{1u}$ <--- $^1A_{1g}$ electronic band of benzene. The bands in the 38,100 cm^{-1} region have been assigned to the $^1B_1$ <--- $^1A_1$ electronic transition (C_{2v} symmetry), being the equivalent of the $^1B_{2u}$ <--- $^1A_{1g}$ transition in benzene (26). Ground state and excited state fundamental vibrational frequencies of liquid toluene are given in Table I (26) (31). In the singlet excited state, the 528(b_1) frequency was the only nontotally symmetric fundamental vibration observed.

The reaction of a ($^3P_1$)Hg atom with a toluene molecule produces a triplet state toluene molecule by intermolecular energy transfer:

$$Hg(^3P_1) + C_6H_5CH_3(^1A_1) \text{ ------> } Hg(^1S_0) + C_6H_5CH_3(^3A_1) \tag{VI}$$

TABLE I

FUNDAMENTAL VIBRATIONAL FREQUENCIES FOR THE GROUND AND FIRST EXCITED STATES OF TOLUENE (/CM^{-1})

	$^1A_1$	$^1B_1$	$^3A_1$
(Ref.	31	26	32)
Symmetry			
a_1	521	456	-
	785	751	785
	1003	932	1002
	1175	1189	1175
	1210	-	1603
b_1	240	-	-
	622	528	-
	1060	-	-
	1155	-	-
a_2	405	-	-
	842	-	-
	985	-	-
b_2	216	-	-
	467	-	467
	730	-	695
	830	-	-
	1190	-	-

Wigner's spin conservation rule, which requires a correlation of spins between reactants and products, is observed. The phosphorescence spectra of toluene in EPA and in a cyclohexane matrix at 90 K is shown in Figure 4 and triplet-excited state fundamental vibrational frequencies are given in Table I (32). The 0,0 band, which is at 28,920 cm^{-1}, places a toluene molecule in the $^3A_1$ state, 3.59 eV above the ground state. Even though the transition, $^3A_1$ ---> $^1A_1$, is spin-forbidden, it is orbitally allowed through spin-orbit coupling with the $^1B_1$ state (20). The quenching cross section of toluene with $(^3P_1)Hg$ is expected to be high (59.9×10^{-16} cm^2 for benzene) as compared to that of some aliphatic hydrocarbons (e.g., ethane: 5.94×10^{-16} cm^2) (33). On the other hand, these aliphatic hydrocarbons unlike toluene and benzene, react appreciably with photoexcited mercury vapor at room temperature (34) (35).

Burton and Noyes (20) obtained the triplet state yield of toluene vapor from 266.8 nm excitation and 298 K as 0.70 ± 0.03 relative to benzene by the technique of Cundall (36). Thus, phosphorescence from the triplet state of toluene (reaction VII) and intersystem crossing to the higher vibrational levels of the ground state, followed by vibrational relaxation with accompanying release of thermal energy (reaction VIII), could be competing reactions causing the low quantum yields of products.

$$C_6H_5CH_3(^3A_1) \longrightarrow C_6H_5CH_3(^1A_1) + h\nu \qquad \text{(VII)}$$

$$C_6H_5CH_3(^3A_1) \longrightarrow C_6H_5CH_3(^1A_1) + \text{heat} \qquad \text{(VIII)}$$

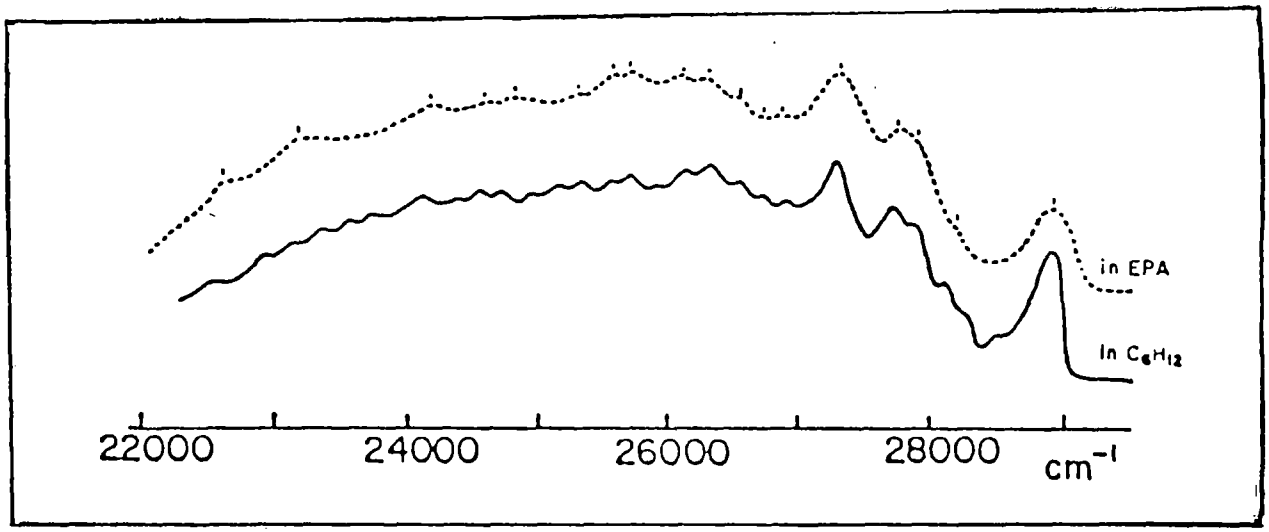


Figure 4. Phosphorescence Spectra of Toluene in EPA and Cyclohexane

Braun et al. (37) have determined the phosphorescence emission spectrum of toluene in the vapor phase and did not observe any emission for excitation to either the second or third electronic states for excitation in the wavelength region of 160.0 - 280.0 nm.

Benzyl Radical

The benzyl radical formed in reaction II as a result of the scission of a C-H bond α to the ring is expected to have a resonance energy greater than the parent toluene molecule and exist in both the benzenoid and the quinonoid canonical forms (8). Figure 5 shows the possible resonance structures of the benzyl radical. A resonance energy of 19 Kcal/mol is obtained when benzylic C-H bond energy is compared to that of methyl. However, resonance contributions from the Kekulé structures of the benzyl radical and toluene molecule will be the same. Bibenzyl should be produced by the recombination of two benzyl radicals via the reaction V, however only Yamamoto et al. (24) have reported identifying it as a product in the Hg photosensitized decomposition of toluene vapor at room temperature. Methyldiphenylmethanes which were also reported in that work will be formed by cross combination of tolyl (quinonoid) and benzyl radicals.

The benzyl radical was first detected by Paneth and Lautsch (38), with the mirror technique. Due to its low reactivity and low equilibrium concentration at room temperature, it is difficult to detect by conventional physical methods. Flash photolysis of toluene vapor by Porter and Wright (8) produced a new banded spectrum during the time of irradiation. Three peaks at 32595, 32755 and 31700 cm^{-1} were resolved and assigned to benzyl radicals formed. Later theoretical calculations

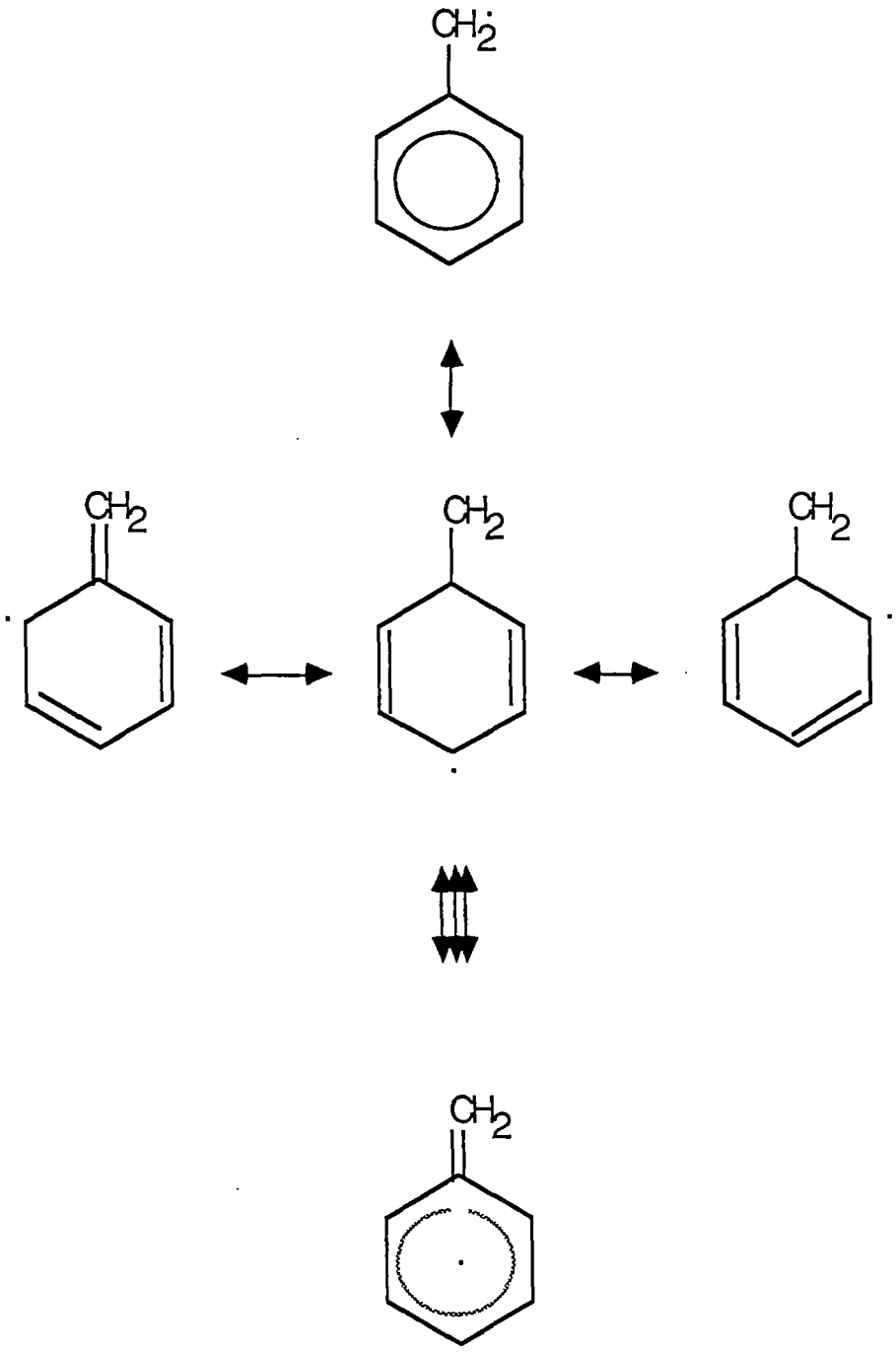


Figure 5. Resonance Structures of the Benzyl Radical

by Longuet-Higgins and Pople (39) placed the two lowest transitions at 27900 and 33700 cm^{-1} while Bingel (40) predicted the lower transition to be between 21300 and 21800 cm^{-1} .

In recent times it has become possible to measure the time-resolved absorption spectra of decaying vibrationally-hot toluene molecules produced either directly by laser flash photolysis of toluene vapor, or indirectly from cycloheptatriene or benzyl chloride (41)-(44). The spectra obtained provide information on the rate of benzyl radical formation. The present status of experimental methods in flash photolysis, including laser flash photolysis, has been extensively reviewed by Rabek (45). Ikeda et al. (41) reported the unimolecular formation rate constant of the benzyl radical as $(2.4 \pm 0.2) \times 10^6$ sec^{-1}, at 193.0 nm, from the nanosecond laser flash photolysis of toluene vapor.

The decadic absorption coefficients of toluene vapor at different temperatures, 295 - 2800 K, and over the wavelength range of 185 - 280 nm have been reported by Hippler et al. (42). Values in the temperature range 860 - 1800 K were obtained from shock wave experiments and at 2800 K from the UV laser induced photoisomerization of cycloheptatriene (CHT):

$$CHT(^1S_0) \xrightarrow{h\nu} CHT(^1S_1) \longrightarrow CHT(^1S_0^*) \qquad (IX)$$

$$CHT(^1S_0^*) \longrightarrow C_6H_5CH_3(^1S_0^*) \qquad (X)$$

$$C_6H_5CH_3(^1S_0^*) \longrightarrow C_6H_5CH_2^{*}\cdot + H\cdot \qquad (XI)$$

" * " represents a vibrationally excited (hot) molecule. The rate constant for benzyl radical formation (reaction XI) was calculated as 1.5×10^6 sec^{-1}.

Molar extinction coefficients of the benzyl radical at three wavelengths have been reported (44). The radicals were obtained from ArF laser photolysis of benzyl chloride at 193 nm, and the time-resolved absorption spectra of the three peaks at 253, 260 and 306 nm showed a slight blue shift.

Object of Research

The purpose of this research is to obtain substantial amounts of the products from the Hg photosensitized decomposition of toluene vapor at room temperature and 253.7 nm and characterize them. In particular bibenzyl, which should be the major product, will be identified by gas chromatography, mass spectrometry, Fourier transform nuclear magnetic resonance and infrared spectroscopy.

The nature of the aerosols formed as a result of irradiation is also investigated. These aerosols can be seen visually when visible light from a He-Ne laser passes through the photolyzed vapor. Particle sizes will be determined from scanning electron micrographs of the aerosols deposited on appropriate substrates, and laser light extinction measurements will used to determine the rates of formation and deposition of the aerosols and the particle size distribution.

Finally, to aid in interpretation of the experimental data, ab initio quantum mechanical calculations at the 3-21G level with almost full optimization will be done on ground state toluene, triplet state toluene and the benzyl radical.

CHAPTER III

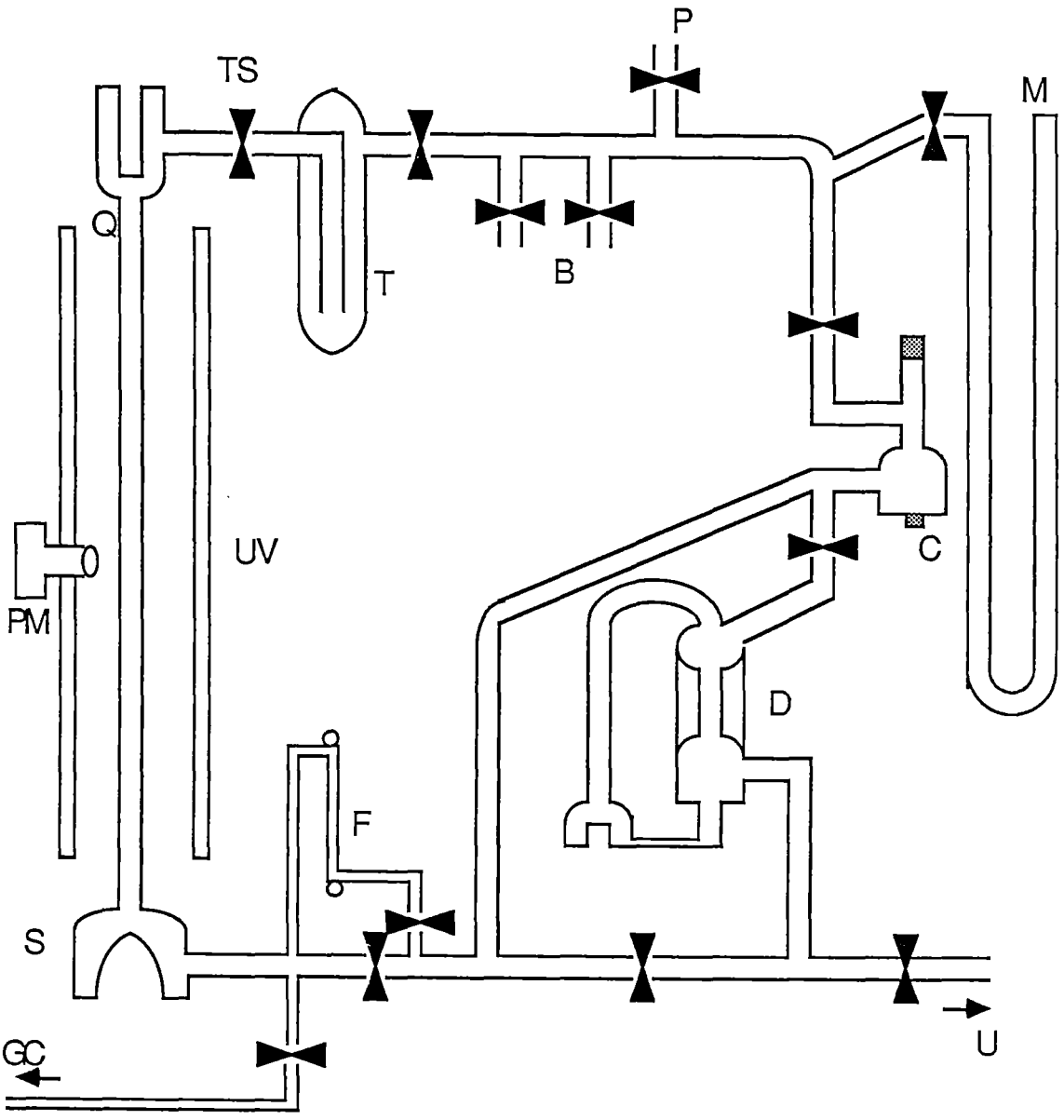
EXPERIMENTAL METHODS

Flow Reactor

In order to obtain large quantities of products for analysis, a large all-glass recirculating flow reactor was used to study the triplet Hg photosensitized decomposition of toluene vapor at room temperature. The reactor was fashioned after that used by Plotkin et al. (46), when they investigated the Hg photosensitized reactions of boranes and carboranes.

A diagram of the reactor used is shown in Figure 6. It had a total volume of 3 liters and was equipped with a flowmeter, a mercury saturator, a mercury manometer, low pressure gauges, Teflon stopcocks and a trap --all connected to a mercury diffusion pump. Circulation of vapors was done with a glass circulating pump (Fig. 7), first designed by Sime et al. (47), which was driven by an external U-magnet attached to a motor. The flow rate was pegged at 10 ml/min for all runs.

The section of the reactor irradiated was a quartz tubing 91.5 cm long and 0.4 liters in volume, the rest of the reactor was constructed from pyrex. Six low pressure mercury lamps (General Electric G36T6) provided the 253.7 nm Hg resonance line, they were of the same height as the quartz tubing and were placed concentrically around it. The Hg lamps were cooled with a flow of compressed air and the temperature profile along the quartz tube monitored with six chromel-alumel



B: Storage Bulb Connection
C: Circulation Pump
D: Mercury Diffusion Pump
F: Flowmeter
M: Mercury Manometer
P: Vacuum Gauge Connection
T: Trap
Q: Quartz Tubing
U: Forepump
S: Mercury Saturator
TS: Teflon Stopcock
UV: Ultra-Violet Lamps
PM: Photomultiplier
GC: GC Connection

Figure 6. Photochemical Flow Reactor

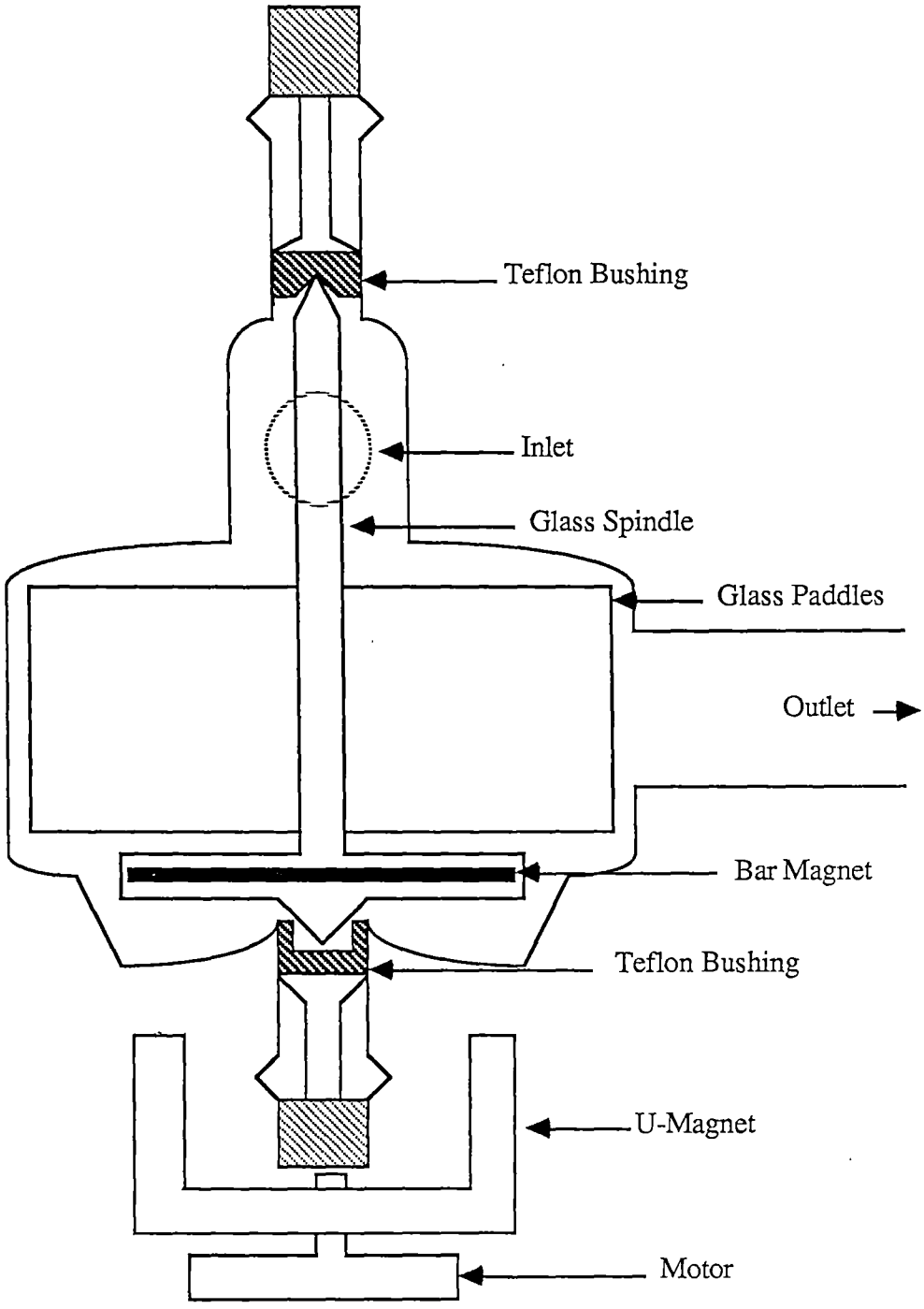


Figure 7. All-Glass Circulating Pump

thermocouples attached to an Omega 2166A Multichannel Digital Thermometer and placed at different locations on the quartz tube. Before introducing the toluene vapor into the irradiated zone via the Teflon stopcocks, the Hg lamps were allowed to attain a steady light output. This was verifiable by monitoring an illuminated portion of the reactor with an Oriel UV photomultiplier tube operating on an Oriel 7010 radiometer.

Toluene used was Fisher research grade, redistilled and the fraction boiling off from 110 ^{o}C to 112 ^{o}C collected and stored over sodium metal in a glass storage bulb. Triply distilled mercury from the Bethlehem Company, meeting the American Chemical Society standards was used without further purification.

A 1/8 inch stainless-steel tubing connected the photochemical reactor to the gas sampling valve of a Hewlett-Packard (HP) 5710A gas chromatograph through a Teflon stopcock. The gas chromatograph was equipped with a flame ionization detector, and the carrier gas was helium flowing at 20 ml/min. Analysis of products was done on a 10ft by 1/8 inch stainless-steel gas chromatograph column, which was packed with 10% SP-2100 on 100/120 Supelcoport. An isothermal run at 100 ^{o}C for 4 mins, followed by a temperature programmed run to 280 ^{o}C at a rate of 4 ^{o}C/min provided a good separation of the products in a reasonable length of time (48). Integration of the peaks was done on a 3385A HP Automation System attached to the gas chromatograph.

Static Reactor

Non-volatile products could not be properly sampled through the gas sampling valve of the gas chromatograph and thus, had to be dissolved in a solvent, methanol, and introduced into the gas chromatograph by syringe. To facilitate the analysis of these products, a static photochemical reactor was used (Fig. 8).

The reaction vessel was cylindrical with a diameter of 3.5 cm and comprised of two compartments. The top part (7 cm long), was constructed from pyrex and fitted with a Teflon stopcock and a socket type joint, by means of which the vessel could be attached to the vacuum line. The lower part of the vessel (22 cm long), was made of quartz. Both parts had a groove for an o-ring seal and kept in place with a screw-type pinch clamp.

Irradiation was made with a four-turn helical low pressure mercury lamp, operating from a 5000V ACME transformer. Only the quartz part of the reaction vessel was irradiated. Before irradiation, the lamp was allowed to attain a steady light output as obtained from the reading on the radiometer attached to the UV photomultiplier tube. The reaction vessel, containing toluene vapor and a drop of mercury, was placed vertically in the center of the the helical lamp, and further enclosed within a cylindrical metallic column. Thus UV light from the lamp to the vessel was cut off by the metal cylinder which was held in place by a solenoid. At the start of irradiation, after the lamp had attained its optimum light output, electric power was switched from the solenoid to the timer and the metal cylinder fell under gravity to expose the reaction vessel to the UV radiation.

At the end of irradiation, the products were condensed to the

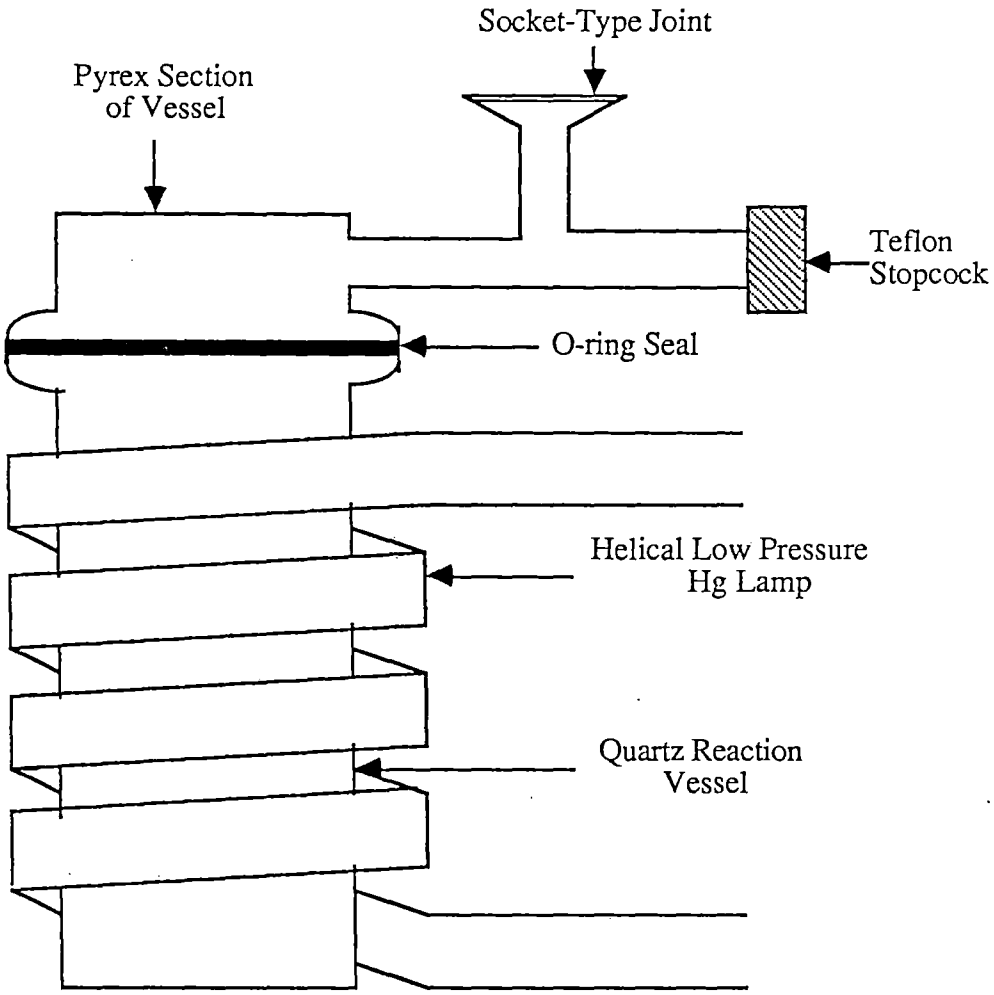


Figure 8. Photochemical Static Reactor

bottom of the reaction vessel with liquid nitrogen, vented to the atmosphere, the top compartment removed and methanol, spiked with an internal standard (naphthalene in this case), quantitatively added to dissolve the products as the vessel the warmed up to ambient temperature. Finally, 2 μL aliquots of the methanol solution were injected into the gas chromatograph. The same column used in the previous section was also used here for separation and identification of the products, but was temperature programmed from 200 °C.

Laser Light Extinction Spectrometer

When a beam of light from a 0.5 mW Metrologic He-Ne laser is passed through the irradiated toluene vapor, it is scattered by aerosols present in the reaction vessel. A diagram of the spectrometer used in measuring light extinction by the aerosol particles is shown in Figure 9.

The laser beam was collimated by the first lens so that a parallel beam of radius 1 cm passed through the reaction vessel. The same static reactor used in the previous section was used here, but the vessel was placed horizontally in the helical low pressure Hg lamp, with its axis parallel and optical windows perpendicular to the light beam. The beam emerging from the vessel was focused by the second lens of diameter 7 cm and focal length 20 cm, onto a 1 mm by 1 mm slit. This optical arrangement easily met the requirements suggested by Hodkinson (49), i.e., the angle subtended by the height of the slit at the lens, 5×10^{-3} radians, was less than one-tenth of the first angular minimum in the Fraunhoffer diffraction pattern of a disc equal to the particle in projected area. If x is the particle size parameter, then the angle

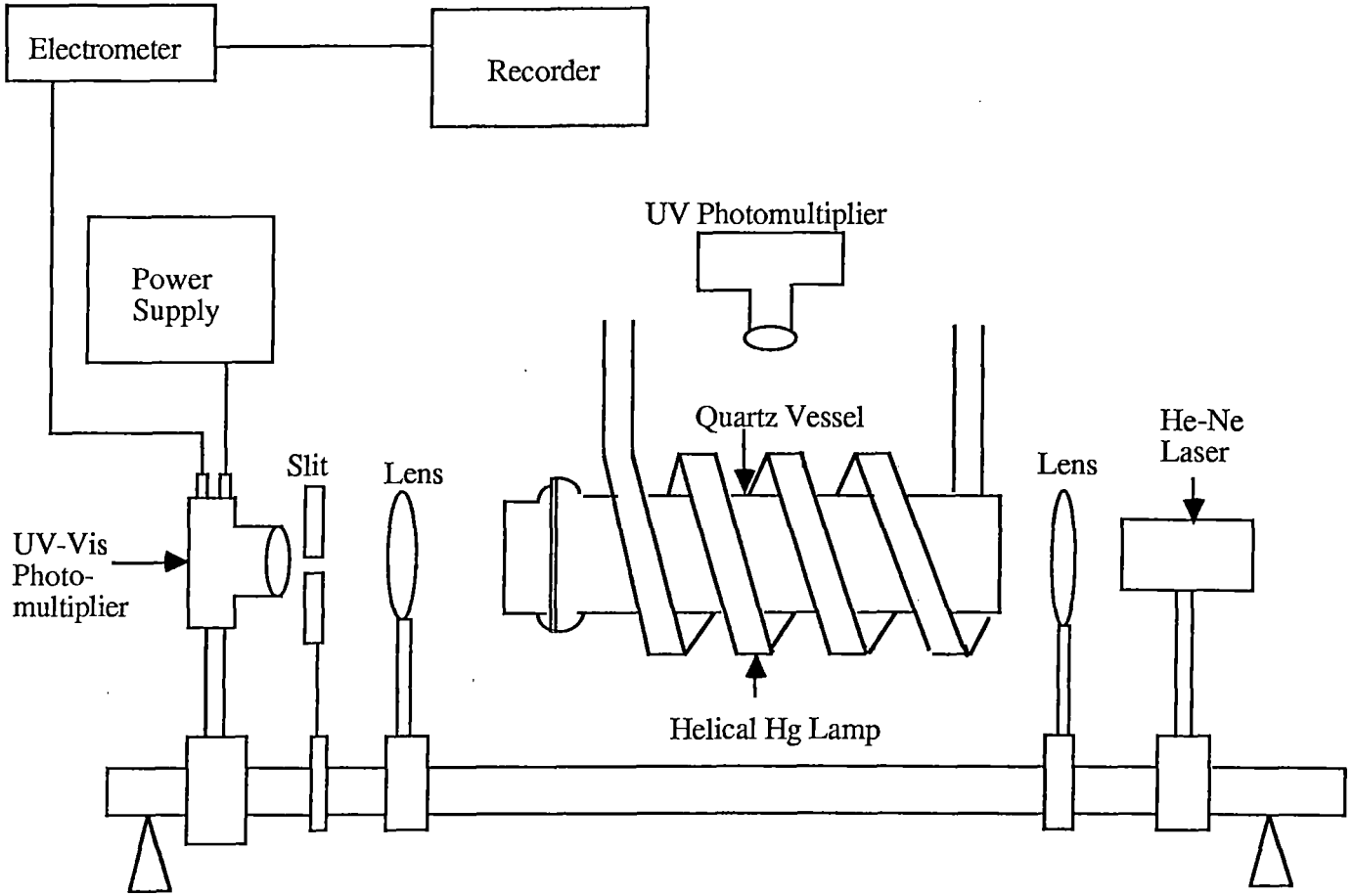


Figure 9. Laser-Light Extinction Spectrometer

referred to had to be less than one-tenth of 3.84/x radians. Behind the slit was the UV-VIS photomultiplier tube connected to a Keithley Instruments 610C Electrometer which in turn was attached to a Keithley Instruments 370 Milliammeter Pen Recorder.

Aerosols were observed to form within 30 seconds when the toluene-mercury mixture was being irradiated with the UV light and remained visible for several minutes after the light had been turned off. Hence, two sets of light extinction measurements were possible: (1) during irradiation, to obtain the rate of aerosol formation and (2) after irradiation to measure the rate at which the aerosols were deposited under gravity.

CHAPTER IV

EXPERIMENTAL RESULTS AND DISCUSSIONS

Product Analysis

The products from the Hg photosensitized decomposition of toluene vapor at 298 K using the 253.7 nm Hg resonance line are listed in Table II with their respective yields. These products were obtained after 30 min irradiation of the toluene vapor (10 mm Hg) in the flow reactor. A gas chromatogram of the volatile products is depicted in Figure 10. Toluene, the substrate, has a peak with a retention time of 7.59 min, retention times for methane, ethane and benzene are 2.16, 2.73 and 3.75 min respectively. O-, m- and p-xylene elute at 10.02, 11.03 and 11.45 min respectively and ethylbenzene at 14.20 min. Hydrogen cannot be detected with a flame ionization detector. However, the amount of it produced could not be any more than that calculated from pressure-volume measurements of residual uncondensed gases after the other products had been condensed in the trap using liquid nitrogen.

Figure 11 shows the peaks due to biphenyl, diphenylmethane and bibenzyl with retention times 30.01, 30.20 and 35.04 min respectively. All peaks were identified by comparing retention times to those of authentic samples. 2-methyldiphenylmethane and 4-methyldiphenylmethane, later identified on a gas chromatograph/mass spectrometer (GC/MS), had retention times of 35.50 and 36.00 min respectively. Other products with retention times between those of ethane and bibenzyl were present,

TABLE II

PRODUCT YIELDS FROM THE Hg PHOTOSENSITIZED DECOMPOSITION OF TOLUENE VAPOR AT 298 K

Product Name	Concentration (/ 10^{-5} M)
Hydrogen	< 0.4036
Methane	0.7996
Ethane	0.0700
Benzene	0.3005
O-xylene	0.0186
P-xylene	0.0335
M-xylene	0.0178
Ethylbenzene	0.0427
Biphenyl	0.0205
Diphenylmethane	0.0147
Bibenzyl	9.1710
2-Methyldiphenylmethane	0.1549
4-Methyldiphenylmethane	0.0712
Unknown (molecular weight 182)	0.2164

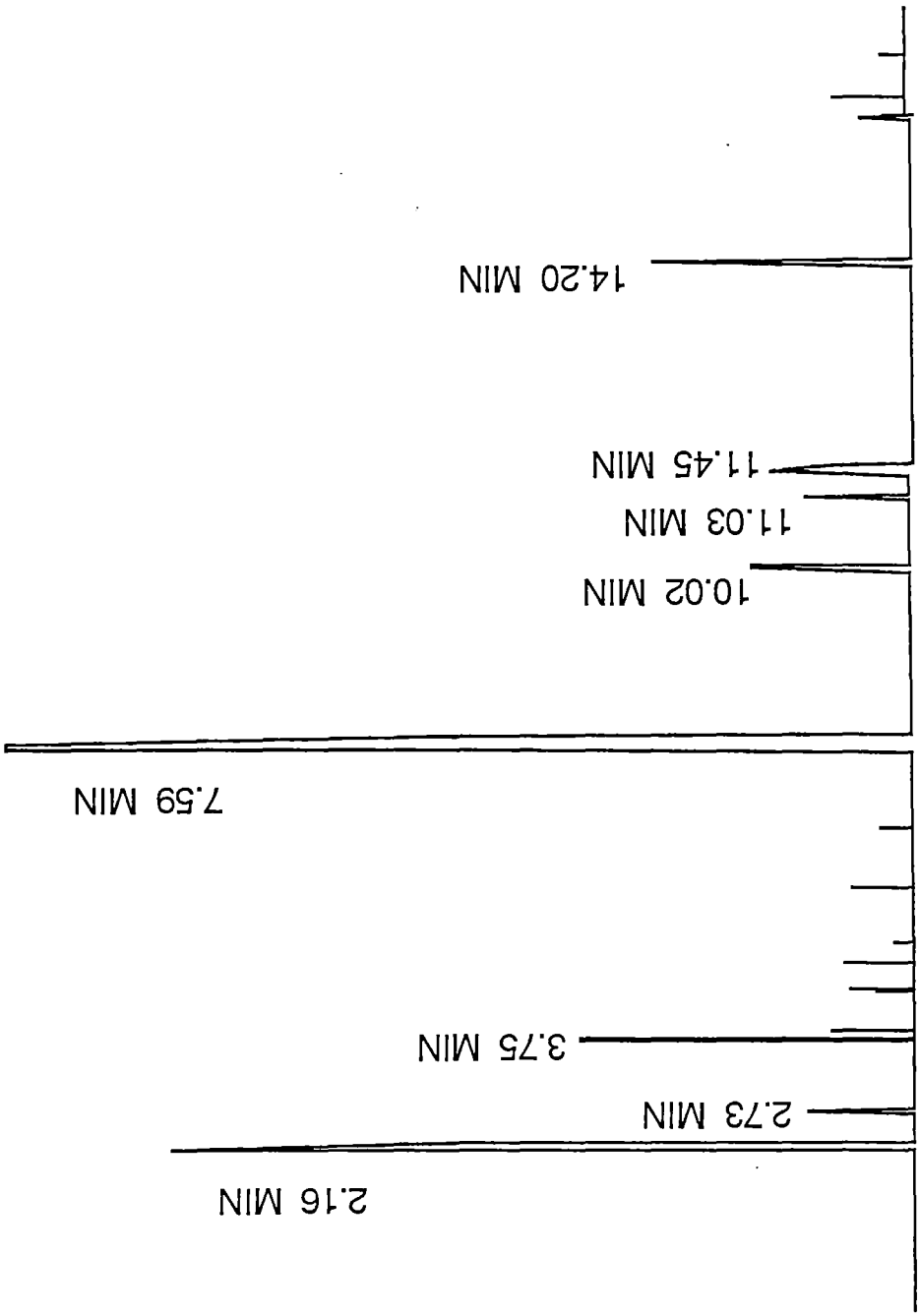


Figure 10. Gas Chromatogram of Volatile Products

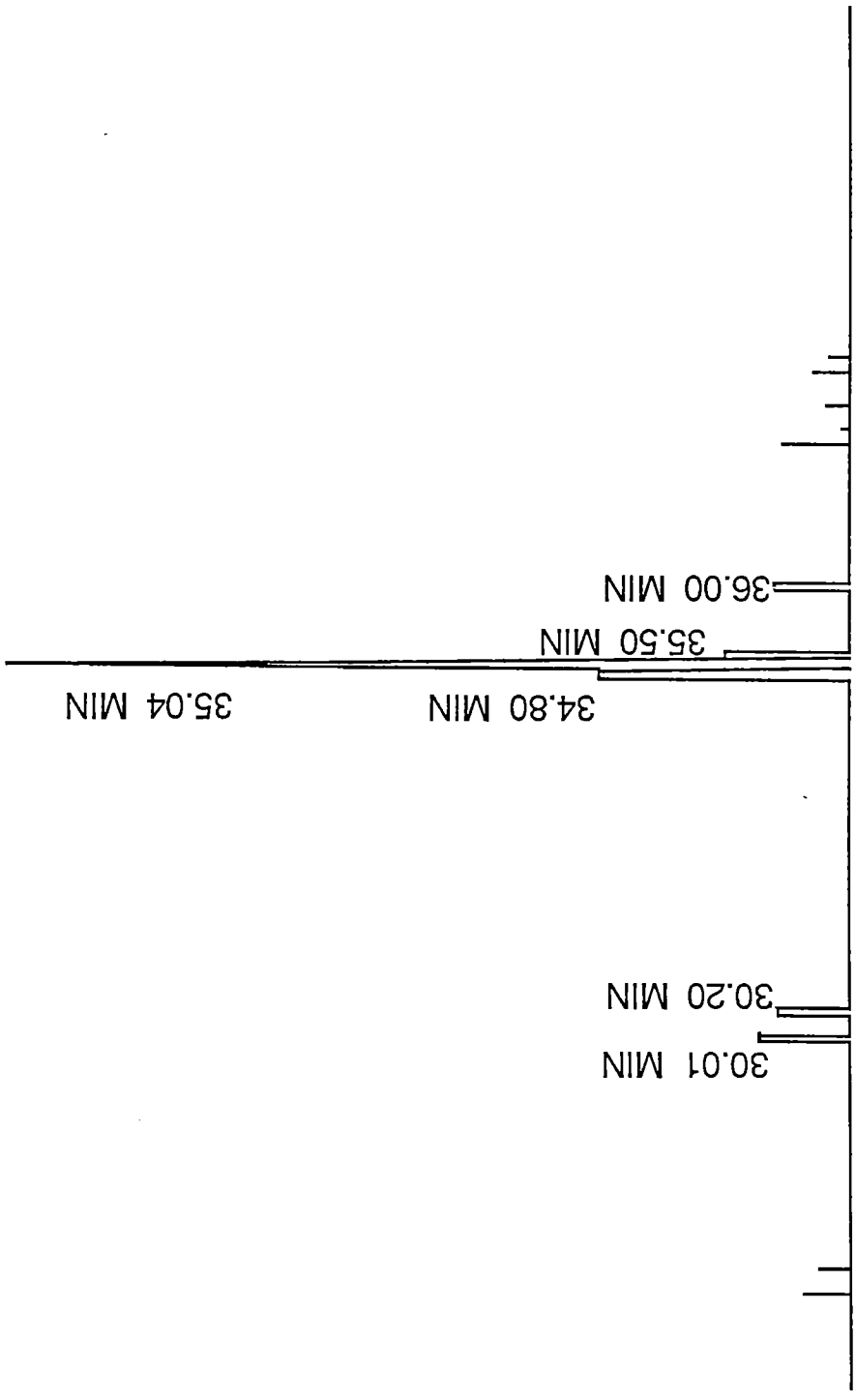


Figure 11. Gas Chromatogram of Nonvolatile Products

but were not identified, due to their very low concentrations.

The products with retention times around 35 min were further analyzed on a Finigan 10-20B GC/MS and identified by library search. Their reconstructed ion chromatogram is shown in Figure 12. Bibenzyl [1,1-(1,2-ethanediyl) bis-benzene], which was the major peak, occurred at 35.37 min. Its mass spectrum (Fig. 13) shows the molecular ion peak at m/e 182 and the base peak at m/e 91. The base peak could be attributed to $C_6H_5CH_2^+$, however, the presence of a peak at m/e 65 suggests that it is due to the tropylium ion ($C_7H_7^+$) formed by rearrangement of the benzylic ion, which then eliminates a neutral acetylene molecule to form $C_5H_5^+$ at m/e 65. Peaks at m/e 77, 78, and 79 are due to $C_6H_5^+$, $C_6H_6^+$ and $C_6H_7^+$ respectively caused by α-cleavage and H rearrangements characteristic of alkylbenzenes (50).

The peak at 35.50 min was attributed to 2-methyldiphenylmethane [1-methyl-2-(phenylmethyl)-benzene] and its mass spectrum is shown in Figure 14. Its molecular ion peak is at m/e 182, but the base peak is at m/e 167, due to $C_6H_4CH_2C_6H_5^+$ formed by the elimination of CH_3 from the benzene ring. The peak at m/e 168 is due to $(C_6H_5)_2CH_2^+$. At 36.02 mins, 4-methyldiphenylmethane [1-methyl-4-(phenylmethyl)-benzene] was identified. It also has a molecular ion peak at m/e 182 and a base peak at m/e 167 (Fig. 15). An unidentified product was found at 35.41 min with a molecular ion peak at m/e 182 and a base peak at m/e 91 (Fig. 16).

Proton nuclear magnetic resonance spectrum of the bibenzyl product dissolved in $CDCl_3$ was obtained from a Varian XL-300 MHz Fourier transform nuclear magnetic resonance (FT-NMR) spectrometer. The spectrometer was run at 4000 Hz and 16,384 G, chemical shifts were measured in ppm

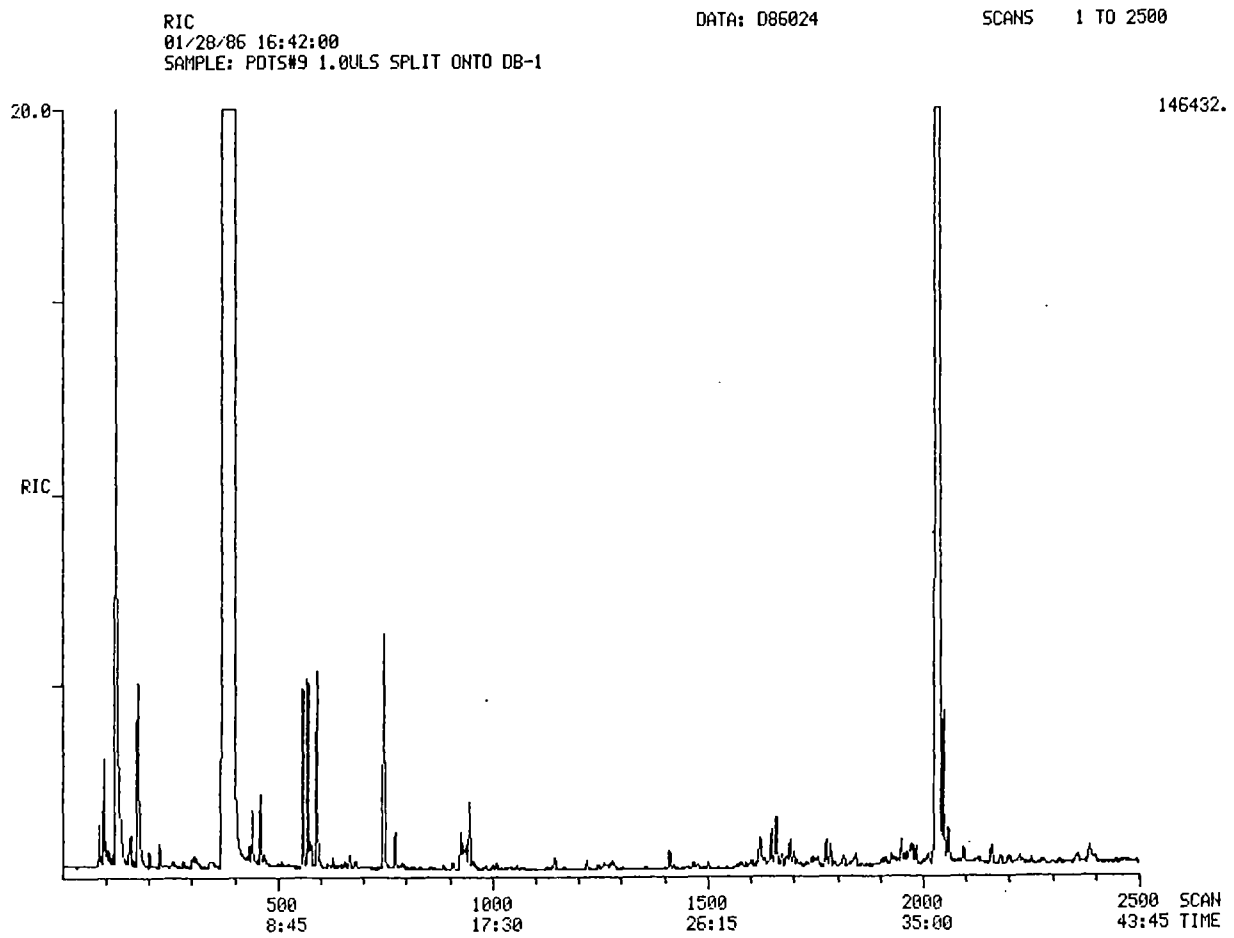


Figure 12. Reconstructed Ion Chromatogram

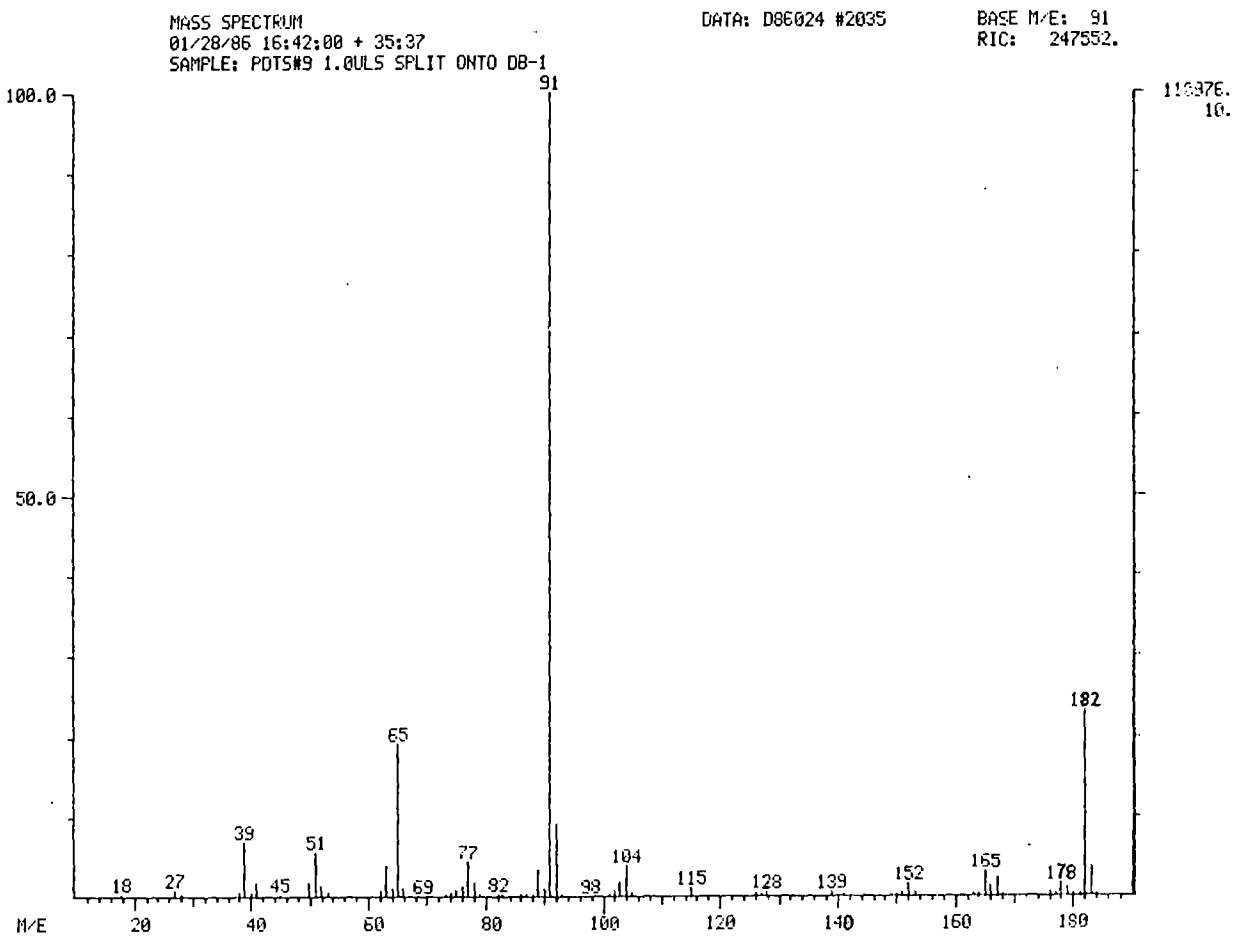


Figure 13. Mass Spectrum of Bibenzyl

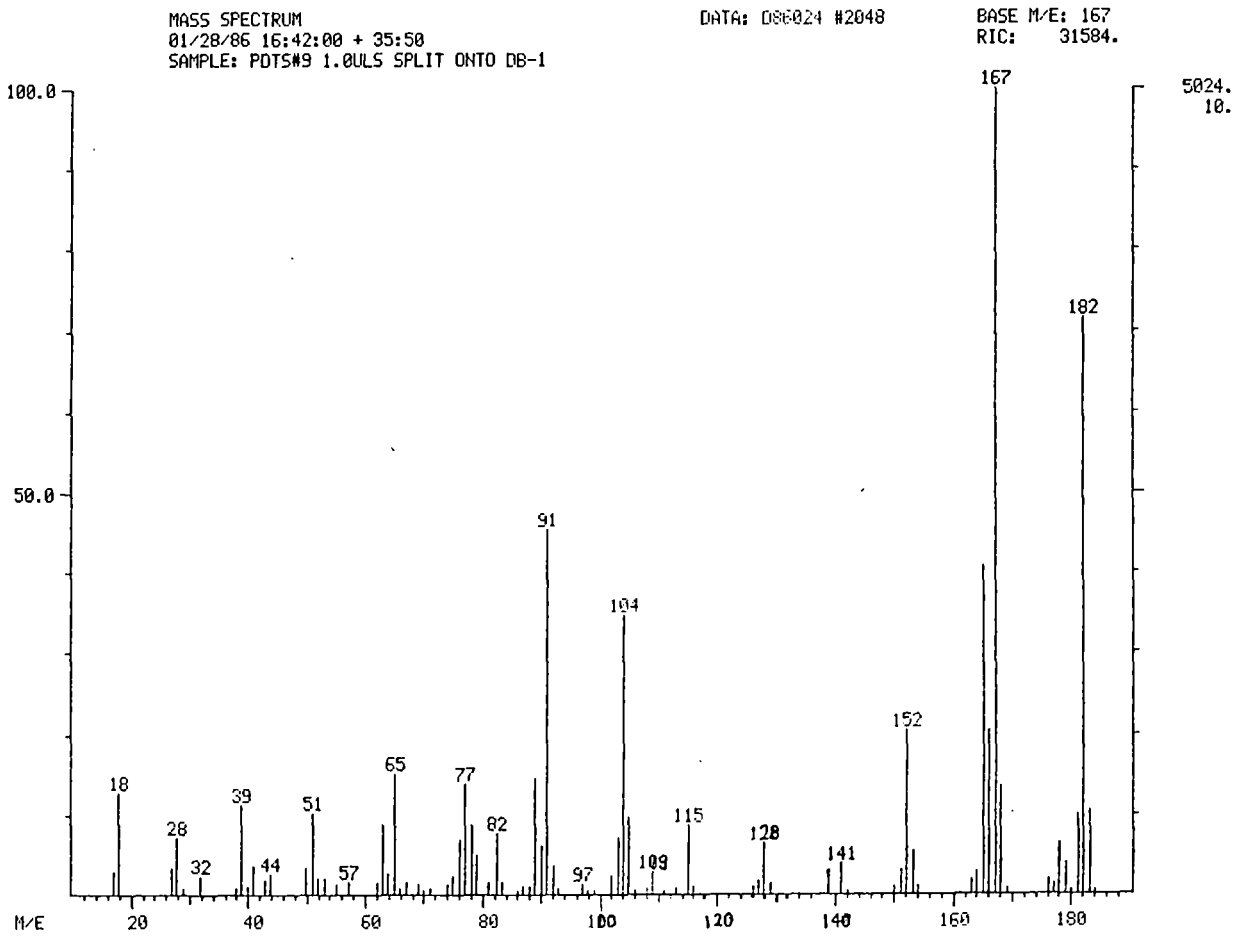


Figure 14. Mass Spectrum of 2-Methyldiphenylmethane

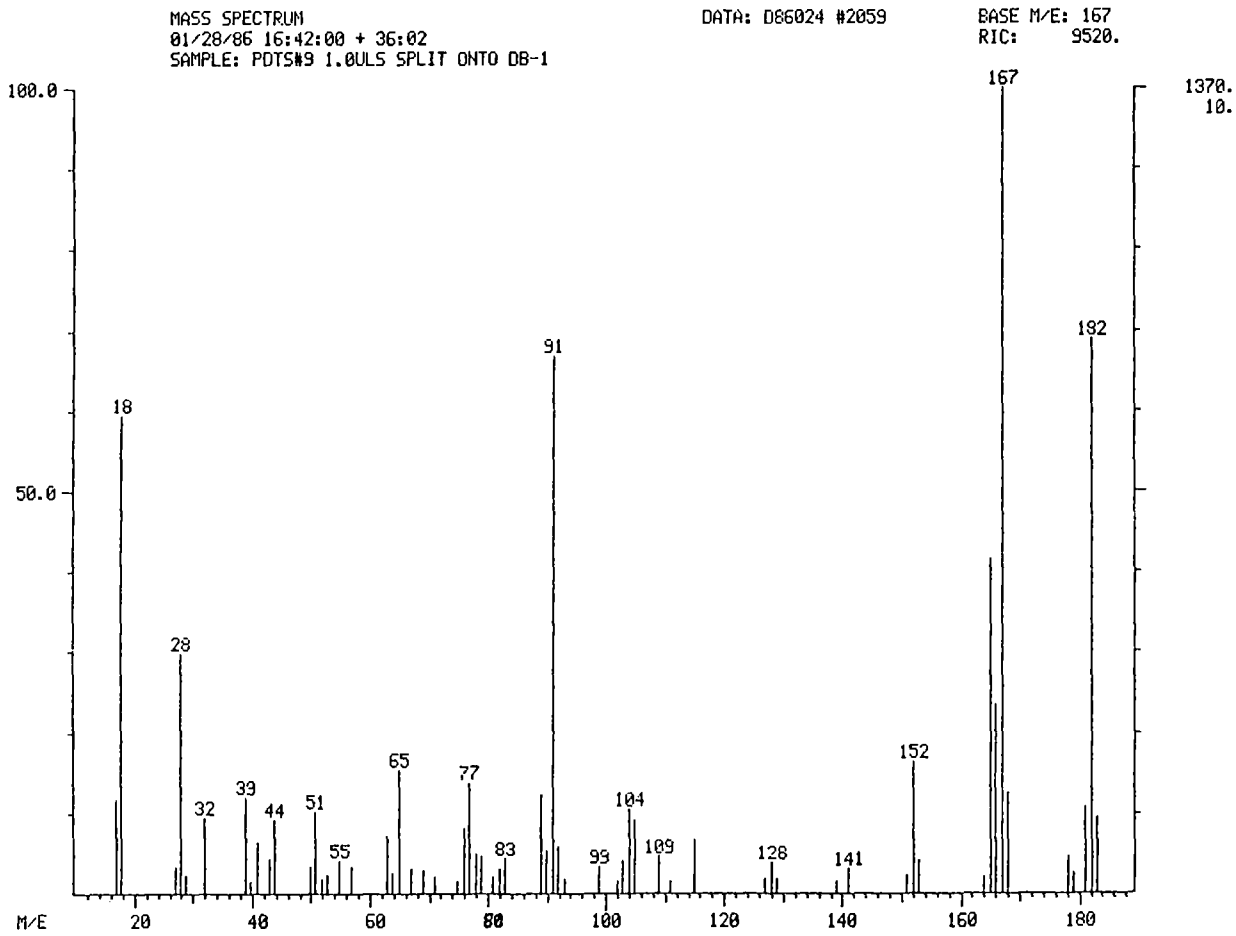


Figure 15. Mass Spectrum of 4-Methyldiphenylmethane

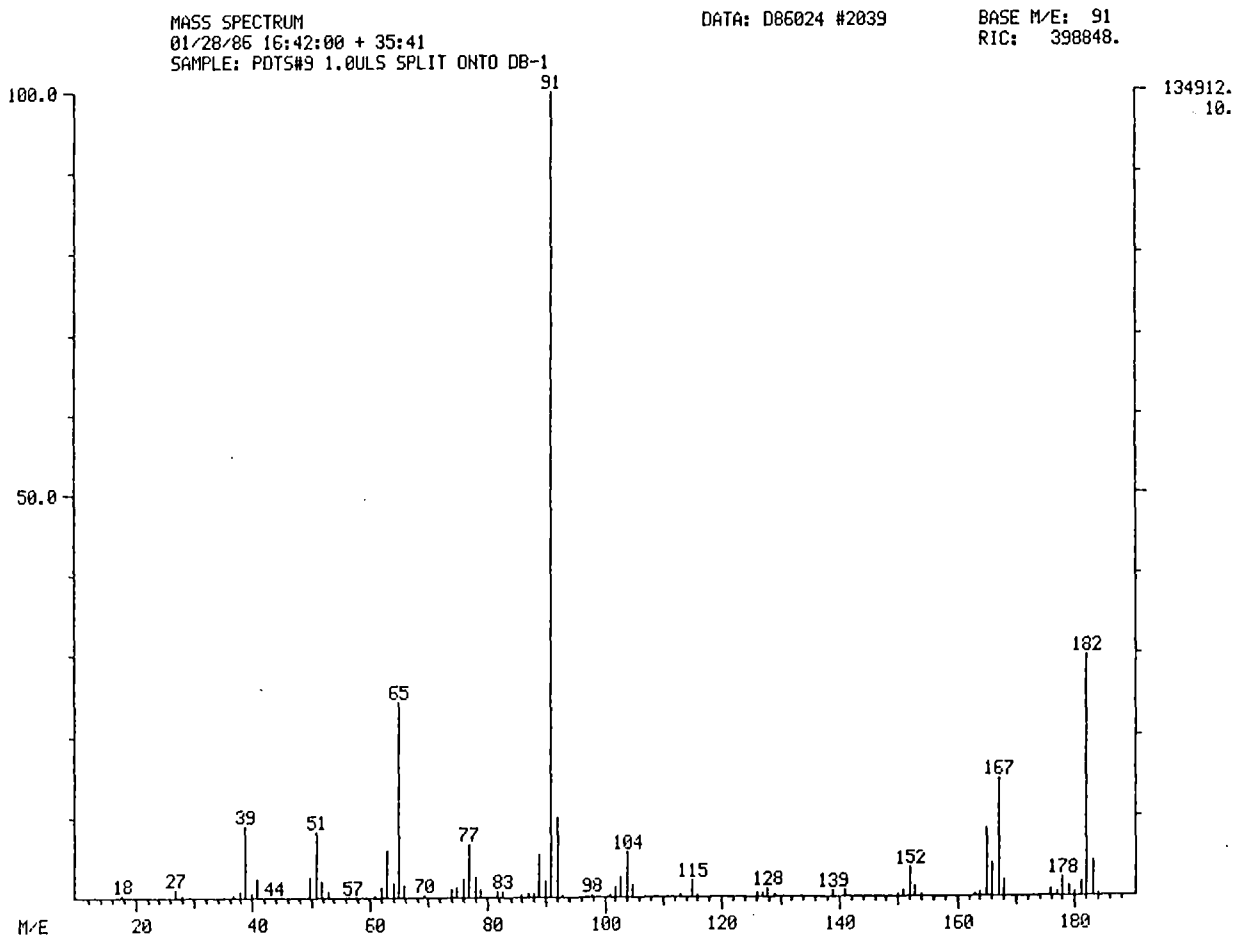


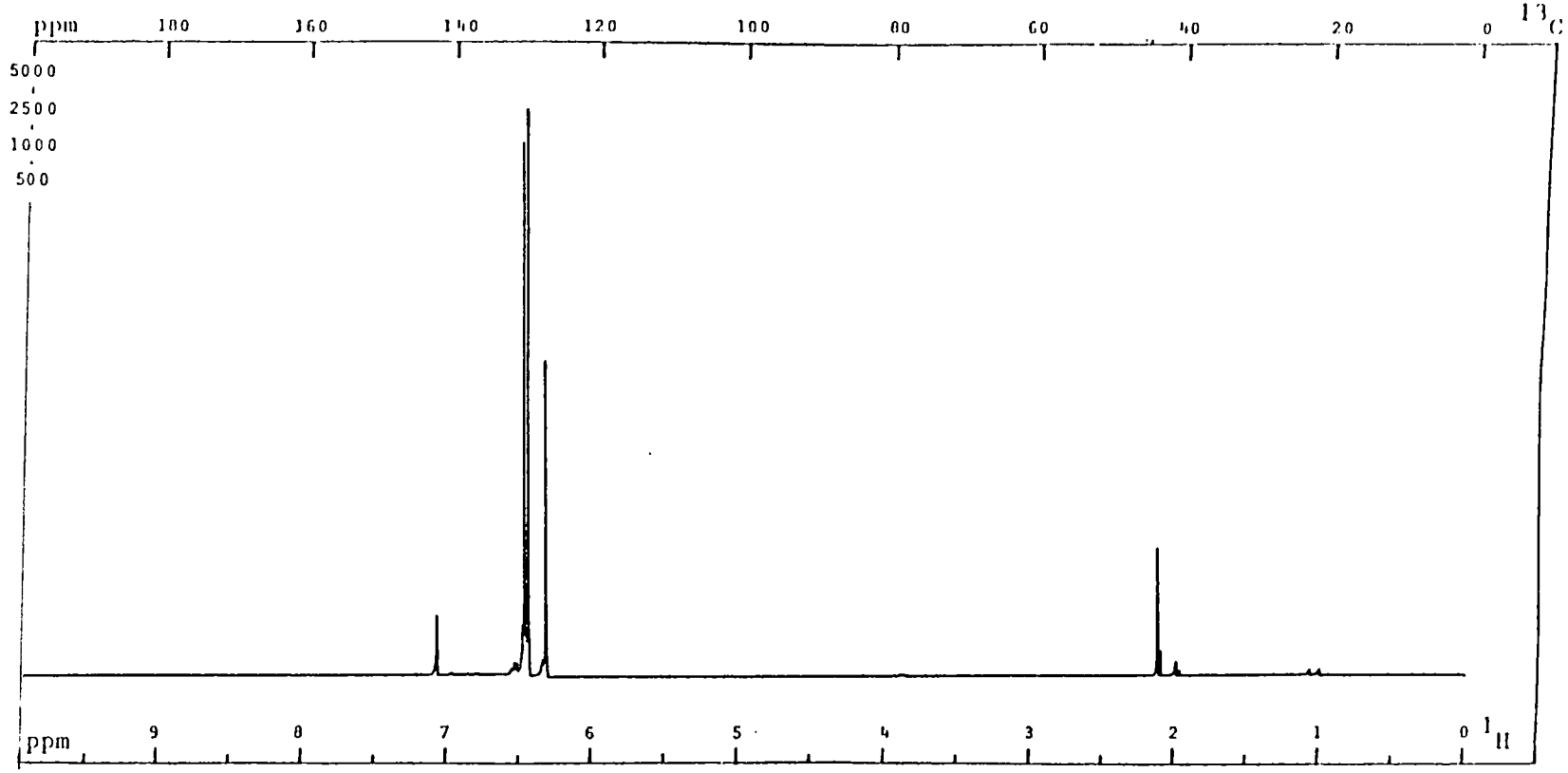
Figure 16. Mass Spectrum of Unidentified Product (Molecular Weight 182)

downfield from $(CH_3)_4Si$. The spectrum (Fig. 17) shows the peaks from the methylene protons at 2.95 ppm, the aromatic protons have peaks at 7.25 ppm. These positions are consistent with quoted literature values (51).

Explanation of the symbols used in the diagram are as follows: PFT - pulsed Fourier transform; CW - continuous wave; Solvent - solvent used; SF - spectrum frequency of nucleus; WC - chart width; T - temperature; NT - number of transients; Size - size of transform; PW/RF - pulse width/ radio frequency; TO - transmitter offset; FB - filter bandwidth; Lock - lock source; D1, D5 - delay after the pulse in the 300 MHz unit (D1), or 100 MHz unit (D5); DC - decoupler on or off; Gated Off - gated decoupling and with decoupler power off during the A(acquisition) or D(delay); DO - decoupler offset; RF(Power) - decoupler power setting; NBW - noise band width; LB - line broadening.

The ^{13}C FT-NMR spectrum of the same sample run on the Varian XL-300 MHz spectrometer is shown in Figure 18, and that of pure bibenzyl (from Aldrich Chemicals) shown in Figure 19. The spectra, which were obtained at 20000 Hz and 32,768 G, show the methylene carbon peaks at 38 ppm and two peaks due to the aromatic carbons centered at 130 ppm. As a result of the low concentration of the bibenzyl product, peaks caused by the coupling of the carbon and deuterium atoms from the solvent show up prominently in its spectrum at 77 ppm.

The Fourier transform infrared (FT-IR) spectrum of the bibenzyl product, obtained from a Nicolet 60-FS spectrometer, is given in Figure 20. Bibenzyl was identified by library search. Ten absorption bands were resolved in the wavelength range of 4000 - 700 cm^{-1}, in Table III, they are compared to the absorption bands of pure bibenzyl obtained from

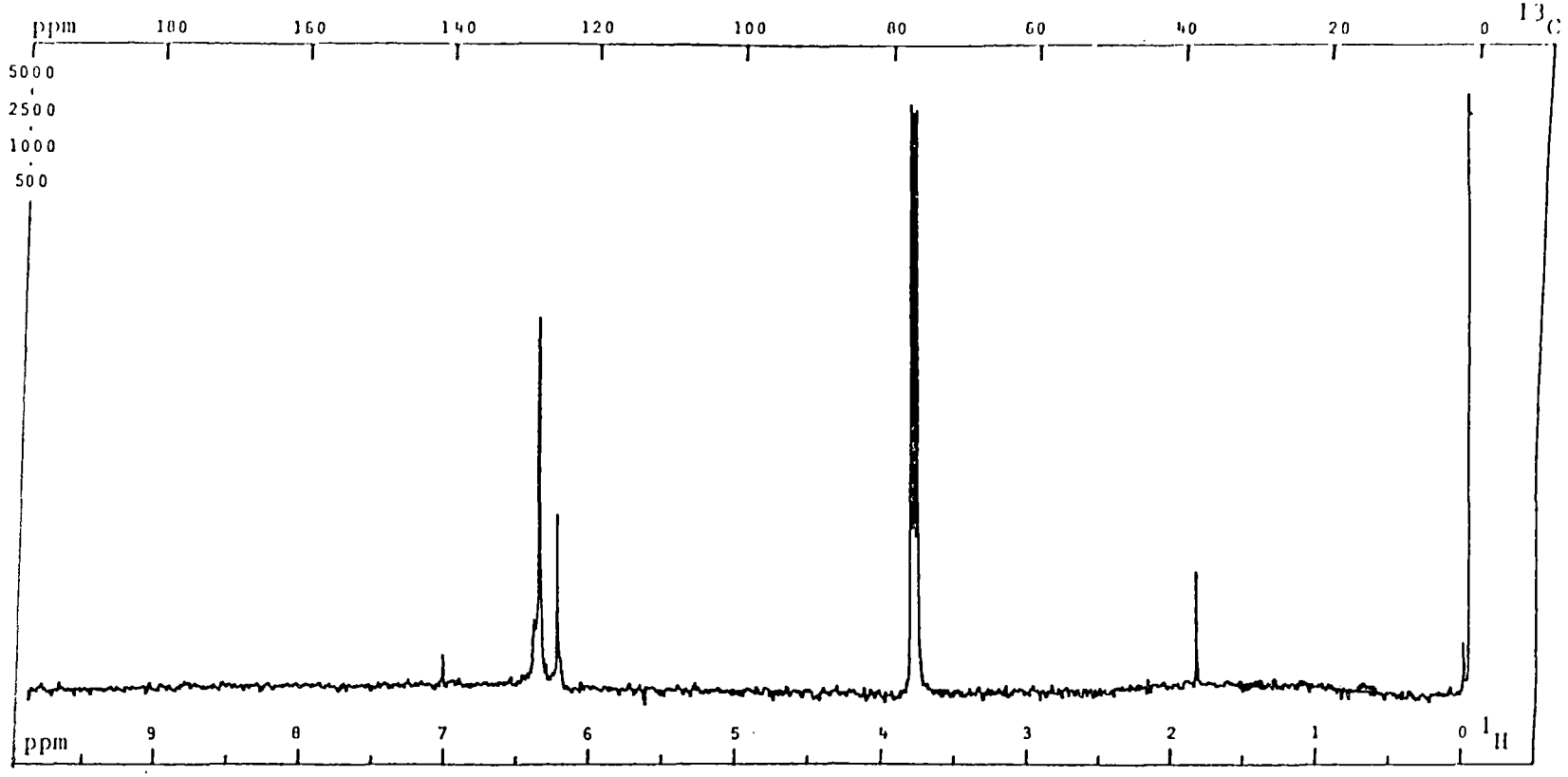


PFT X CW _ ; Solvent: $CDCl_3$; SF: 299.944 MHz; WC: 500 Hz; T: 25 °C; NT: 16

Size: 16 K; PW/RF: 5 µs/dB; TO: 0 Hz; FB: - Hz; Lock: $DCCl_3$; D1,D5: D1, 0 s.

DC: Y, N ; Gated Off: A or D ; DO: 0 Hz; RF(Power): 0 W/dB; NBW: - Hz; LB: - Hz.

Figure 17. Proton NMR Spectrum of the Bibenzyl Product

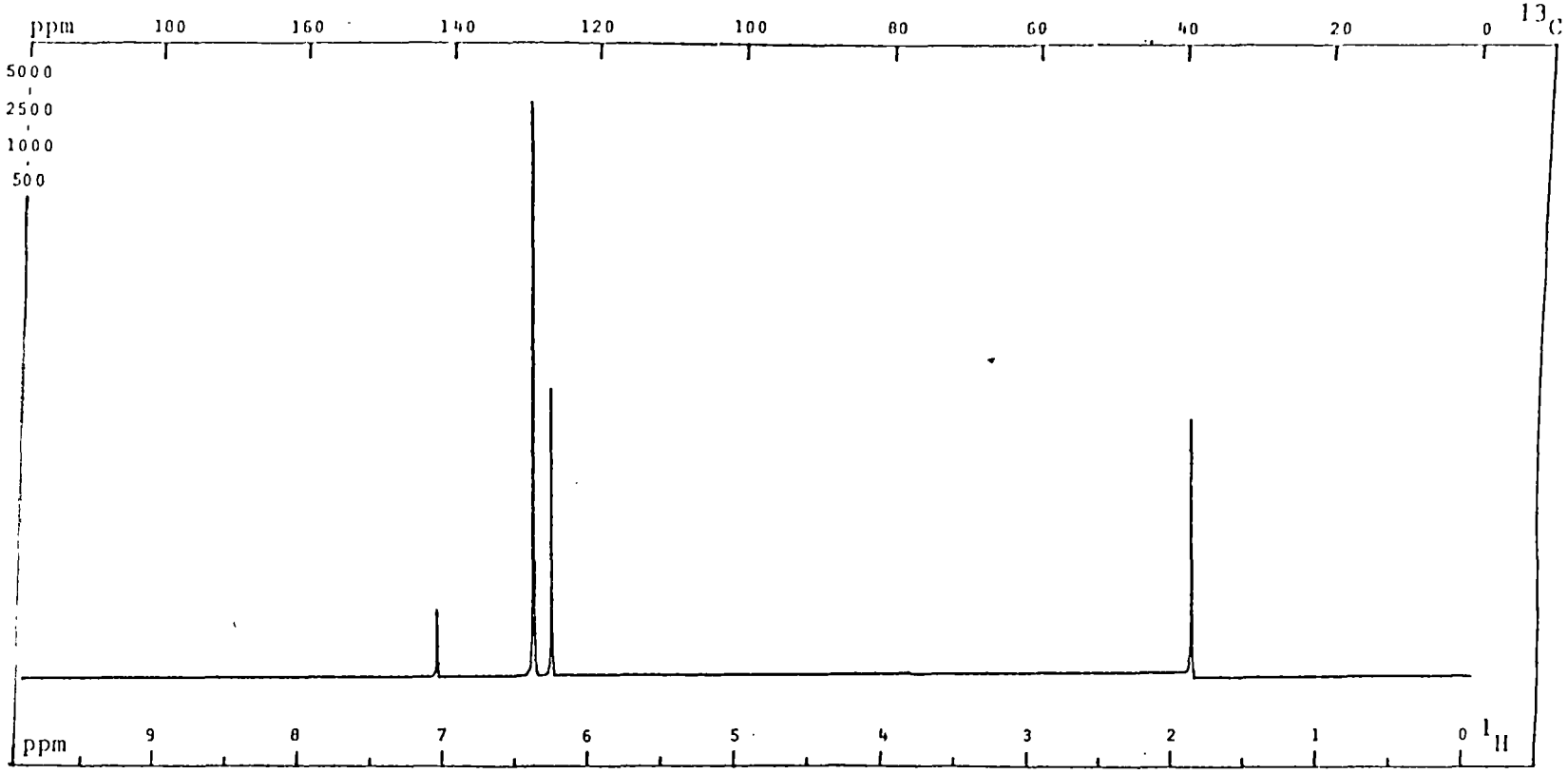


PFT X CW _ ; Solvent: $CDCl_3$; SF: 75.429 MHz; WC: 200 Hz; T: 25 °C; NT: 5000

Size: 8 K; PW/RF: 5 μs/dB; TO: 1000 Hz; FB: - Hz; Lock: $DCCl_3$; D1,D5: D1, 0 s.

DC: Y, N ; Gated Off: A or D ; DO: 0 Hz; RF(Power): 0 W/dB; NBW: - Hz; LB: 2.00 Hz.

Figure 18. Carbon-13 NMR Spectrum of the Bibenzyl Product



PFT X CW _ ; Solvent: $CDCl_3$; SF:75.429 MHz; WC: 200 Hz; T: 25 °C; NT: 400

Size: 40 K; PW/RF: 12.5 μs/dB; TO: 1000 Hz; FB: - Hz; Lock: $DCCl_3$; D1,D5: D1, 4.000 s.

DC: Y, N ; Gated Off:A or D ; DO: 0 Hz; RF(Power): 0 W/dB; NBW: - Hz; LB: 2.000 Hz.

Figure 19. Carbon-13 NMR Spectrum of Pure Bibenzyl

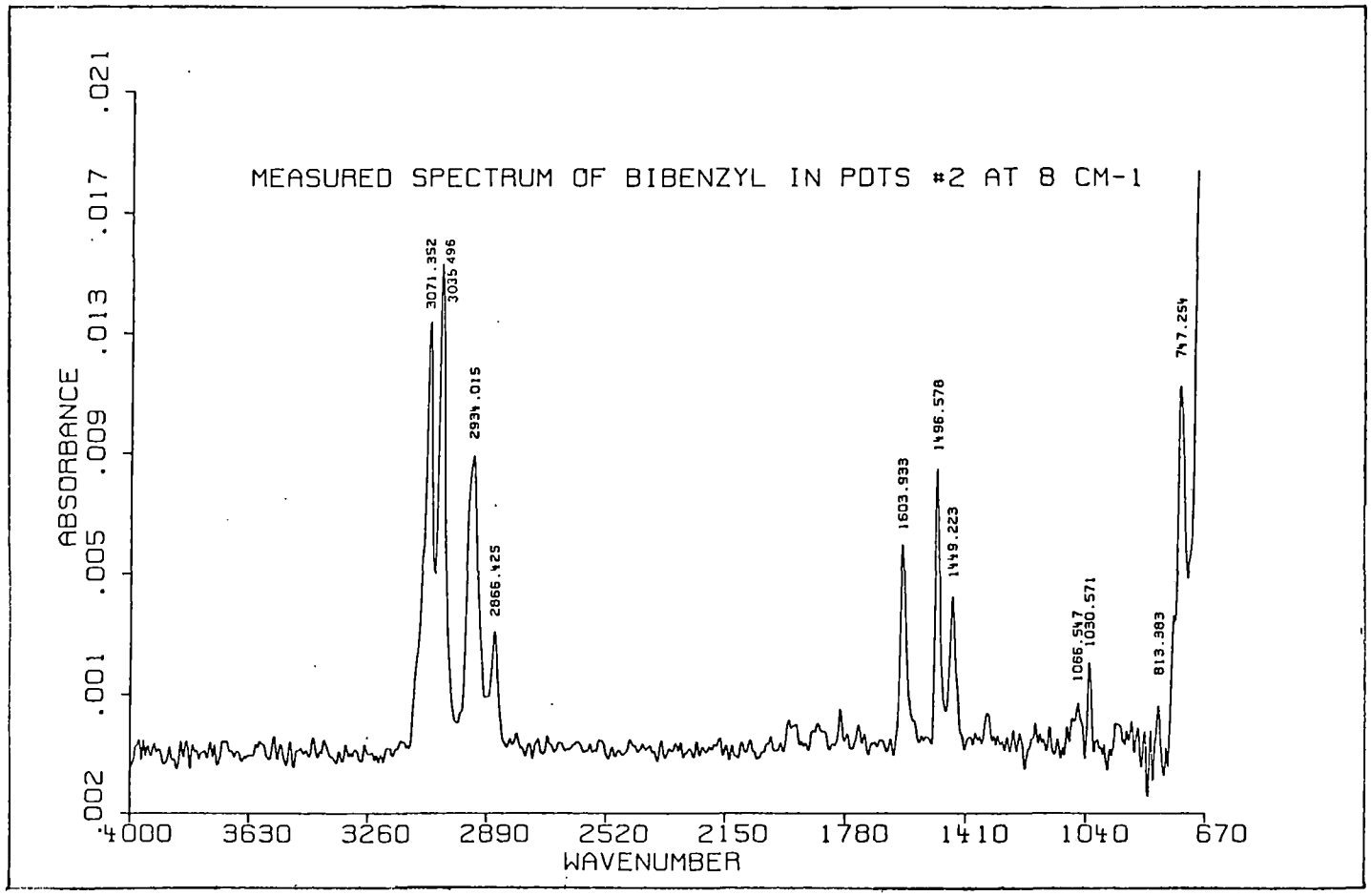


Figure 20. FT-Infrared Spectrum of the Bibenzyl Product

TABLE III

INFRARED ABSORPTION BANDS OF BIBENZYL(/CM^{-1})

Vibration Mode	Bibenzyl Product	Pure Bibenzyl
Ring C-H Stretching	3071.362	3080
"	3035.496	3050
Asymmetric CH_2 stretching	2934.015	2910
Symmetric CH_2 stretching	2866.425	2840
Ring C-C stretching	1603.933	1600
Ring deformation	1496.933	1490
CH_2 scissoring	1449.223	1450
In-plane C-H bending	1066.547	1070
"	1030.571	1030
"	813.383	900
Out-of-plane C-H bending	747.254	730
"	-	700

literature (51).

Bands resulting from aromatic C-H stretching vibrations occur at 3071 and 3035 cm^{-1}. Asymmetric C-H stretching vibrations of the methylenes give an absorption band at 2934 cm^{-1} and the symmetric stretching band which is expected to be weaker is at 2866 cm^{-1}. The C-C aromatic ring stretching bands occur at 1603, 1496 and 1449 cm^{-1}. In-plane C-H bending vibrations are at 1066 and 1030 cm^{-1} and out-of-plane ring C-H bending vibrations bands characteristic of polynuclear aromatics occur at 747 cm^{-1}, the other band around 690 cm^{-1} is out of the wavelength region surveyed (52) (53).

Thus the major dimeric product, bibenzyl, formed during triplet-mercury photosensitization of toluene vapor at 25 °C, has been unequivocally characterized by gas chromatography, mass spectrometry, nuclear magnetic resonance spectroscopy and infrared spectroscopy.

Kinetics of Product Formation

The yield of bibenzyl as a function of time is plotted in Figure 21. Bibenzyl was produced from toluene vapor (10 mm Hg) at 298 K using the static photochemical reactor, its rate of formation was found to be 0.0960 μmol/min.

Quantum yield of bibenzyl was determined by actinometry using the quantum yield of hydrogen formation from the Hg photosensitized decomposition of n-butane at 25 °C (54). In Table IV, the quantum yield decreases by only 10% over a period of 180 sec, suggesting that the bibenzyl molecules formed do not undergo any major reactions. The low values are consistent with previously reported yields (23) (24).

Nitric oxide inhibited the rate of bibenzyl formation. The effect

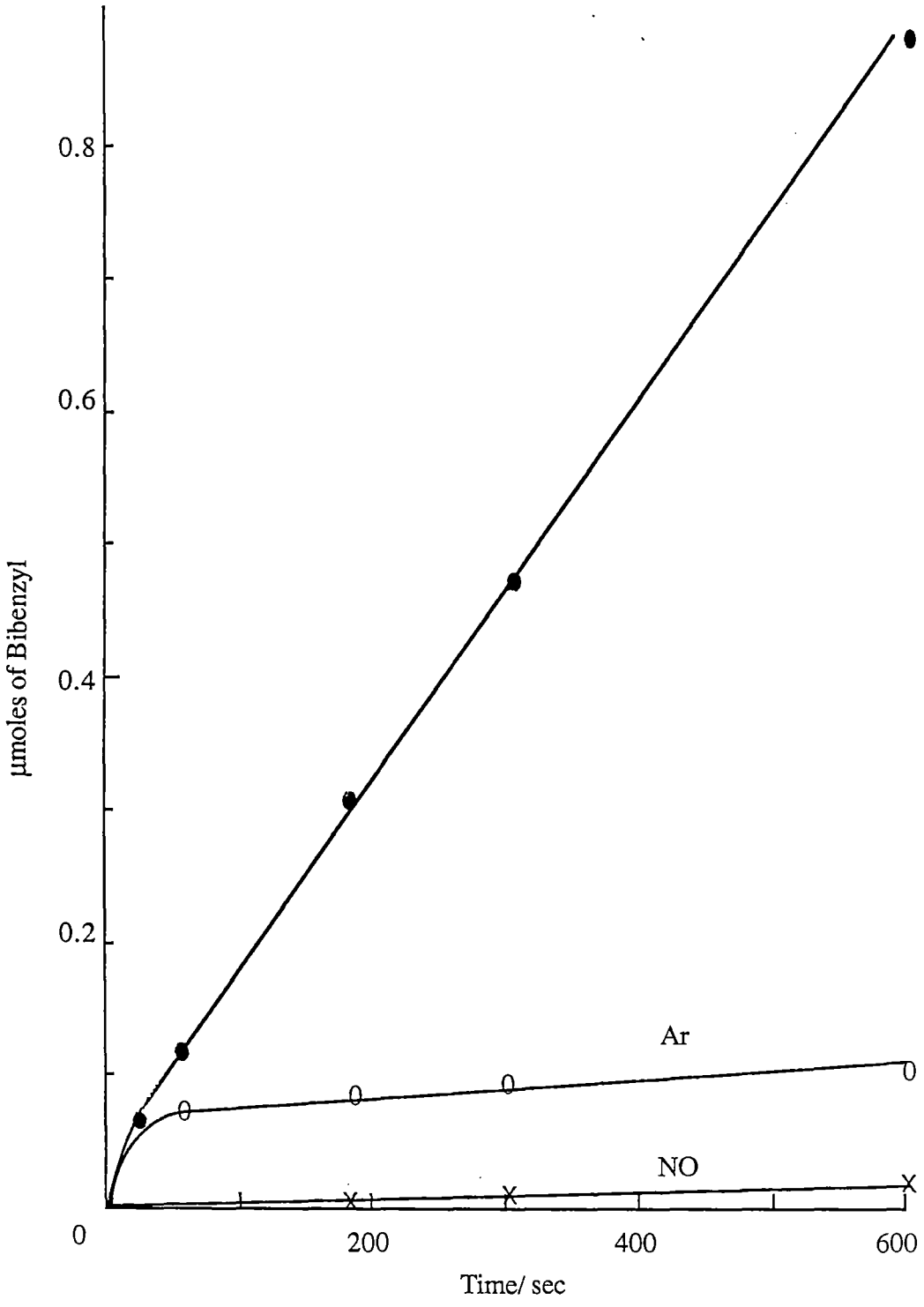


Figure 21. Bibenzyl Yield from the Hg Photosensitization of Toluene Vapor (10 mm Hg)

TABLE IV

QUANTUM YIELD OF BIBENZYL FORMATION

Time of irradiation (/sec)	Quantum Yield (/ 10^{-2})
30	1.0450
60	0.9854
180	0.8655
300	0.8226
600	0.7530

of 10% nitric oxide on bibenzyl yield is shown on the graph in Figure 21. On the same graph is depicted the effect of added inert gas, argon (100 mm Hg), even though the yield of bibenzyl is decreased considerably, it is greater than the yield from the addition of NO. The quantum yield of bibenzyl formation in the presence of NO was found to be 1.714×10^{-4} and 1.542×10^{-3} in the presence of Ar.

Figure 22 depicts the rate of bibenzyl formation as a function of toluene pressure. It increases steadily with substrate pressure, this is in line with the results of Yamamoto et al. (24), who found the benzyl radical concentration to increase with pressure. Bibenzyl is formed from the combination of two benzyl radicals:

$$2\ C_6H_5CH_2\cdot \quad \text{---------}> \quad C_6H_5CH_2CH_2C_6H_5 \qquad \text{(XII)}$$

Bibenzyl has also been reported as a major product in the pyrolysis of toluene (55) (56). At low temperatures the benzyl radical is present in large quantities, but the amount falls off at high temperatures as a result of its decomposition. Ingold and Lossing (57) estimate the activation energy for its disappearance as 68 ± 4 Kcal/mol. Using the flow technique, Horrex and Miles (56) calculated the unimolecular rate constant for bibenzyl decomposition as $2 \times 10^9 \exp -48000/RT\ sec^{-1}$. The rather low frequency factor and high activation energy preclude its decomposition at room temperature.

Kinetics of two volatile products, methane and benzene were determined at 298 K on the flow reactor. The vapor pressure of toluene used was 10 mm Hg, and the yields are shown as a function of time in Figure 23. Nitric oxide inhibited the rate of methane formation but did

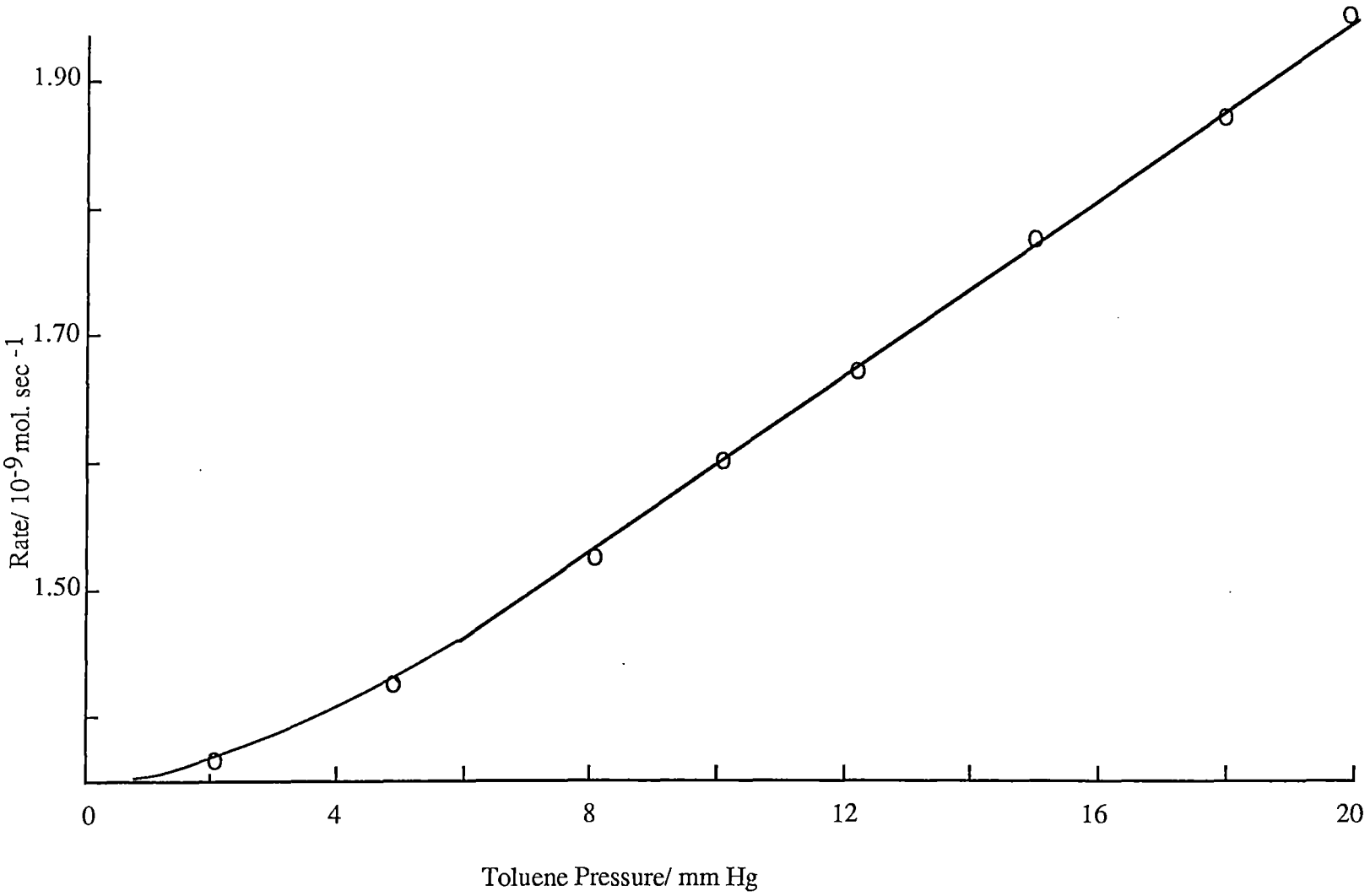


Figure 22. Effect of Toluene Pressure on the Rate of Bibenzyl Formation

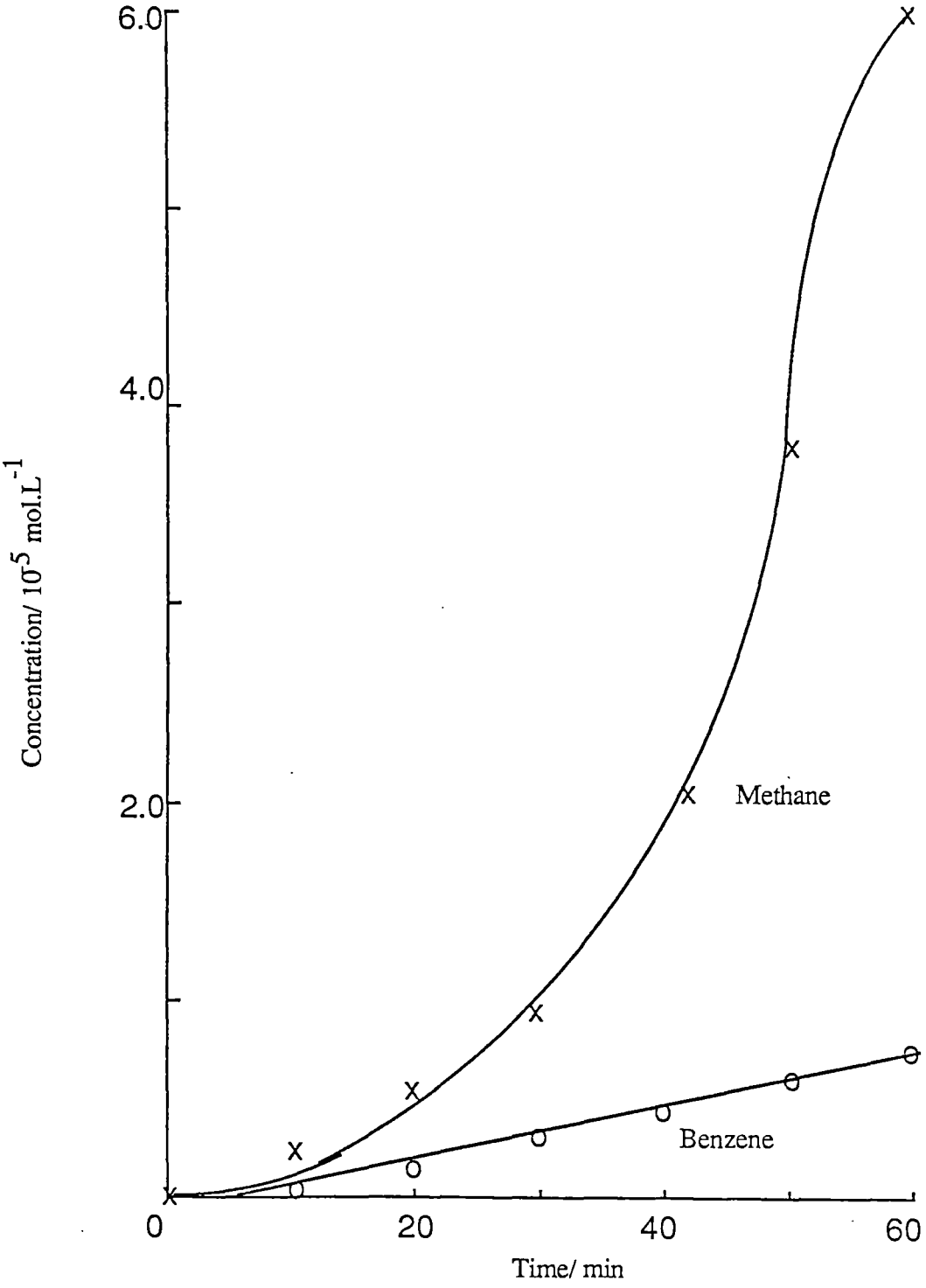


Figure 23. Methane and Benzene Yields from the Hg Photosensitization of Toluene Vapor (10 mm Hg)

not inhibit the rate of benzene formation to any great extent, as the graph in Figure 24 depicts. The initial rates of formation and quantum yields are reported in Table V. Hay (58) has pointed out that radical reactions with NO will be reversible unless the adduct formed is stabilized by efficient energy transfer through hybridization or resonance effects. The consequence of this is that σ-radicals do not react appreciably with NO as compared to π-radicals. Hence, it is not suprising that NO greatly inhibited the rates of formation of bibenzyl and methane, which are formed from π-radicals (benzyl and methyl radicals respectively). However, the rate of formation of benzene, which is formed from a σ-radical (phenyl) is not appreciably inhibited by NO.

The rates of formation of methane, benzene and the xylenes are shown as functions of toluene pressure in Figure 25. These rates tended to decrease in the pressure range of 2 - 20 mm Hg. Methane and benzene are formed from methyl and phenyl radicals. Though both, with the benzyl radical, are formed from excited toluene molecules, one type of the excited species forms the methyl and phenyl radicals and the other forms the benzyl radical, resulting in the difference in activities (23) (24).

Methane can be formed from the following reactions:

$$H\cdot + CH_3\cdot \longrightarrow CH_4 \qquad \text{(XIII)}$$

$$CH_3\cdot + C_6H_5CH_3 \longrightarrow CH_4 + C_6H_5CH_2\cdot \qquad \text{(XIV)}$$

Reaction XIII is expected to be exothermic with a small activation

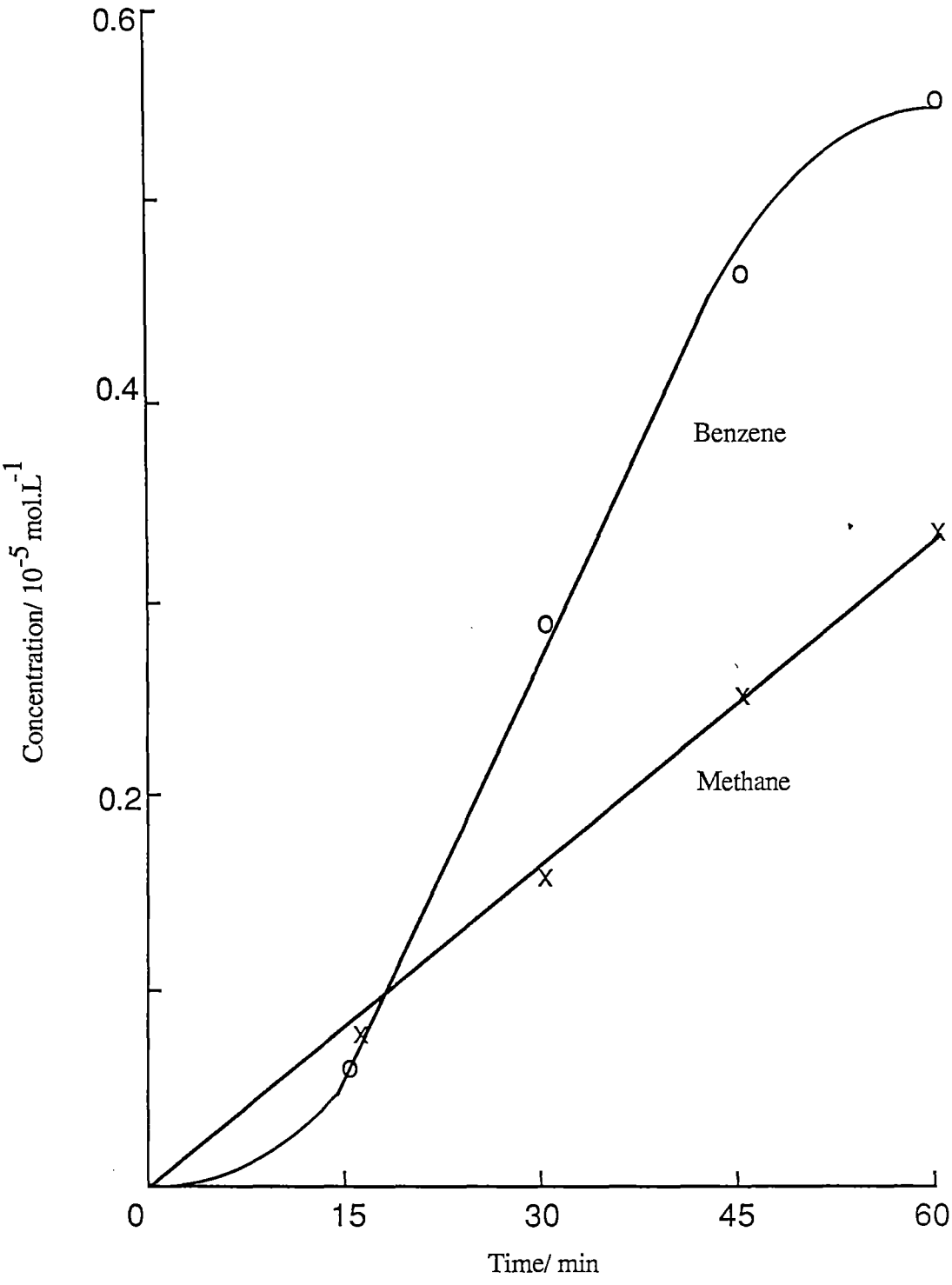


Figure 24. Effect of NO on Methane and Benzene Yields

TABLE V

INITIAL RATES OF FORMATION AND QUANTUM YIELDS
OF METHANE AND BENZENE

Name	Rate ($/10^{-7}$ $mol.L^{-1}\cdot min^{-1}$)	Quantum Yield ($/10^{-4}$)
Methane	2.667	8.105
Benzene	1.026	3.041
10% NO added:		
Methane	0.5185	1.554
Benzene	0.8889	2.838

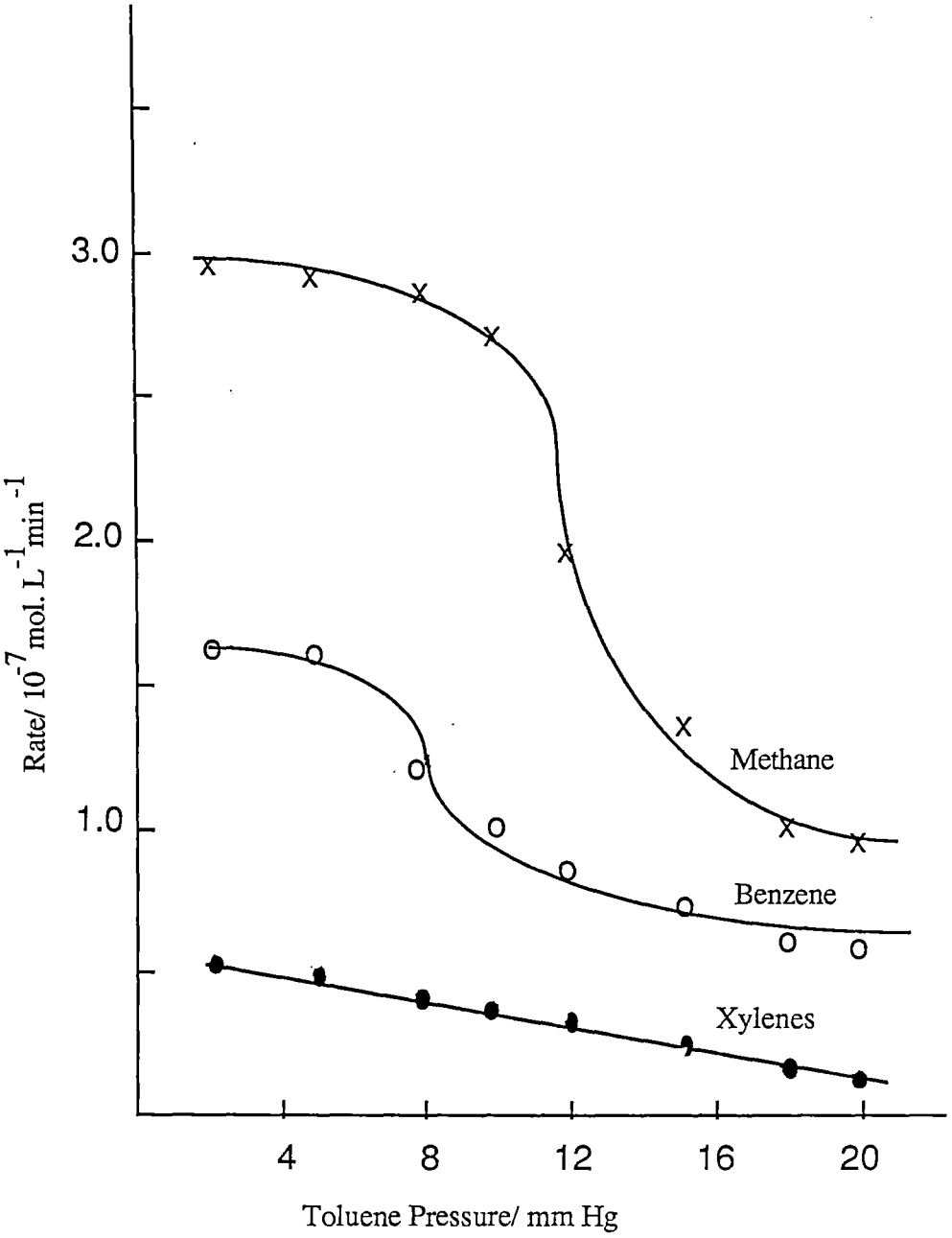


Figure 25. Effect of Toluene Pressure on the Rate of Formation of Methane, Benzene and the Xylenes

energy (59). The activation energy for reaction XIV is only 8.3 Kcal/mol and was determined from the photolysis of acetone (60). Reactions leading to benzene formation are:

$$H\cdot + C_6H_5\cdot \longrightarrow C_6H_6 \qquad \text{(XV)}$$

$$C_6H_5\cdot + C_6H_5CH_3 \longrightarrow C_6H_6 + C_6H_5CH_2\cdot \qquad \text{(XVI)}$$

The formation of benzene by the reaction,

$$H\cdot + C_6H_5CH_3 \longrightarrow C_6H_6 + CH_3\cdot \qquad \text{(XVII)}$$

was ruled out by Blade et al. (61), who found only hydrogen but no methane to form during the pyrolysis of bibenzyl in the presence of toluene.

The rate of hydrogen formation was taken as the rate of residual gas production. Its dependence on toluene pressure is shown in Figure 26, and as expected, it goes through a maximum (23). Hydrogen quantum yield will be less than 4.091×10^{-4}. The reactions which account for hydrogen formation are:

$$H\cdot + C_6H_5CH_3 \longrightarrow C_6H_5CH_2\cdot + H_2 \qquad \text{(XVIII)}$$

$$H\cdot + H\cdot + M \longrightarrow H_2 + M \qquad \text{(XIX)}$$

Steiner (62) has calculated the frequency factor as 10^{10} $L.mol^{-1}.sec^{-1}$ and estimated E_a as approximately zero for reaction XIX, with errors

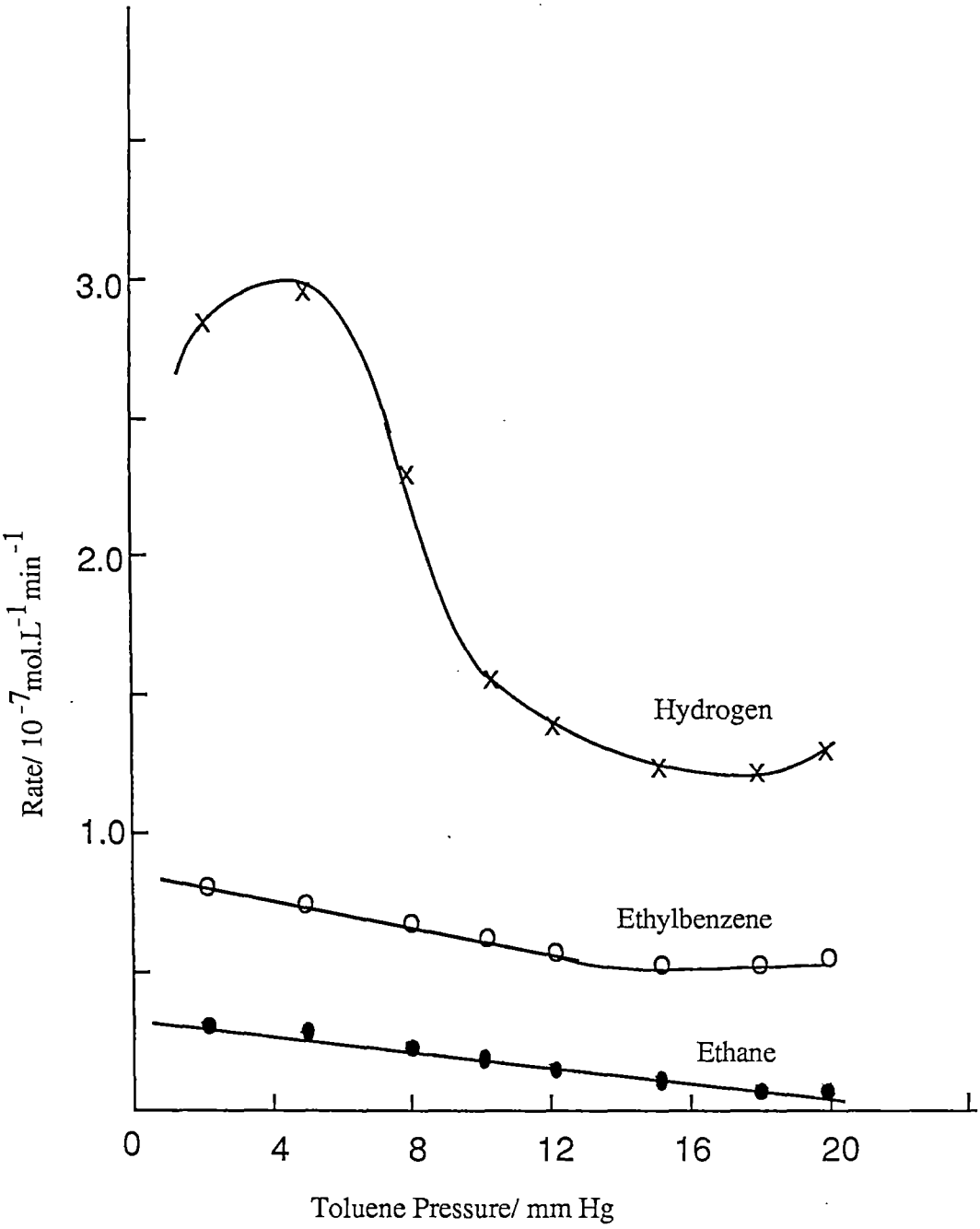


Figure 26. Effect of Toluene Pressure on the Rate of Formation of Hydrogen, Ethane and Ethylbenzene

introduced by wall-effects (M).

Ethane, a minor product, is formed from the recombination of two methyl radicals:

$$2\ CH_3\cdot \longrightarrow C_2H_6 \qquad \text{(XX)}$$

The half-life of the methyl radical at room temperature is 0.006 sec (63). Despite the the disagreement in reported activation energy values for reaction XX, it is expected to be low enough for the reaction to occur at room temperature (59). Ingold and Lossing (64) obtained E_a = -2.2 $\pm$ 0.5 Kcal/mole and suggest a collision efficiency of unity at room temperature. The effect of toluene pressure on the rate of ethane and ethylbenzene formation is also shown in Figure 26, and like the other volatile products formed via methyl or phenyl radicals, the rates tend to decrease with increasing substrate pressure.

Ethylbenzene and the xylenes will be formed by reactions between methyl radicals and benzyl or tolyl radicals:

$$CH_3\cdot + C_6H_5CH_2\cdot \longrightarrow C_6H_5C_2H_5 \qquad \text{(XXI)}$$

$$CH_3\cdot + C_6H_5CH_2\cdot \longrightarrow C_6H_4(CH_3)_2 \qquad \text{(XXII)}$$

The pressure dependency exhibited by the volatile products can be interpreted as resulting from competitive collisional stabilization of their vibrationally excited precursors in either the ground or the excited triplet state.

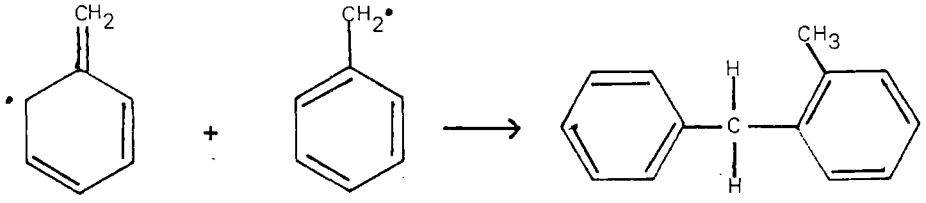
Biphenyl is formed from two phenyl radicals:

$$2\ C_6H_5\cdot \longrightarrow (C_6H_5)_2 \qquad \text{(XXIII)}$$

An activation energy of 13 Kcal/mol was suggested for reaction XXIII from the Hg photosensitized decomposition of benzene (65). The reaction between a phenyl and a benzyl radical will result in the formation of diphenylmethane.

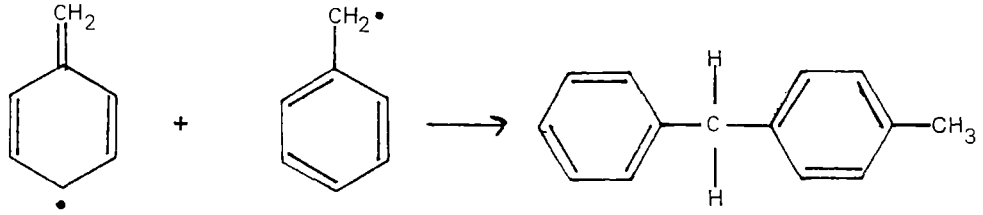
$$C_6H_5\cdot + C_6H_5CH_2\cdot \longrightarrow C_6H_5CH_2C_6H_5 \qquad \text{(XXIV)}$$

It must be mentioned that Blades et al. (61) found the "large amounts of bibenzyl" formed during the pyrolysis of toluene to be rather a mixture of isomeric dimethyl diphenyls, the formation of which they attribute to the secondary decomposition of benzyl radicals. In this experiment, formation of the methyldiphenylmethanes have been attributed to cross combination reactions between tolyl and benzyl radicals.



(XXV)

2-MDPM



(XXVI)

4-MDPM

2-methyldiphenylmethane (2-MDPM) was formed via an o-tolyl radical, and 4-methyldiphenylmethane (4-MDPM) from a p-tolyl radical. Yamamoto et al. (24) did report the formation of 3-methyldiphenylmethane (3-MDPM), however, this would be formed via a m-tolyl radical, which is not a preferred canonical resonance form.

Formation of Bibenzyl Aerosols

A quartz infrared gas cell fitted with sodium chloride windows was filled with toluene vapor (10 mm Hg), argon (15 mm Hg) and a drop of mercury added, then subjected to ultra-violet radiation from the helical low pressure Hg-lamp for 15 mins. The argon present, prolonged the time of suspension of the aerosols formed and thus enabled the infrared spectrum of the aerosols to be obtained in situ, by use of a Digilab FTS-20 infrared spectrometer. The spectrum, corrected for toluene absorption is shown in Figure 27 and the bands resolved are listed in Table VI with the absorption bands of toluene, obtained from the literature (66). Comparison with Table III proves that bibenzyl forms the aerosol particles in the reaction vessel.

Aerosols formed in the static reactor were allowed to deposit on aluminum plates and analyzed on a scanning electron microscope (Cambridge Instruments Stereo Scan SEM-90B) after coating with a gold film. An electron micrograph of some of the aerosols formed after 5 mins of irradiating 10 mm Hg toluene vapor is shown in Figure 28. Uniform spheres of diameter 5.6×10^{-7} m were obtained. After 15 mins of irradiation, the aerosols coalesced into larger particles of varying sizes ranging from 4×10^{-6} m to 10^{-5} m agglomerates (Fig 29). Much larger flakes were produced after 30 mins of irradiation (Fig. 30).

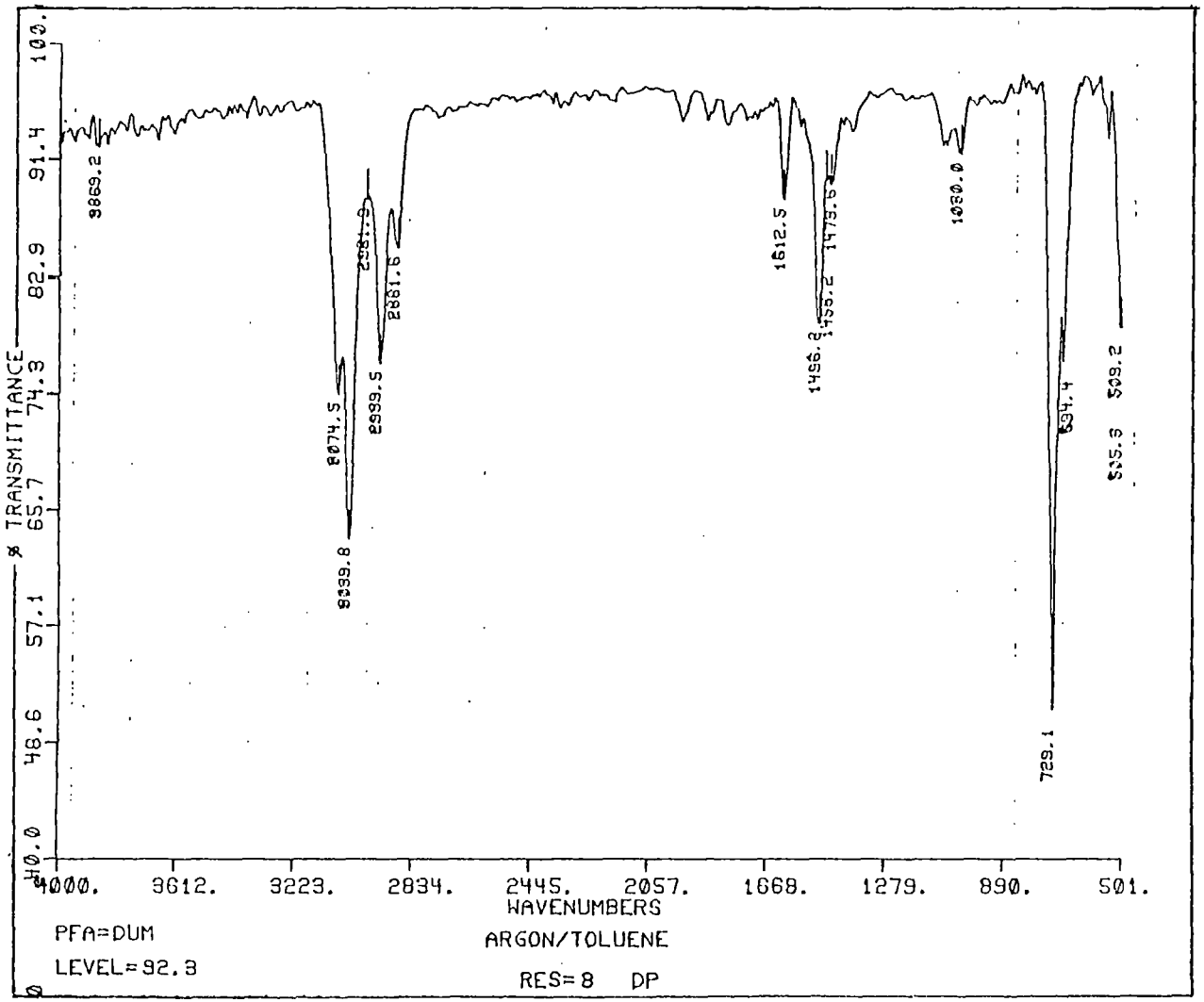


Figure 27. FT-Infrared Spectrum of Bibenzyl Aerosols

TABLE VI

INFRARED ABSORPTION BANDS OF THE AEROSOLS AND TOLUENE ($/CM^{-1}$)

Vibration Mode	Bibenzyl Aerosols	Toluene Vapor
Ring C-H stretching	3074.5	-
"	3039.8	3040
"	-	2930
Asymmetric CH_2 stretching	2939.5	-
Symmetric CH_2 stretching	2881.6	-
Ring C-C stretching	1612.5	1610
Ring deformation	1496.8	1500
CH_2 scissoring	1458.2	-
In-plane CH_3 bending	-	1460
"	-	1380
"	-	1180
In-plane C-H bending	-	1090
"	1030.0	1040
"	-	900
Out-of-plane C-H bending	729.0	730
"	694.4	700

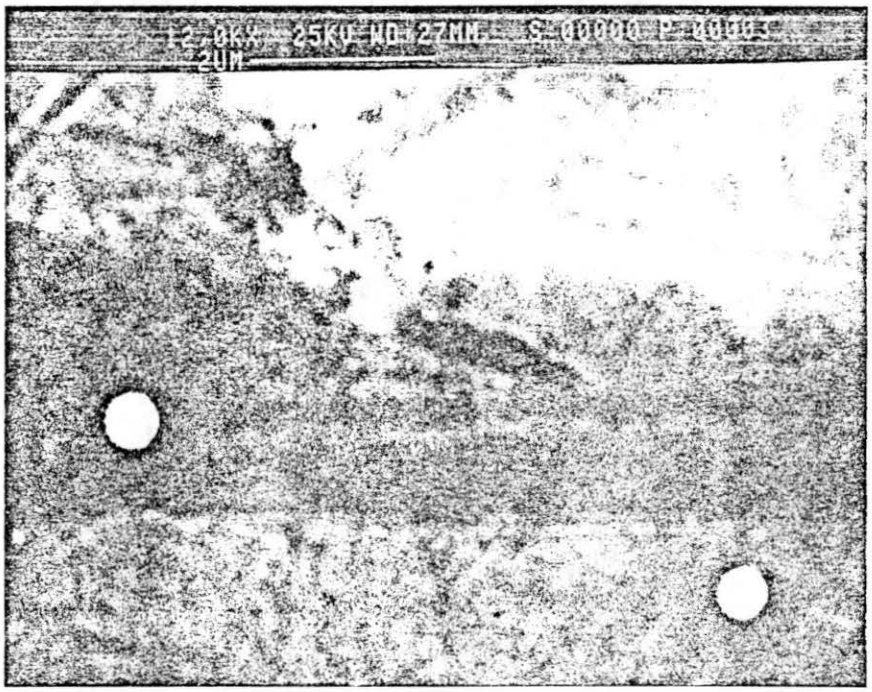


Figure 28. Scanning Electron Micrograph of Aerosols Formed after 5 min of Irradiation

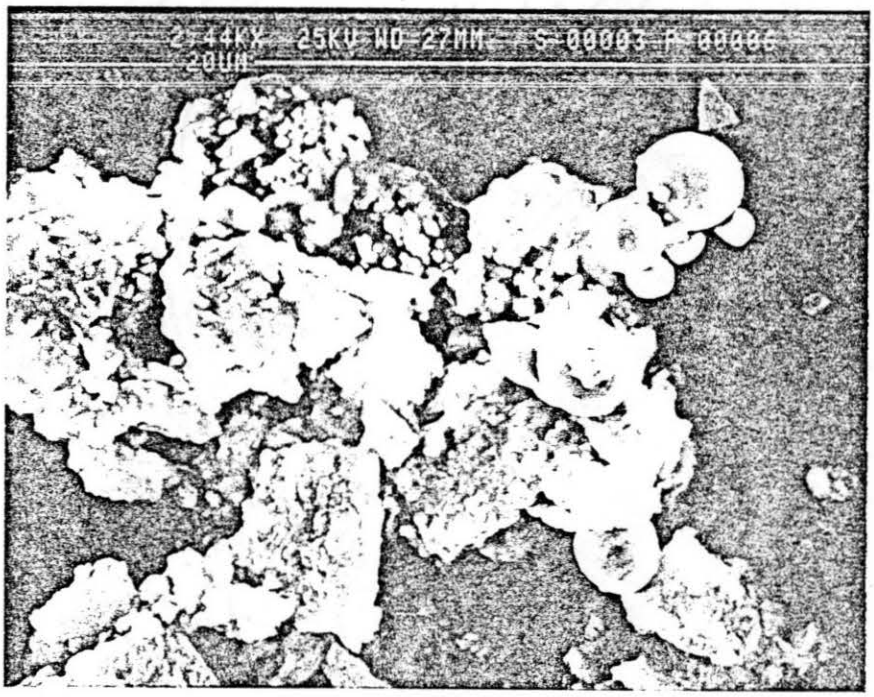


Figure 29. Scanning Electron Micrograph of Aerosols Formed after 15 min of Irradiation

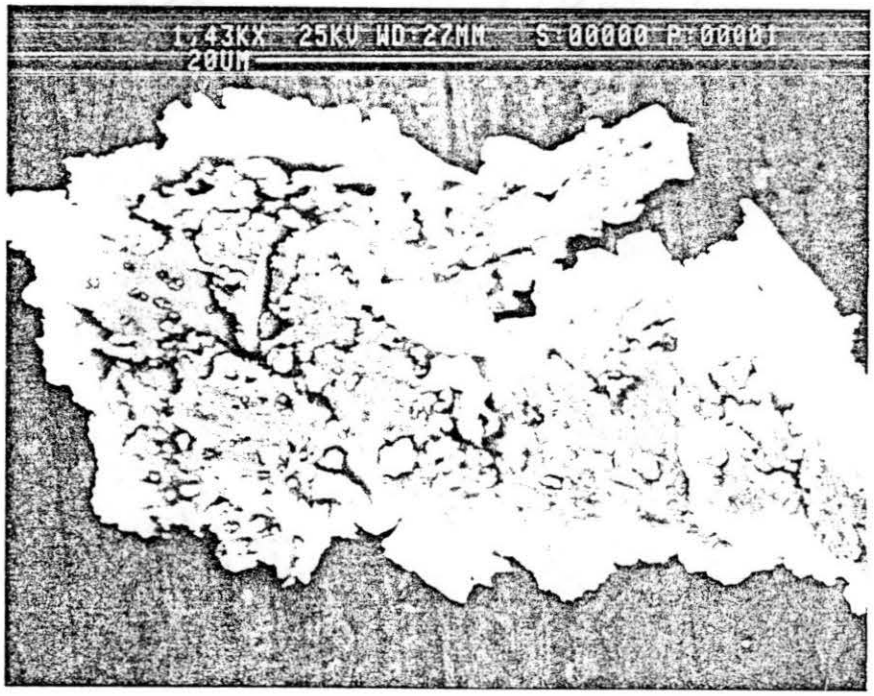


Figure 30. Scanning Electron Micrograph of Aerosols Formed after 30 min of Irradiation

The Total Mie Scattering Coefficient

In the light extinction spectrometer, a suspension of aerosol particles removes light from the illuminating laser beam by scattering or absorption. Light extinction can be represented by the Beer-Lambert law:

$$I/I_o = \exp(-naEl) \tag{3}$$

I/I_o: is the light transmittance,

l: is the length of the reaction vessel,

n: is the number of particles per unit volume,

a: is the projected area of a particle against the light beam,

E: is the particle extinction efficiency (The Total Mie Scattering coefficient).

The transmittance is obtained from the ratio of the light intensity measurement after aerosols are formed (I), to the light intensity before irradiation (I_o), when no aerosols are present.

If E_{scat}, the scattering efficiency, is defined as the light scattered by a particle divided by the light intercepted by the particle, and E_{abs}, the absorption efficiency, defined as the fraction of the incident beam absorbed per unit cross-sectional area of the particle, then the total scattering efficiency is given by,

$$E = E_{scat} + E_{abs} \tag{4}$$

When the particle size is much less than the wavelength of the incident light, Rayleigh scattering takes place and the scattering and absorption

efficiencies are governed by the Rayleigh theory (49). In this work, the particle size after 5 mins of UV irradiation has been shown to be around 0.560 μm (from SEM measurements), which is of the same order of magnitude as the wavelength of the laser beam, 0.6328 μm and the Rayleigh theory is inapplicable.

The particle size is normally represented by its size parameter,

$$x = 2\pi r/\lambda \tag{5}$$

r is the particle radius and λ is the wavelength of the incident light. Thus the Rayleigh theory holds for $x << 1$, but for x~1, E has to be calculated by the Mie theory (67). The latter involves the exact solution of the Maxwell equations for scattered electromagnetic radiation using spherical Bessel functions and associated Legendre polynomials. However, Penndorf (68) has proposed an approximation method for obtaining E from the Mie Theory.

The normalized size parameter, p, is defined as:

$$p = 2x(m-1) \tag{6}$$

which is the phase retardation of a diametric ray passing through a spherical particle (m is the refractive index of the particle). A plot of the total Mie scattering coefficient against p passes through various maxima and minima. The maxima correspond to the reinforcement of transmitted and diffracted light and the minima due to their interference. For particles with $1 \leqslant m \leqslant 2$, Van de Hulst (69) has shown that the maxima and minima occur at the same p values and are

independent of the refractive indices. A satisfactory approximation to the positions of maxima and minima for particles with m approximately equal to one will be:

$$p_y\{m\} = p_y\{m-1\} + 0.3(m-1) \tag{7}$$

The subscript y, refers to the order of the maxima or minima. Values for $p_y\{m-1\}$ given by Penndorf are shown in Table VII, for y = 1 - 10. The relationship between E and the maxima and minima is:

$$E\{m-1\} = 2 - 4(\sin p)/p + 4(1-\cos p)/p^2 \tag{8}$$

hence for the maxima,

$$E'_y = 2 + 4/p'_y + 4/p'^2_y + 29M/p'_y - 51M/p'^2_y \tag{9}$$

and for the minima,

$$E''_y = 2 - 4/p''_y + 4/p''^2_y + 8.01M/p''_y - 27.3M/p''^2_y \tag{10}$$

M is given by the Lorentz - Lorentz equation,

$$M = (m^2 - 1)/(m^2 + 2) \tag{11}$$

m = 1.5478 for bibenzyl (51).

The points between the maxima and the minima can be interpolated graphically, and p_y values can be scaled to the size parameter x using

TABLE VII

POSITIONS OF MAXIMA AND MINIMA OF THE TOTAL MIE SCATTERING COEFFICIENT (REFRACTIVE INDEX-1)

Position (y)	Maxima (p_y')	Minima (p_y'')
1	4.0856	7.6231
2	10.7923	14.0041
3	17.1551	20.3266
4	23.4730	26.6312
5	29.7756	32.9270
6	36.0713	39.2202
7	42.3632	45.5101
8	48.6527	51.7984
9	54.9408	58.0856
10	61.2278	64.3720

(y is the order of the extrema)

equation 6. In Figure 31 a plot is given of the total Mie scattering coefficient E, as a function of the size parameter for bibenzyl particles, calculated by the above approximation method. Assuming the particles were of the same size after 5 mins of irradiation, the size parameter for bibenzyl aerosols in a laser beam of wavelength λ = 632.8 nm, calculated from equation 5 is 2.78. This corresponds to an E value of 3.70 $\pm$ 3%, which means a bibenzyl particle removes from the light beam, about four times the amount of light intercepted by its geometrical cross-sectional area.

Rates of Aerosol Formation

Transmittance of the laser beam as a function of the time of UV light irradiation of toluene vapor (10 mm Hg), is shown in Figure 32. The transmittance decreases with time as a result of the formation of aerosols which attenuate the light intensity by scattering. The He-Ne laser, equipped with fixed internal mirrors, produces an elliptically polarized light beam, consequently the light intensity tended to vary sinoisudally with time. Only maximum intensity readings of the pen recorder were used and this restricted the number of readings to four or five during 5 mins of irradiation.

The initial rate of aerosol formation (calculated from the absolute value of the change in transmittance per unit time) for different pressures of toluene vapor, each exposed to UV radiation for 5 mins, is depicted in Figure 33. A linear correlation was made between these rates and the rates of bibenzyl formation (obtained previously) for different substrate pressures. The correlation factor of 0.9857 and an error parameter of 0.07 obtained, confirms that light extinction was

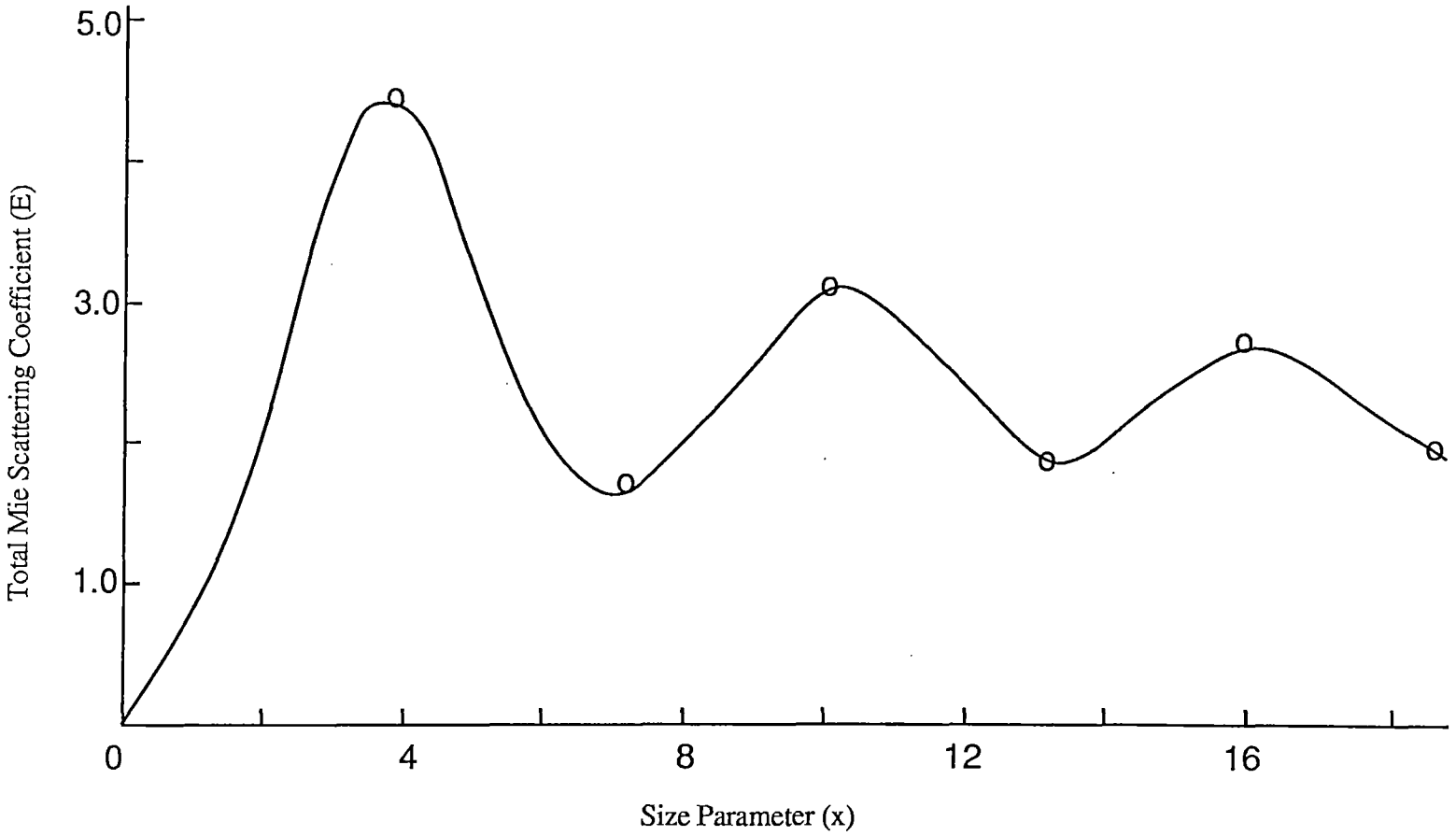


Figure 31. Calculated Total Mie Scattering Coefficients of Bibenzyl Aerosols

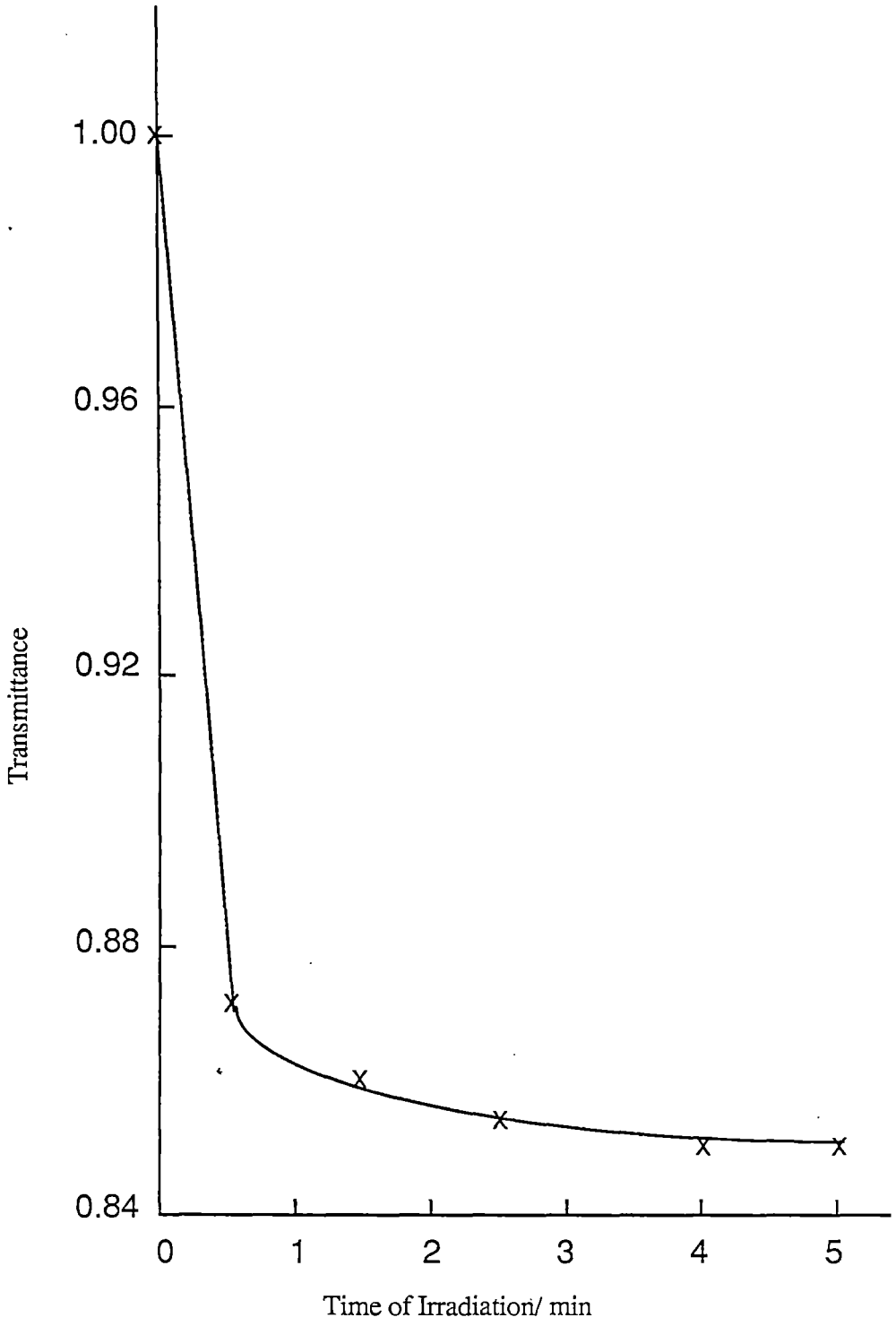


Figure 32. Effect of Aerosol Formation on Transmittance (10 mm Hg Toluene Vapor)

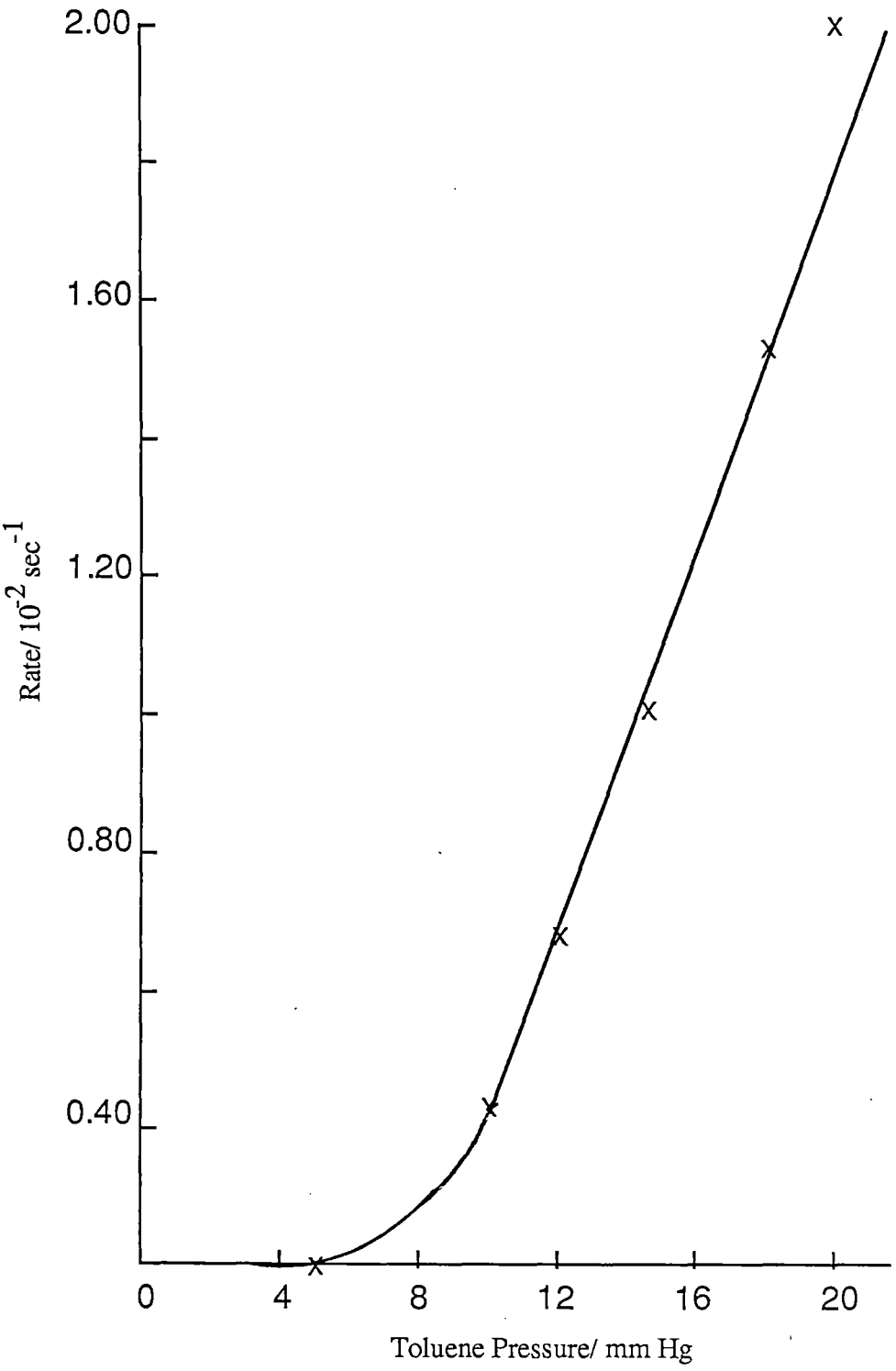


Figure 33. Effect of Toluene Pressure on the Rate of Aerosol Formation

mainly by the the bibenzyl particles. The linear regression line is shown in Figure 34.

Particle Size Distribution

It is possible to determine the particle radius size distribution by combining transmittance measurements with the differential settling of the aerosol particles. This method, first used by Gumprecht and Sliepcevich (70), does not require an a priori assumption of the form of the distribution function.

In photochemical production of aerosols, the particles are uniformly distributed in the reaction vessel. For such a system, the transmittance T, is related to the distribution function p(r) by,

$$-\ln T = \pi l \int E r^2 p(r) dr \qquad (12)$$

where r is the particle radius and the other parameters have their usual meaning (71). As the particles settle, there will be a decrease in scattering and hence an increase in transmittance. The particular radius corresponding to each time can be calculated from Stokes law:

$$r = \left[\frac{9h\eta}{2g(\rho - \rho_m)t} \right]^{1/2} = \frac{k}{t^{1/2}} \qquad (13)$$

h: the distance a particle falls through the light beam, was taken to be 1 cm, the radius of the light beam.

η: is the viscosity of the medium, the low pressure viscosity of toluene vapor is 698 μP (72).

$(\rho - \rho_m)$: is the difference in density between the dispersed

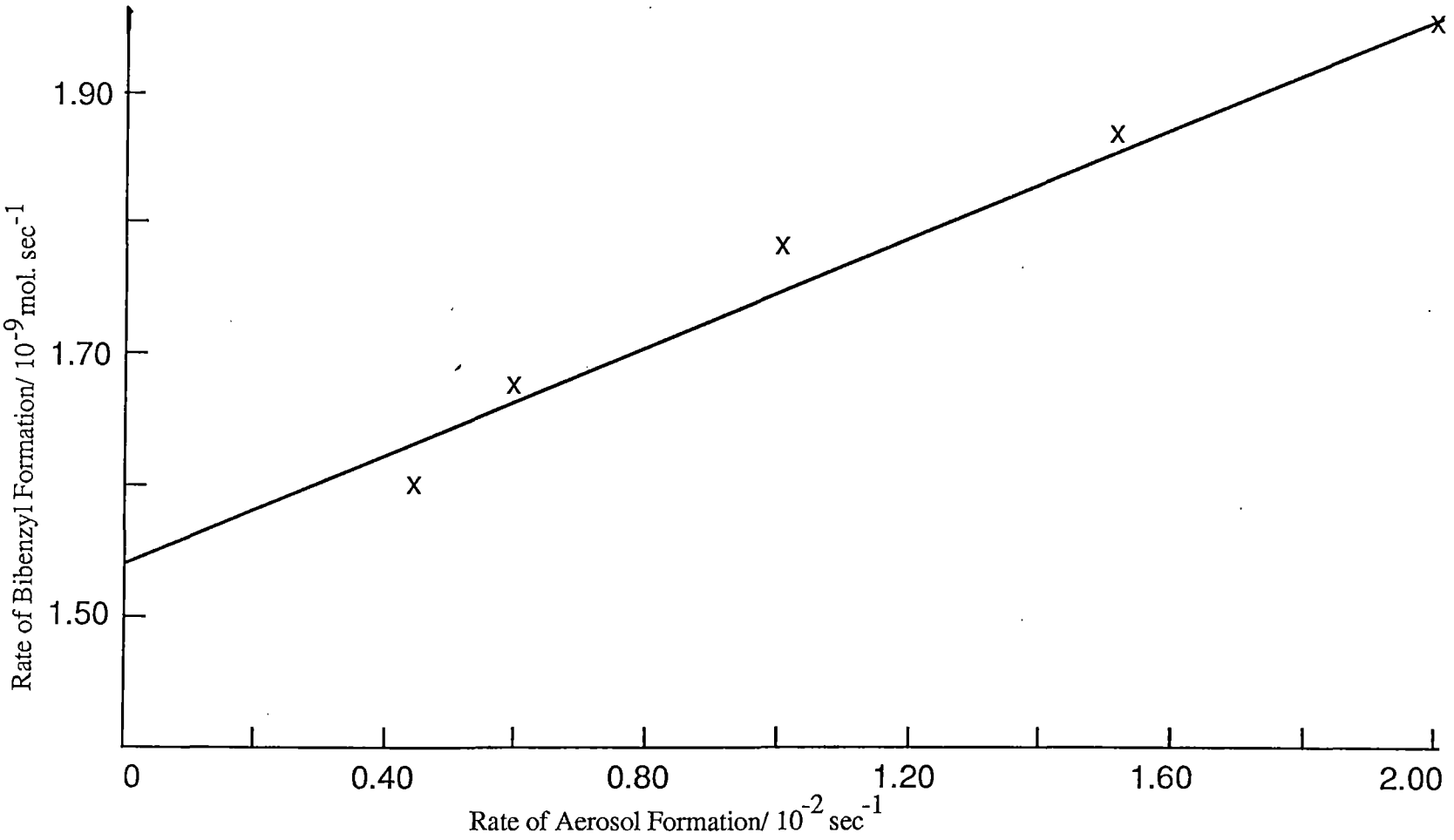


Figure 34. Linear Correlation between the Rates of Bibenzyl Formation and Aerosol Formation

bibenzyl particles and the toluene vapor. However, since the latter is negligible compared to the former, the value used was the density of bibenzyl, 0.9583 $g.cm^{-3}$ (51).

g: is the acceleration due to gravity, 980 $g.cm^{-1}.sec^{-2}$.

t: is the time.

k: is a constant.

The rate of change of transmittance due to settling is,

$$-d(\ln T)/dt = \pi l E r^2 p(r) dr/dt \qquad (14)$$

where p(r)dr is the number of particles per unit volume, in the size range between r and r + dr, which drop out of the light beam during the time interval t + dt (71).

If r in equation 14 is replaced by equation 13 and d(lnT)/dt is taken as the slope of the logarithmic transmittance curve at time t, then,

$$p(r) = \frac{2t^{5/2}}{\pi l k^3 E} \frac{d(\ln T)}{dt} \qquad (15)$$

giving an expression for the number of particles of each particular size.

The transmittance as function of settling time of aerosols formed after 5 mins of irradiation of 10 mm Hg toluene vapor is shown in Figure 35. There is an increase in transmittance resulting from the removal of particles from the path of the light beam as they are deposited under gravity. In Figure 36, the graph for the corresponding radius size distribution is depicted. On the same graph is shown the size

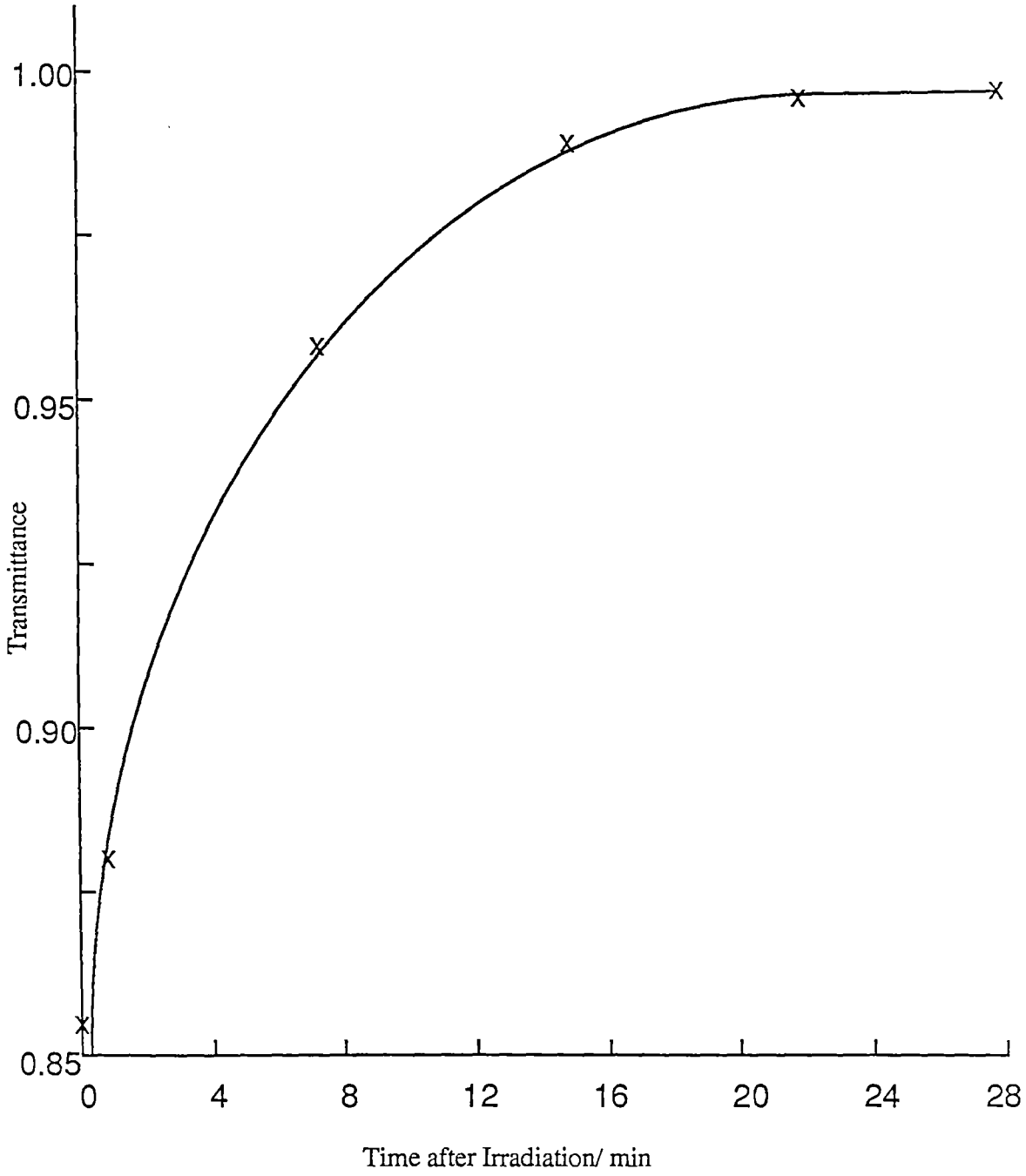


Figure 35. Effect of Aerosol Deposition on Transmittance (10 mm Hg Toluene Vapor)

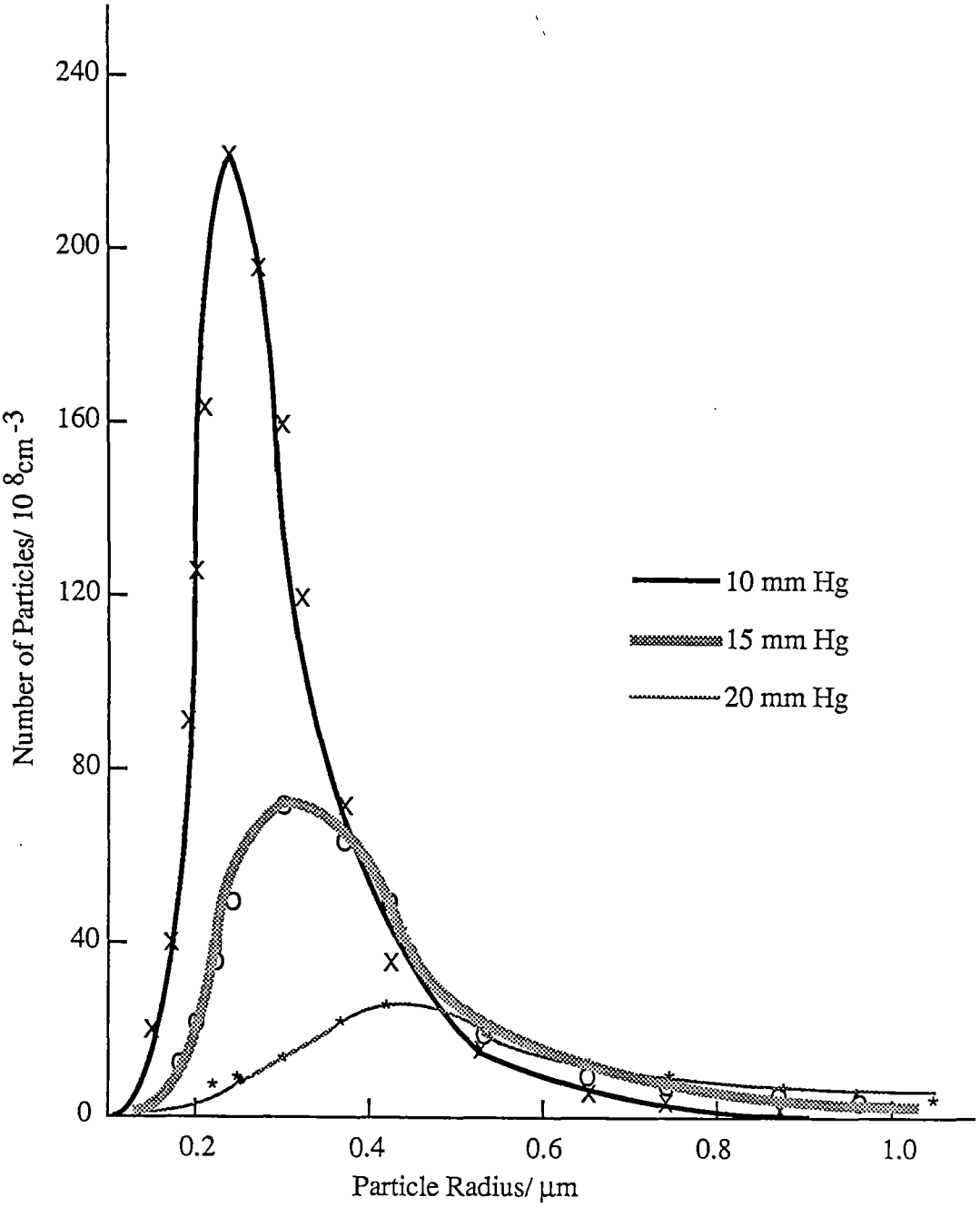


Figure 36. Particle Size Distribution at Different Substrate Pressures

distributions for aerosols produced from 15 and 20 mm Hg of toluene vapor.

The maximum radius size distribution for 10 mm Hg of toluene vapor occurs at a radius of 0.236 μm which is comparable to the value obtained from SEM measurements, 0.280 μm. The latter is actually the settled projected-area radius, and for quartz particles, has been reported to be as much as 30% larger than the mean radius of randomly oriented particles (73). At higher substrate pressures, the size corresponding to the maximum distribution shifts to larger radii (Table VIII) and a broader size distribution is obtained. Qualitatively, this trend could be attributed to the the fact that at higher pressures, the aerosol particles are closer to each other and the chance of their coalescing to form larger particles is enhanced.

The main draw back to this method of particle size analysis is that, with small particles in the μm range, Brownian motion could be significant, and the equations do not take into account the possibility of this phenomenon occurring.

TABLE VIII

PARTICLE RADII WITH MAXIMUM SIZE DISTRIBUTION
AT DIFFERENT SUBSTRATE PRESSURES

Substrate Pressure (/ mm Hg)	Maximum Distribution (/ 10^8 cm^{-3})	Corresponding Radius (/ μm)
10	223.0	0.236
15	72.0	0.300
20	23.0	0.430

CHAPTER V

AB INITIO QUANTUM MECHANICAL CALCULATIONS

Ground State Toluene

Toluene with benzene and other derivatives of benzene have been the subject of many quantum mechanical calculations. Earlier semi-empirical SCF-MO work on toluene include MINDO/3 calculations by Bingham et al. (74) and CNDO/2 calculations by Pople and Gordon (75). These took into consideration both π-electrons and σ-electrons contributions to charge distribution and electronic dipole moments, as against much earlier calculations which considered only π-electron interactions (76).

Ab initio molecular orbital calculations performed by Hehre et al. (77) with a STO-3G minimal basis set produced a toluene energy of -266.47382 a.u. Using a large contracted basis set (11s 7p 1d/7s 1p)/ [5s 3p 1d/3s 3p], Ermler and Mulliken (78) obtained a lower value of -269.8245 a.u. The optimized geometry of toluene was determined by Pang et al. (79) using a 4-21G basis set and also by Bock et al. (80) with a 6-21G basis set. The former found the methyl C-H bonds to be on the average 0.011 $\mathring{A}$ longer than the ring C-H bonds and the bond lengths identical to those of benzene.

In this work an almost full geometrical optimization was performed on the toluene molecule with the standard 3-21G split valence basis set (81) (82). Calculations were carried out on a VAX11/780 computer using the GAUSSIAN82 program (83). The restricted Hartree-Fock energy

calculated for the ground state singlet toluene molecule was -268.24022 a.u., assuming a C_s symmetry.

The optimized geometrical coordinates given in Table IX, place one methyl hydrogen in the plane of the ring and the other two symmetrically above and below the plane. Maximum forces in the distance and angle coordinates in the final optimization were less than 1.80×10^{-4} hartrees/bohr and 2.50×10^{-4} hartrees/radian respectively. Eigenvalues and molecular orbital coefficients for the 79 basis functions used are listed in Appendix A.

In Figure 37 is shown the electron population at the atomic sites and between adjacent atoms in the molecule. The atoms are numbered in a manner consistent with the computer output and the electron populations were obtained by Mulliken population analysis (84). Of primary importance is the π-electron distribution in the ring (Figure 38): the ortho and para positions have greater π-electron populations, which is consistent with experimentally known ortho and para directing properties of the methyl group during electrophilic substitution reactions. However, the inductive effect from the methyl is small and is depicted by an increase of only 0.0070 in the total π-electron charge of the ring. The total atomic charge distribution (Figure 39), also gives higher charge distributions at the ortho and para carbons, being the result of ring polarization by the methyl group. The net charge contribution from the methyl to the ring ($\sigma + \pi$) is 0.0658, the resulting dipole moment calculated was 0.3289 D which is close to the experimental value of 0.360 D (85). The above results are compared with those of other workers in Table X.

TABLE IX

STANDARD ORIENTATION FOR GROUND STATE TOLUENE

Center #	Atom	Coordinates (/Angstroms) X	Y	Z
1	C	0.000000	0.899550	0.000000
2	C	-0.012685	-1.889530	0.000000
3	C	-1.195303	0.198288	0.000000
4	C	-1.203244	-1.187642	0.000000
5	C	1.192294	0.184964	0.000000
6	C	1.187654	-1.196913	0.000000
7	C	0.022191	2.416844	0.000000
8	H	-0.016959	-2.961619	0.000000
9	H	-2.137402	-1.714064	0.000000
10	H	-2.124343	0.735332	0.000000
11	H	2.116055	-1.733296	0.000000
12	H	2.125872	0.715430	0.000000
13	H	-0.982543	2.820968	0.000000
14	H	0.536938	2.791939	0.878307
15	H	0.536938	2.791939	-0.878307

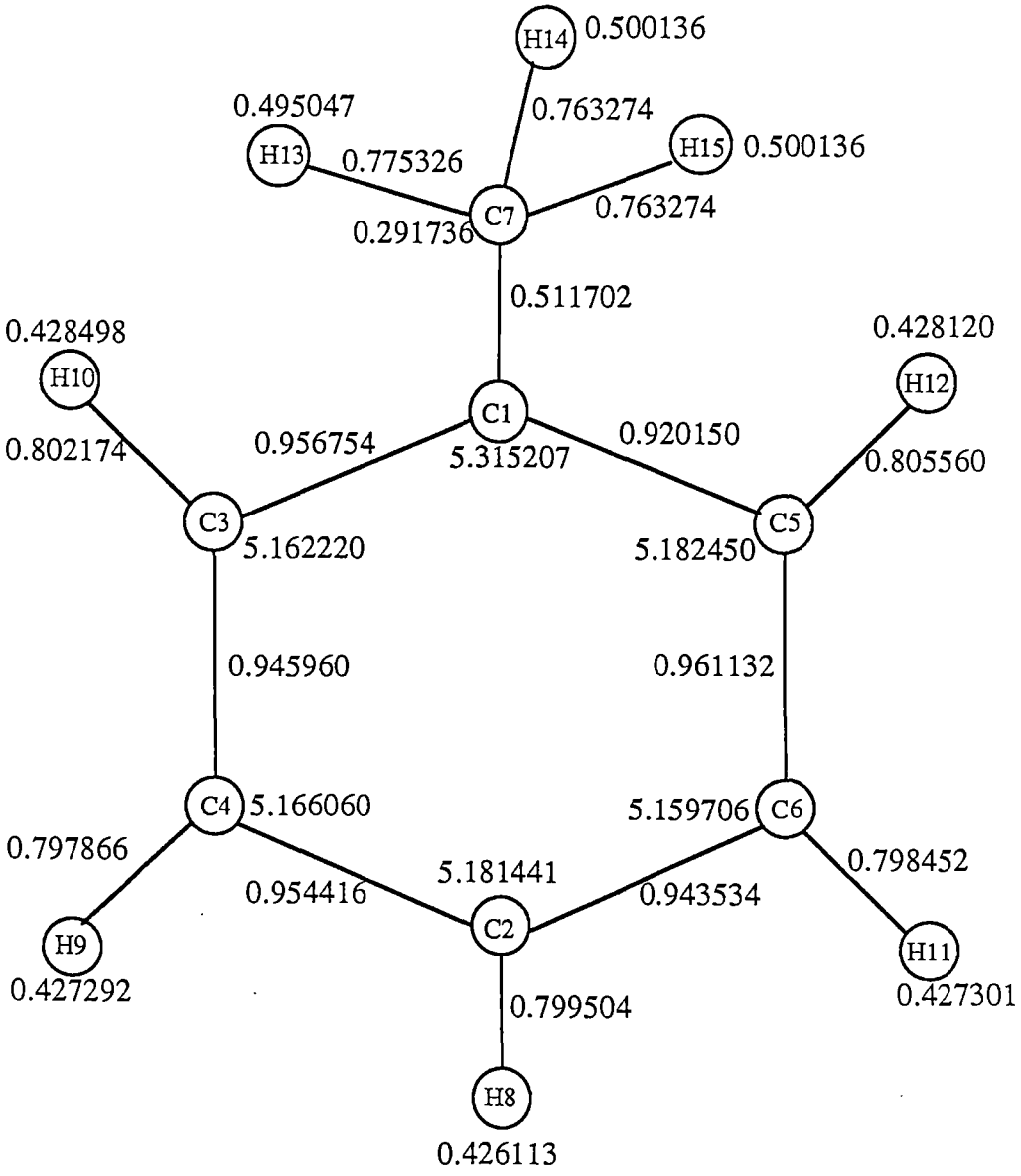


Figure 37. Total Electron Population of Ground State Toluene

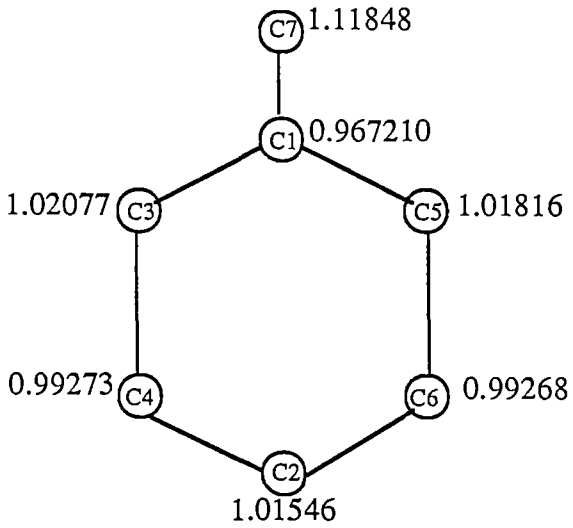


Figure 38. Π-Electron Distribution in Ground State Toluene

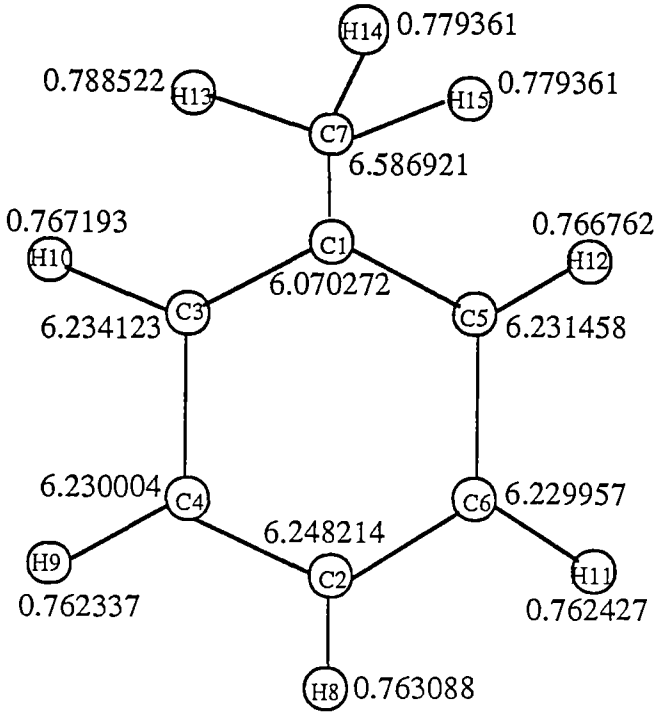


Figure 39. Total Charge Distribution in Ground State Toluene

TABLE X

COMPARISON OF CALCULATED GROUND STATE TOLUENE PARAMETERS WITH OTHER RESULTS

Method	Ref.	Energy (/a.u.)	π-e*	($\sigma + \pi$)-e*	IP (/eV)	Dipole Moment(/D)
STO-3G	77	-266.47382	0.008	0.015	-	0.25
6-31G	80	-	0.008	0.036	-	-
4-21G	86	-269.3528	-	-	8.68	-
Large basis	78	-269.82450	0.018	-0.102	8.87	0.33
3-21G	**	-268.24022	0.008	0.066	8.88	0.33
Expt.	85	-	-	-	-	0.36
"	86	-	-	-	8.83	-

* Electron contribution from methyl group to ring
** From this work
IP: First Ionization Potential

Triplet State Toluene

A 3-21G ab initio calculation on the electronically excited triplet toluene molecule gave an unrestricted Hartree-Fock energy of -268.13720 a.u., which is 2.803 eV above the ground state, the experimentally determined value is 3.59 eV (32). The theoretical value would be expected to be less in magnitude since unrestricted Hartree-Fock energies tend to be more negative than the corresponding restricted Hartree-Fock energies (87). Yet, there is no doubt that the 4.86 eV transferred by collision with $(^3P_1)Hg$ is enough to convert a ground state toluene molecule to its triplet state. The excess energy results in the formation of a vibrationally excited molecule in the triplet state.

Molecular orbital coefficients and eigenvalues are listed in Appendix B separately for α and β-electron contributions to triplet toluene. Table XI lists the optimized geometrical coordinates of $^3A_1$ toluene and the bond lengths and angles are compared with ground state toluene in Table XII obtained from this work and from 6-31G calculation of Bock et al. (80). There is a considerable amount of agreement in values obtained from the two types of basis sets used for the ground state molecule, the 6-31G bond lengths and angles have been shown to be close to experimental values obtained from microwave spectroscopy (88). In triplet toluene, the methyl shows a greater distortion to the right of the ring: angle <C7C1C3 is 124.1° in the $^3A_1$ state and 121.2° in the $^1A_1$ state. The ring itself is distorted and bonds C1-C5 and C2-C4 in $^3A_1$ toluene are greater than their $^1A_1$ counterparts by 0.144 and 0.149 Å respectively. However, the rest of the bond lengths and angles remain almost the same for both states, differing by only $\pm$ 0.05 Å or $\pm$ 0.5°.

TABLE XI

STANDARD ORIENTATION FOR TRIPLET STATE TOLUENE

Center #	Atom	Coordinates (/Angstroms) X	Y	Z
1	C	0.000000	0.993960	0.000000
2	C	-0.067108	-1.942798	0.000000
3	C	-1.224257	0.293593	0.000000
4	C	-1.343342	-1.092711	0.000000
5	C	1.264933	0.085491	0.000000
6	C	1.158270	-1.296543	0.000000
7	C	0.155880	2.435763	0.000000
8	H	-0.136532	-3.013453	0.000000
9	H	-2.301876	-1.580505	0.000000
10	H	-2.119889	0.885365	0.000000
11	H	2.056181	-1.882632	0.000000
12	H	2.219892	0.571963	0.000000
13	H	0.808098	2.928937	0.000000
14	H	0.712035	2.764883	0.876123
15	H	0.712035	2.764883	-0.876123

TABLE XII

COMPARISON OF OPTIMIZED GEOMETRIES FOR GROUND AND TRIPLET STATE TOLUENE MOLECULES FROM 3-21G AND 6-31G CALCULATIONS

Bond /Angle	Ground State 6-31G	Ground State 3-21G	Triplet State 3-21G
Bond lengths(/Å):			
C1-C3	1.3907	1.3858	1.3869
C1-C5	1.3943	1.3900	1.5343
C1-C7	1.5105	1.5175	1.5016
C2-C4	1.3856	1.3821	1.5306
C2-C6	1.3890	1.3858	1.3849
C3-C4	1.3892	1.3860	1.3875
C5-C6	1.3856	1.3819	1.3886
C2-H8	1.0771	1.0721	1.0704
C3-H10	1.0782	1.0731	1.0747
C4-H9	1.0776	1,0723	1.0708
C5-H12	1.0788	1.0738	1.0719
C6-H11	1.0776	1.0722	1.0737
C7-H13	1.0827	1.0830	1.0832
C7-H14	1.0850	1.0849	1.0884
C7-H15	1.0850	1.0849	1.0884
Bond angles(/°):			
<C1C3C4	120.92	120.73	121.95
<C2C6C5	120.19	120.18	121.31
<C3C4C2	120.18	120.19	119.26
<C4C2C6	119.45	119.49	119.24
<C5C1C3	118.35	118.66	118.49
<C5C1C7	120.44	120.10	117.38
<C6C5C1	120.91	120.74	119.76
<C7C1C3	121.21	121.24	124.14
<C1C3H10	119.52	119.57	118.89
<C1C5H12	120.01	119.46	118.37
<C2C4H9	120.08	120.08	118.91
<C2C6H11	120.01	120.00	119.34
<C4C2H8	120.31	120.29	118.92
<H13C7C1	111.21	111.07	111.50
<H14C7C1	111.21	110.65	110.64
<H15C7C1	111.21	110.65	110.64
<H13C7H14	107.77	108.13	108.34
<H13C7H15	107.77	108.13	108.34
<H14C7H15	107.77	108.10	107.22

Distortion of the benzene molecule from its regular hexagonal geometry in the $^3B_{1u}$ state has been reported by de Groot and Van der Waals (89). The large difference between the bond lengths in the triplet and singlet states suggest that there might be some excess energy deposited in the vibrational energy of the ring. The effect of Ar on product yield further shows that even an inert gas can partially deactivate the source of benzyl radicals.

Mulliken population analysis (Fig. 40) shows a considerable decrease in the electron populations at the C1-C5 and C2-C4 bonds. Though Mulliken population analysis has its shortcomings, there is a possibility of ring rupture at those bonds resulting in the formation of the unidentified products with molecular structures between C_2 and C_{14}, as obtained in the gas chromatograms (Figs. 10 and 11). The total π-electron population in the ring (Fig. 41) is exactly 6.000 for triplet toluene, indicating little or no contribution from the π-electrons of the methyl group to the ring. Figure 42 depicts the total charge distribution in the molecule, the ortho and para carbons do not have higher charges. The net charge contribution to the ring is only 0.04248 and the dipole moment is 0.2295 D.

The Benzyl Radical

Ab initio molecular orbital calculation on the benzyl radical using the 3-21G standard basis set and almost full optimization, gave an unrestricted Hartree-Fock energy of -267.64118 a.u. It is thus possible to estimate a theoretical energy change for the reaction,

$$C_6H_5CH_3 \text{ -------> } C_6H_5CH_2\cdot + H\cdot \qquad \text{(XXVII)}$$

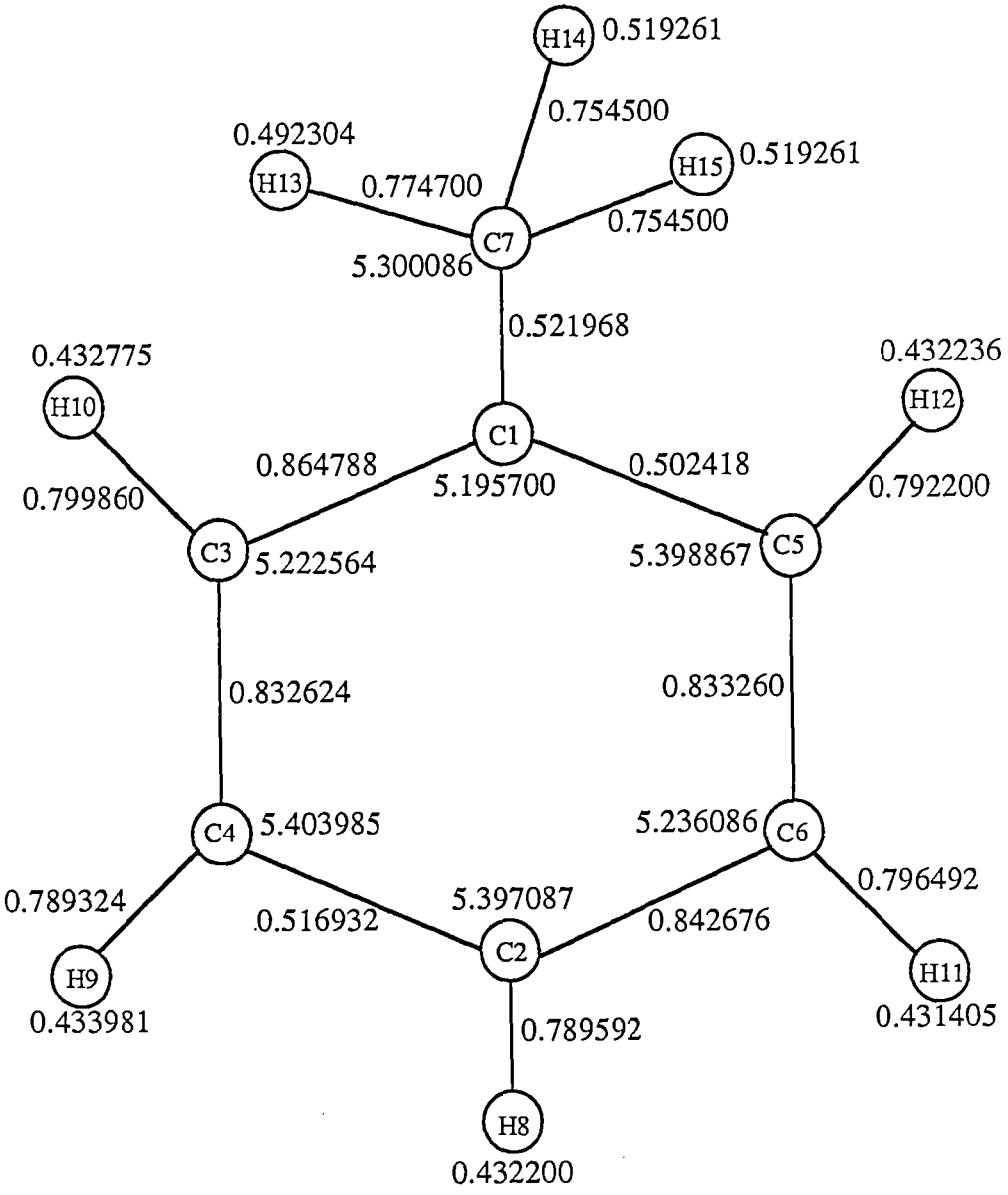


Figure 40. Total Electron Population of Triplet State Toluene

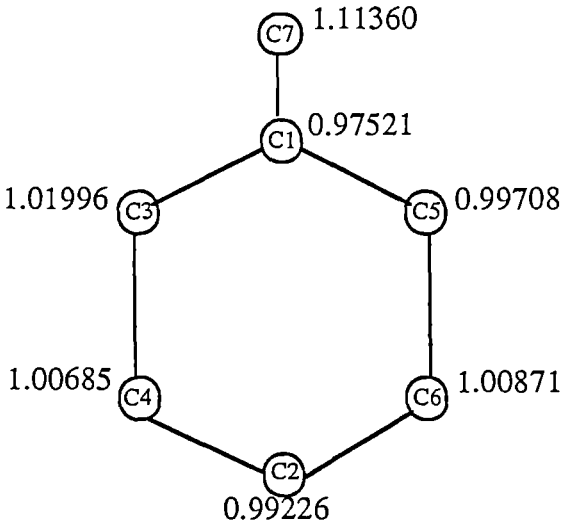


Figure 41. Π-Electron Distribution in Triplet State Toluene

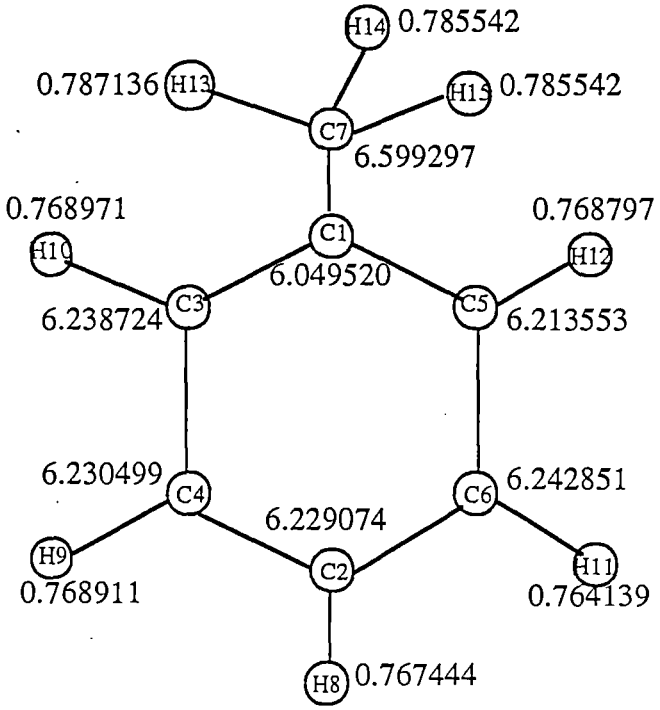


Figure 42. Total Charge Distribution in Triplet State Toluene

using 3-21G optimized energy of ground state toluene (from the previous section) and 3-21G energy of hydrogen atom, -0.49620 a.u. (90). It will be assumed that the heat of reaction is equal to the difference in energies for the reactant and products. This assumption is justifiable only if the kinetic (thermal plus zero point) energies of the species are additive functions of the atoms in them (91). The value obtained, 0.10284 a.u. or 64.533 Kcal/mol, is not greatly different from the experimental energy of 78 Kcal/mol (19). The difference can be attributed to the fact that the calculated energies were just HF energies which do not take into account correlation between the motions of electrons with opposite spins. Also, restricted Hartree-Fock and unrestricted Hartree-Fock energies are being compared.

The optimized geometrical coordinates of the benzyl radical are given in Table XIII and the bond angles and lengths in Table XIV. A planar molecule results and except for the C3-C4 and C5-C6 bond lengths which are comparable to their analogues in ground state toluene, the rest of the ring C-C bonds are longer by 0.04 Å, but the C1-C7 bond is less by 0.11 Å. The ring angles do not differ by more than 1° for both species. Molecular orbitals and corresponding eigenvalues for the α and β-electrons are listed in Appendix C.

Several valence bond and semi-empirical SCF-MO calculations have been done on the benzyl radical, some involving configuration interaction (92)-(94). Carrington and Smith (94) have compared the calculated π-electron spin densities ρ_i, with proton hyperfine coupling constants a_i, obtained from electron spin resonance spectroscopy. They accomplished this by calculating theoretical hyperfine constants a_i' from the ρ_i values, using the McConnell equation (95):

TABLE XIII

STANDARD ORIENTATION FOR THE BENZYL RADICAL

Center #	Atom	Coordinates (/Angstroms) X	Y	Z
1	C	0.000000	0.995389	0.000000
2	C	0.000580	-1.839805	0.000000
3	C	1.219717	0.254551	0.000000
4	C	1.212738	-1.134473	0.000000
5	C	-1.219573	0.254510	0.000000
6	C	-1.212523	-1.134461	0.000000
7	C	-0.000336	2.399269	0.000000
8	H	0.000026	-2.911645	0.000000
9	H	2.141035	-1.671196	0.000000
10	H	2.150273	0.788559	0.000000
11	H	-2.140724	-1.671191	0.000000
12	H	-2.150301	0.788269	0.000000
13	H	0.918167	2.953810	0.000000
14	H	-0.918963	2.953514	0.000000

TABLE XIV

3-21G OPTIMIZED GEOMETRY FOR THE BENZYL RADICAL

Bond	Distance(/Å)	Bond angle	Angle(/°)
C1-C3	1.4271	<C1C3C4	120.99
C1-C5	1.4270	<C2C6C5	120.48
C1-C7	1.4039	<C3C4C2	120.47
C2-C4	1.4029	<C4C2C6	119.63
C2-C6	1.4028	<C5C1C3	117.45
C3-C4	1.3890	<C5C1C7	121.26
C5-C6	1.3890	<C6C5C1	120.99
C2-H8	1.0718	<C7C1C3	121.29
C3-H10	1.0729	<C1C3H10	118.86
C4-H9	1.0723	<C1C5H12	118.89
C5-H12	1.0729	<C2C4H9	119.78
C6-H11	1.0722	<C2C6H11	119.78
C7-H13	1.0729	<C4C2H8	120.19
C7-H14	1.0726	<H13C7C1	121.11
		<H14C7C1	121.13
		<H13C7H14	119.73

$$a_i' = \rho_i Q \qquad (16)$$

Q is a constant chosen to be in the range of 22.5 - 30.0 gauss.

Π-electron spin densities calculated in this work and from others are given in Table XV. Aside from the 3-21G spin densities, the rest show the C7 atom to have a relatively high spin density. Though this is in line with the magnitudes of experimental coupling constants, one would expect that delocalization of the odd electron in the benzyl radical will lead a more even distribution of spin densities as obtained by 3-21G calculations, further, the planar configuration of the molecule allows an even greater interaction between the p_z orbital of methylene and the π-system of the ring. From Table XV, it can be seen that the C4 (meta) and C1 positions have negative spin densities since they do not contribute to resonance in the radical. Experimental results indicate that there should be a larger proton hyperfine splitting constant from the para position (C2) than from the ortho position (C3), due to possible interactions from protons on adjacent carbons (94). Most of the results on the table do not predict this trend of affairs.

Electron distribution in the radical is shown in Figure 43. The π-electron contribution to the ring is 0.00592 (Fig. 44), and the total charge contribution is 0.06974. These values are greater than those from toluene and can be attributed to enhanced resonance effects in the benzyl radical. The charge distribution is shown in Figure 45, and it gives a dipole moment of 0.0223 D along the y-axis.

TABLE XV

CALCULATED SPIN DENSITIES FOR THE BENZYL RADICAL

Method	Ref.	Spin Density at Carbon #: 1	2	3	4	7
Valence bond	91	-0.323	0.370	0.407	-0.256	0.651
HMO with C.I.	91	-0.076	0.089	0.149	-0.048	0.785
SCF-MO, no C.I.	89	0.000	0.052	0.088	0.000	0.772
SCF-MO with C.I.	91	-0.067	0.095	0.131	-0.032	0.774
SCF-MO, UHF with C.I.	90	-0.103	0.208	0.200	-0.089	0.673
3-21G, UHF	*	-0.482	0.559	0.566	-0.506	0.804

HMO: Huckel Molecular orbitals
SCF-MO: self-consistent field molecular orbitals
C.I.: configuration interaction
UHF: unrestricted Hartree-Fock
*: this work

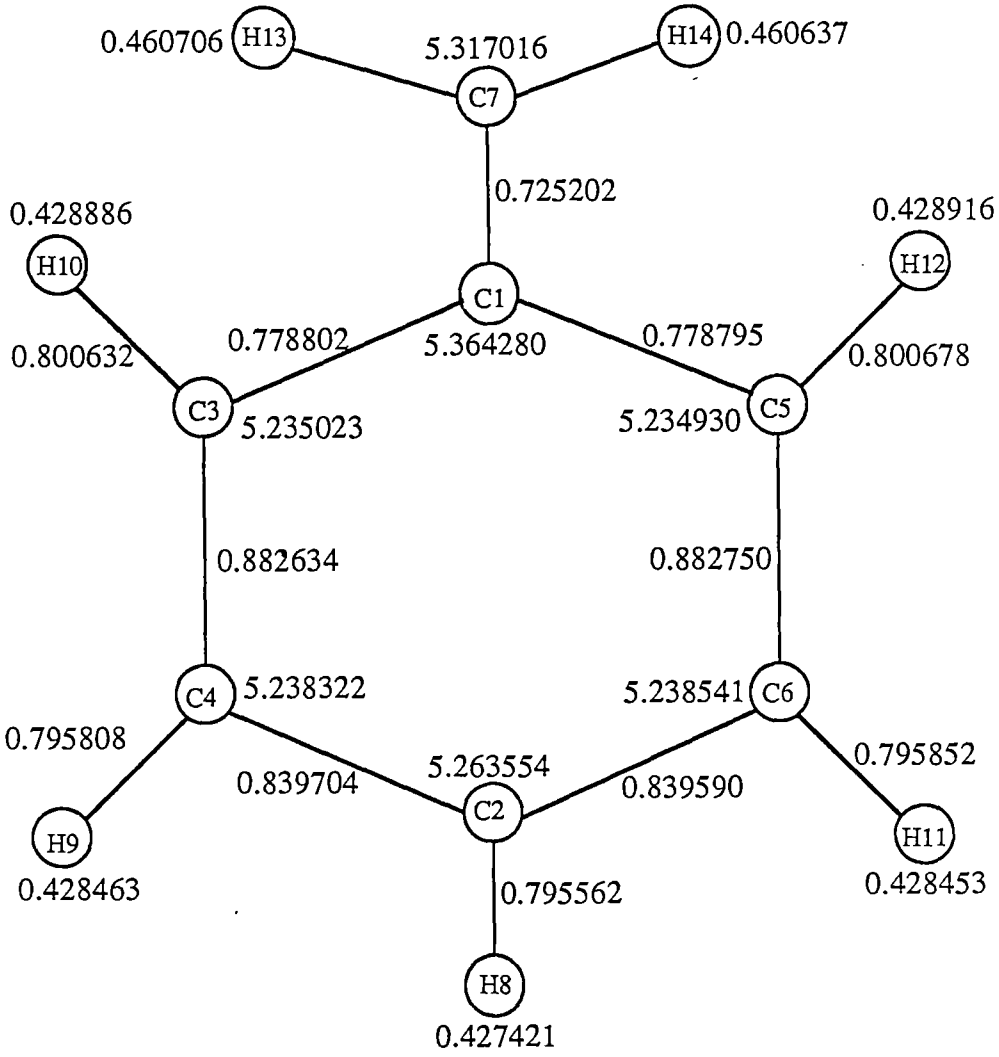


Figure 43. Total Electron Population of the Benzyl Radical

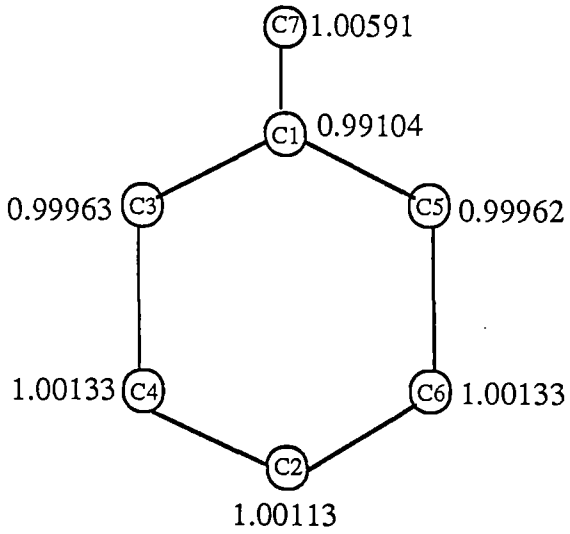


Figure 44. Π-Electron Distribution in the Benzyl Radical

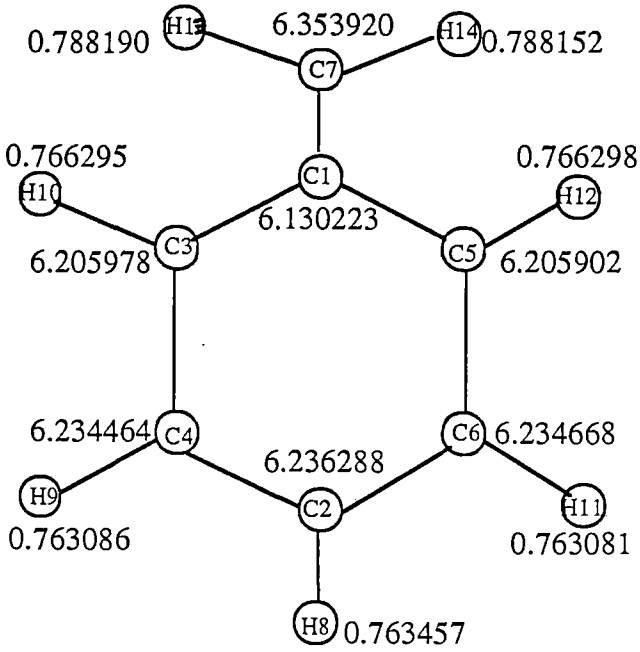


Figure 45. Total Charge Distribution in the Benzyl Radical

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

It has been possible to separate and analyze most of the products from the triplet Hg photosensitized decomposition of toluene vapor at 25 ^{o}C, despite their low quantum yields. No doubt bibenzyl was the major product and has been characterized completely.

The mechanism of photosensitization can be considered as one involving energy transfer from triplet excited Hg to a low lying triplet state of toluene, 3.59 eV above the ground state. There is a very efficient transfer of electronic energy, σ^2 is about 60 $\mathring{A}^2$ and primary reactions will originate from the vibrationally excited triplet formed. Unlike benzene, there is no evidence that the "hot" toluene molecule isomerizes (96). It dissociates to a small extent to form a benzyl radical and a hydrogen atom or even to a smaller extent to form phenyl and methyl radicals. The total quantum yield of product formation is less than 0.013, thus the major processes occurring after excitation could be either radiative transition to the ground state (phosphorescence), or a radiationless transition (intersystem crossing). The former not being an important process in the vapor phase, leaves intersystem crossing from the $^3A_1$ state to higher vibrational levels in the $^1A_1$ state with release of thermal energy, as the major route for electronic energy degradation.

The aerosols formed were bibenzyl particles and a good correlation

was obtained between the rates of aerosol and bibenzyl formation at different substrate pressures. Differential settling method for determining particle size distribution, gave particle radii consistent with scanning electron microscope results. Light extinction measurement is not the most versatile technique for determining particle properties, recent advances in the quasi-elastic light scattering technique should be mentioned. This involves the measurements of time-averaged intensities of light scattered by particle dispersions (97). The light intensities measured in the μsec range using photon correlation spectroscopy, or the heterodyne technique, provide information on particle size distribution and particle dynamics. Most of these measurements have been made on colloidal systems and few on aerosols (98). The reason being that aerosols have been found to perturb light intensities appreciably, only over long path lengths (49). Yet in this work, it has been shown that when toluene vapor is irradiated with UV light in the presence of Hg, it produces aerosols which are capable of attenuating a laser light beam by as much as 30% over a sample length of 30 cm. Also, the production of aerosols by UV light is unique, in that, a uniform distribution of particles is achieved almost instantaneously.

The 3-21G basis set is presently being used as a starting point for more detailed ab initio calculations involving polarization basis sets like the 3-21G*, 6-31G* and the 6-31G** (87). It is used to optimize the geometry of molecules before SCF calculations are done with the polarization sets. Nevertheless, results from this work show that the 3-21G split-valence basis set reasonably predicted experimental properties of the molecules studied.

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APPENDIX A:

MOLECULAR ORBITALS AND EIGENVALUES FOR THE GROUND STATE TOLUENE MOLECULE

ORBITAL SYMMETRIES.

OCCUPIED (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
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VIRTUAL (A") (A") (A') (A') (A') (A") (A') (A') (A') (A')
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THE ELECTRONIC STATE IS 1-A'.

MOLECULAR ORBITAL COEFFICIENTS

					1 (A')	2 (A')	3 (A')	4 (A')	5 (A')
EIGENVALUES --					-11.18452	-11.17320	-11.17285	-11.16995	-11.16959
1	1	C	1S		0.98730	-0.00277	-0.00264	-0.00211	0.00779
2			2S	(I)	0.10055	-0.00099	-0.00121	-0.00039	-0.00182
3			2PX	(I)	-0.00013	0.00056	-0.00050	0.00011	0.00181
4			2PY	(I)	-0.00046	-0.00043	-0.00049	-0.00023	0.00110
5			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
6			2S	(O)	-0.09695	0.01773	0.02232	-0.00153	0.02248
7			2PX	(O)	0.00240	0.00222	-0.00131	-0.00106	-0.01858
8			2PY	(O)	0.01322	-0.01015	-0.01293	0.00337	-0.01713
9			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
10	2	C	1S		-0.00517	0.05552	0.07245	-0.96583	0.12042
11			2S	(I)	-0.00137	0.00962	0.01224	-0.09716	0.01206
12			2PX	(I)	-0.00002	0.00106	-0.00090	0.00005	0.00110
13			2PY	(I)	-0.00027	0.00114	0.00141	-0.00136	-0.00030
14			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
15			2S	(O)	0.01183	-0.04100	-0.05075	0.08560	-0.01852
16			2PX	(O)	-0.00026	-0.01146	0.00930	-0.00001	-0.00112
17			2PY	(O)	0.00696	-0.02194	-0.02703	0.02128	-0.00793
18			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
19	3	C	1S		-0.01244	0.01651	0.06439	0.16491	0.91936
20			2S	(I)	-0.00535	0.00226	0.01115	0.01671	0.09297
21			2PX	(I)	-0.00151	0.00028	0.00059	0.00029	0.00130
22			2PY	(I)	-0.00055	-0.00005	-0.00157	-0.00121	-0.00037
23			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
24			2S	(O)	0.03507	-0.01127	-0.04885	-0.00500	-0.08734
25			2PX	(O)	0.02043	-0.00677	-0.01712	0.00339	-0.02116
26			2PY	(O)	0.00391	0.00409	0.02107	-0.00046	0.00874
27			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
28	4	C	1S		-0.00344	0.09698	-0.97811	-0.05240	0.05783
29			2S	(I)	-0.00010	0.00920	-0.09962	-0.00174	0.00144
30			2PX	(I)	-0.00003	0.00098	-0.00124	0.00144	-0.00061
31			2PY	(I)	-0.00075	-0.00035	-0.00077	-0.00063	-0.00119
32			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
33			2S	(O)	-0.00972	0.00930	0.10181	-0.02515	0.03148
34			2PX	(O)	-0.00813	0.00727	0.02663	-0.01932	0.01316
35			2PY	(O)	-0.00176	0.00502	0.01487	0.00285	0.01632
36			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
37	5	C	1S		-0.01225	0.04938	0.02827	0.09517	-0.33363
38			2S	(I)	-0.00514	0.00951	0.00436	0.00965	-0.03385
39			2PX	(I)	0.00146	-0.00052	-0.00039	-0.00016	0.00128
40			2PY	(I)	-0.00059	-0.00160	-0.00034	-0.00118	0.00008
41			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
42			2S	(O)	0.03236	-0.04537	-0.02115	0.00105	0.01989
43			2PX	(O)	-0.01868	0.01542	0.01056	-0.00463	-0.00035
44			2PY	(O)	0.00279	0.01975	0.00779	-0.00071	0.00313
45			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
46	6	C	1S		-0.00393	-0.97965	-0.09065	-0.05170	0.01109
47			2S	(I)	-0.00021	-0.09960	-0.00993	-0.00148	0.00112
48			2PX	(I)	0.00008	0.00138	-0.00071	-0.00143	0.00032
49			2PY	(I)	-0.00073	-0.00071	-0.00047	-0.00052	0.00041

50			2PZ (I)	0.00000	0.00000	0.00000	0.00000	0.00000
51			2S (O)	-0.00960	0.09777	0.02877	-0.02668	0.00319
52			2PX (O)	0.00726	-0.02431	-0.01251	0.01975	-0.00451
53			2PY (O)	-0.00216	0.01392	0.00791	0.00159	-0.00219
54			2PZ (O)	0.00000	0.00000	0.00000	0.00000	0.00000
55	7	C	1S	-0.00423	0.00553	0.00577	-0.00019	-0.01148
56			2S (I)	-0.00180	0.00118	0.00121	0.00011	-0.00198
57			2PX (I)	0.00042	0.00023	-0.00007	0.00001	0.00026
58			2PY (I)	0.00037	-0.00028	-0.00034	0.00014	-0.00002
59			2PZ (I)	0.00000	0.00000	0.00000	0.00000	0.00000
60			2S (O)	0.01154	0.00035	0.00109	-0.00196	0.00760
61			2PX (O)	-0.00293	-0.00197	0.00069	0.00021	0.00227
62			2PY (O)	-0.00843	0.00026	0.00016	0.00080	-0.00301
63			2PZ (O)	0.00000	0.00000	0.00000	0.00000	0.00000
64	8	H	1S (I)	0.00016	-0.00025	-0.00032	0.00235	-0.00061
65			1S (O)	0.00174	-0.00467	-0.00566	-0.00627	0.00012
66	9	H	1S (I)	-0.00052	0.00021	0.00256	0.00014	-0.00010
67			1S (O)	-0.00130	0.00227	-0.00454	-0.00443	0.00543
68	10	H	1S (I)	-0.00045	-0.00041	-0.00029	0.00005	-0.00223
69			1S (O)	0.00299	-0.00185	-0.00505	0.00191	0.00559
70	11	H	1S (I)	-0.00045	0.00248	0.00071	0.00014	0.00014
71			1S (O)	-0.00110	-0.00496	0.00147	-0.00463	0.00103
72	12	H	1S (I)	-0.00034	-0.00018	-0.00045	0.00018	0.00022
73			1S (O)	0.00266	-0.00461	-0.00296	0.00141	-0.00377
74	13	H	1S (I)	-0.00082	-0.00015	0.00031	0.00007	0.00001
75			1S (O)	-0.00155	-0.00079	-0.00032	0.00014	-0.00002
76	14	H	1S (I)	-0.00102	0.00026	0.00002	0.00005	-0.00032
77			1S (O)	0.00244	0.00032	-0.00007	0.00004	-0.00046
78	15	H	1S (I)	-0.00102	0.00026	0.00002	0.00005	-0.00032
79			1S (O)	0.00244	0.00032	-0.00007	0.00004	-0.00046

				6 (A')	7 (A')	8 (A')	9 (A')	10 (A')
	EIGENVALUES --			-11.16932	-11.16254	-1.15872	-1.04506	-1.01357
1	1	C	1S	0.01551	-0.00426	-0.10783	0.12176	0.00085
2			2S (I)	-0.00366	0.00118	0.11936	-0.13026	-0.00099
3			2PX (I)	-0.00083	-0.00023	-0.00036	-0.00054	0.10554
4			2PY (I)	0.00223	0.00070	-0.05116	-0.03300	-0.00009
5			2PZ (I)	0.00000	0.00000	0.00000	0.00000	0.00000
6			2S (O)	0.04547	-0.01666	0.20073	-0.26772	-0.00194
7			2PX (O)	0.00869	0.00267	0.00153	-0.00440	0.01711
8			2PY (O)	-0.03485	-0.01711	0.00825	-0.00412	0.00051
9			2PZ (O)	0.00000	0.00000	0.00000	0.00000	0.00000
10	2	C	1S	0.13823	-0.00314	-0.09072	-0.11724	0.00036
11			2S (I)	0.01387	-0.00018	0.10152	0.12697	-0.00042
12			2PX (I)	-0.00052	0.00002	-0.00001	-0.00070	0.10236
13			2PY (I)	-0.00074	0.00018	0.05733	0.03740	-0.00062
14			2PZ (I)	0.00000	0.00000	0.00000	0.00000	0.00000
15			2S (O)	-0.02891	0.00163	0.17184	0.25476	-0.00072
16			2PX (O)	0.00035	-0.00085	-0.00040	0.00140	0.00934
17			2PY (O)	-0.01429	0.00187	0.01670	0.00699	0.00002
18			2PZ (O)	0.00000	0.00000	0.00000	0.00000	0.00000
19	3	C	1S	0.31248	-0.01624	-0.09796	0.03505	0.11905
20			2S (I)	0.03147	-0.00093	0.10937	-0.03742	-0.12763
21			2PX (I)	-0.00060	0.00017	0.05339	-0.04048	0.00477
22			2PY (I)	-0.00035	0.00072	-0.02279	-0.07527	0.05483
23			2PZ (I)	0.00000	0.00000	0.00000	0.00000	0.00000
24			2S (O)	-0.04380	0.00158	0.19057	-0.08846	-0.27492
25			2PX (O)	-0.01557	-0.00093	0.01734	-0.00838	-0.00520
26			2PY (O)	0.01117	-0.00041	-0.01426	0.00115	0.01019
27			2PZ (O)	0.00000	0.00000	0.00000	0.00000	0.00000
28	4	C	1S	0.05056	-0.00663	-0.09211	-0.07364	0.11806
29			2S (I)	0.00201	0.00015	0.10439	0.07858	-0.12677
30			2PX (I)	-0.00071	0.00017	0.04930	0.05051	0.00447
31			2PY (I)	-0.00051	0.00037	0.02963	-0.04044	-0.05658
32			2PZ (I)	0.00000	0.00000	0.00000	0.00000	0.00000
33			2S (O)	0.02661	-0.00312	0.15810	0.17637	-0.27621

34			2PX (O)	0.01394	-0.00250	0.00509	0.01533	-0.00742
35			2PY (O)	0.01054	-0.00209	0.00020	0.00817	-0.00965
36			2PZ (O)	0.00000	0.00000	0.00000	0.00000	0.00000
37	5	C	1S	0.92247	-0.01379	-0.09821	0.03512	-0.11914
38			2S (I)	0.09324	-0.00077	0.10959	-0.03750	0.12765
39			2PX (I)	-0.00067	-0.00026	-0.05327	0.03962	0.00533
40			2PY (I)	-0.00055	0.00089	-0.02287	-0.07597	-0.05679
41			2PZ (I)	0.00000	0.00000	0.00000	0.00000	0.00000
42			2S (O)	-0.09601	0.00076	0.19085	-0.08803	0.27549
43			2PX (O)	0.02616	0.00339	-0.01645	0.00536	-0.00558
44			2PY (O)	0.01374	-0.00427	-0.01630	0.00814	-0.01024
45			2PZ (O)	0.00000	0.00000	0.00000	0.00000	0.00000
46	6	C	1S	0.06342	-0.00715	-0.09230	-0.07284	-0.11875
47			2S (I)	0.00115	0.00023	0.10469	0.07743	0.12754
48			2PX (I)	0.00086	-0.00013	-0.04866	-0.05033	0.00566
49			2PY (I)	-0.00134	0.00037	0.03086	-0.03962	0.05784
50			2PZ (I)	0.00000	0.00000	0.00000	0.00000	0.00000
51			2S (O)	0.04118	-0.00474	0.15755	0.17792	0.27791
52			2PX (O)	-0.01813	0.00116	-0.00564	-0.01349	-0.00703
53			2PY (O)	0.01980	-0.00429	-0.00100	0.01249	0.00993
54			2PZ (O)	0.00000	0.00000	0.00000	0.00000	0.00000
55	7	C	1S	-0.01959	-0.98727	-0.03804	0.11551	0.00011
56			2S (I)	-0.00339	-0.10220	0.03991	-0.11100	-0.00019
57			2PX (I)	-0.00010	-0.00013	-0.00067	0.00098	0.01358
58			2PY (I)	0.00006	-0.00004	-0.02723	0.04210	-0.00026
59			2PZ (I)	0.00000	0.00000	0.00000	0.00000	0.00000
60			2S (O)	0.01388	0.08500	0.07359	-0.31073	0.00027
61			2PX (O)	-0.00134	-0.00013	0.00233	-0.00380	0.00410
62			2PY (O)	-0.00628	-0.00625	0.00758	0.00990	0.00043
63			2PZ (O)	0.00000	0.00000	0.00000	0.00000	0.00000
64	8	H	1S (I)	-0.00101	0.00024	0.03109	0.05546	-0.00013
65			1S (O)	-0.00056	0.00025	-0.00361	0.00608	0.00004
66	9	H	1S (I)	0.00012	-0.00007	0.03150	0.03479	-0.06314
67			1S (O)	0.00506	-0.00142	-0.00693	0.00743	-0.01273
68	10	H	1S (I)	-0.00148	-0.00010	0.03483	-0.02209	-0.06388
69			1S (O)	-0.00016	0.00014	-0.00040	-0.00932	-0.01257
70	11	H	1S (I)	0.00003	0.00003	0.03162	0.03436	0.06350
71			1S (O)	0.00714	-0.00126	-0.00693	0.00741	0.01273
72	12	H	1S (I)	-0.00264	0.00024	0.03507	-0.02278	0.06376
73			1S (O)	0.00431	-0.00105	-0.00085	-0.00806	0.01282
74	13	H	1S (I)	-0.00056	-0.00027	0.01657	-0.05667	-0.00586
75			1S (O)	-0.00038	-0.01448	-0.00160	-0.00304	-0.00488
76	14	H	1S (I)	-0.00044	-0.00032	0.01652	-0.05648	0.00281
77			1S (O)	0.00003	-0.01451	-0.00566	0.00372	0.00171
78	15	H	1S (I)	-0.00044	-0.00032	0.01652	-0.05648	0.00281
79			1S (O)	0.00003	-0.01451	-0.00566	0.00372	0.00171

				11 (A')	12 (A')	13 (A')	14 (A')	15 (A')
EIGENVALUES --				-0.93565	-0.82730	-0.80029	-0.70209	-0.63891
1	1	C	1S	-0.03037	-0.00030	0.10413	0.02299	-0.00581
2			2S (I)	0.03247	0.00005	-0.10780	-0.01918	0.00517
3			2PX (I)	-0.00306	0.19183	0.00017	-0.00006	0.21377
4			2PY (I)	-0.14170	-0.00149	0.05150	-0.08956	0.00264
5			2PZ (I)	0.00000	0.00000	0.00000	0.00000	0.00000
6			2S (O)	0.08298	0.00209	-0.34077	-0.09355	0.02355
7			2PX (O)	-0.00814	0.08078	0.00107	0.00136	0.15285
8			2PY (O)	-0.02033	0.00090	0.03106	-0.06061	0.00971
9			2PZ (O)	0.00000	0.00000	0.00000	0.00000	0.00000
10	2	C	1S	0.09857	0.00078	0.09041	0.02832	0.00470
11			2S (I)	-0.10377	-0.00078	-0.09343	-0.02407	-0.00521
12			2PX (I)	0.00117	-0.17994	-0.00060	0.00194	0.21956
13			2PY (I)	0.00762	0.00146	0.03894	0.21287	-0.00152
14			2PZ (I)	0.00000	0.00000	0.00000	0.00000	0.00000
15			2S (O)	-0.26458	-0.00250	-0.29700	-0.12216	-0.01325
16			2PX (O)	0.00233	-0.06304	-0.00098	0.00073	0.11803
17			2PY (O)	-0.00722	0.00077	0.00107	0.13719	0.00396

18			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
19	3	C	1S		-0.07392	0.08954	-0.03409	0.02101	-0.01006
20			2S	(I)	0.07813	-0.09276	0.03399	-0.01760	0.00893
21			2PX	(I)	0.02846	-0.00866	-0.13820	0.11660	-0.09473
22			2PY	(I)	-0.00447	-0.10831	-0.11805	-0.11975	-0.19369
23			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
24			2S	(O)	0.19217	-0.27979	0.11578	-0.08748	0.05316
25			2PX	(O)	0.01416	-0.00775	-0.05350	0.08315	-0.03951
26			2PY	(O)	-0.01441	-0.03202	-0.03413	-0.06787	-0.10869
27			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
28	4	C	1S		0.01667	-0.09332	-0.06246	-0.00984	0.00063
29			2S	(I)	-0.01845	0.09681	0.06378	0.01482	0.00014
30			2PX	(I)	-0.04397	0.00425	-0.11898	0.13016	-0.10080
31			2PY	(I)	0.09130	-0.09566	0.09557	0.09512	0.20472
32			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
33			2S	(O)	-0.03939	0.29608	0.21066	0.01582	-0.01203
34			2PX	(O)	-0.00114	0.00875	-0.04683	0.08418	-0.06116
35			2PY	(O)	0.02226	-0.02838	0.03948	0.06010	0.11360
36			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
37	5	C	1S		-0.07251	-0.09032	-0.03380	0.02168	0.01768
38			2S	(I)	0.07626	0.09345	0.03384	-0.01804	-0.01694
39			2PX	(I)	-0.02738	-0.00842	0.13614	-0.11904	-0.10978
40			2PY	(I)	-0.00676	0.10823	-0.11921	-0.11822	0.19065
41			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
42			2S	(O)	0.19129	0.28374	0.11480	-0.09106	-0.07153
43			2PX	(O)	-0.01948	-0.00855	0.05404	-0.08384	-0.05621
44			2PY	(O)	-0.00398	0.03015	-0.03723	-0.06892	0.09113
45			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
46	6	C	1S		0.01522	0.09357	-0.06159	-0.01022	-0.00874
47			2S	(I)	-0.01722	-0.09692	0.06308	0.01525	0.00855
48			2PX	(I)	0.04425	0.00538	0.11949	-0.12996	-0.07775
49			2PY	(I)	0.09011	0.09753	0.09504	0.09468	-0.21567
50			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
51			2S	(O)	-0.03123	-0.29878	0.20648	0.01644	0.03108
52			2PX	(O)	0.00425	0.00916	0.04651	-0.08446	-0.03903
53			2PY	(O)	0.02791	0.02820	0.03746	0.05915	-0.13059
54			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
55	7	C	1S		0.15835	0.00092	-0.05459	-0.02799	0.00068
56			2S	(I)	-0.14801	-0.00112	0.05017	0.02245	-0.00054
57			2PX	(I)	-0.00082	0.04566	0.00055	0.00458	0.14863
58			2PY	(I)	-0.02312	-0.00202	0.08470	0.09451	-0.01333
59			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
60			2S	(O)	-0.49705	-0.00257	0.19646	0.12012	-0.00724
61			2PX	(O)	-0.00057	0.02703	-0.00069	0.00119	0.10430
62			2PY	(O)	0.00037	0.00008	0.03697	0.05280	-0.00531
63			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
64	8	H	1S	(I)	-0.06879	-0.00094	-0.08982	-0.14608	-0.00413
65			1S	(O)	-0.02345	-0.00038	-0.04618	-0.09141	-0.00098
66	9	H	1S	(I)	-0.01392	0.09103	0.07695	-0.08224	-0.00861
67			1S	(O)	-0.00151	0.04326	0.03820	-0.05488	-0.00776
68	10	H	1S	(I)	0.03723	-0.09036	0.05708	-0.11011	-0.00313
69			1S	(O)	0.00830	-0.04320	0.03117	-0.06793	-0.00325
70	11	H	1S	(I)	-0.01327	-0.09166	0.07590	-0.08180	0.03432
71			1S	(O)	-0.00155	-0.04366	0.03757	-0.05465	0.02299
72	12	H	1S	(I)	0.03544	0.09057	0.05632	-0.11113	-0.01524
73			1S	(O)	0.01002	0.04351	0.03000	-0.06848	-0.00705
74	13	H	1S	(I)	-0.09673	-0.02443	0.05425	0.03587	-0.09549
75			1S	(O)	-0.01687	-0.01630	0.02422	0.01738	-0.07693
76	14	H	1S	(I)	-0.09652	0.01076	0.05162	0.04004	0.04302
77			1S	(O)	-0.01674	0.00626	0.02516	0.02352	0.03316
78	15	H	1S	(I)	-0.09652	0.01076	0.05162	0.04004	0.04302
79			1S	(O)	-0.01674	0.00626	0.02516	0.02352	0.03316
					16	17	18	19	20
					(A')	(A')	(A")	(A')	(A')
	EIGENVALUES --				-0.62772	-0.58881	-0.57836	-0.56901	-0.53982
1	1	C	1S		-0.07394	0.00073	0.00000	-0.01054	-0.00046

2			2S	(I)	0.07657	-0.00092	0.00000	0.00572	0.00260
3			2PX	(I)	-0.02005	-0.09988	0.00000	0.00532	0.04472
4			2PY	(I)	0.03405	0.00011	0.00000	0.24834	-0.01231
5			2PZ	(I)	0.00000	0.00000	-0.13754	0.00000	0.00000
6			2S	(O)	0.23821	-0.00087	0.00000	0.06331	-0.01436
7			2PX	(O)	-0.00851	-0.06744	0.00000	0.00660	0.03881
8			2PY	(O)	0.08203	-0.00029	0.00000	0.21528	-0.01325
9			2PZ	(O)	0.00000	0.00000	-0.10727	0.00000	0.00000
10	2	C	1S		0.05796	-0.00052	0.00000	-0.01201	0.00155
11			2S	(I)	-0.06262	0.00064	0.00000	0.01538	-0.00173
12			2PX	(I)	-0.02004	-0.10726	0.00000	0.00326	0.12804
13			2PY	(I)	0.02261	0.00227	0.00000	0.27032	-0.00197
14			2PZ	(I)	0.00000	0.00000	-0.03432	0.00000	0.00000
15			2S	(O)	-0.16699	0.00064	0.00000	0.02324	-0.00276
16			2PX	(O)	-0.01145	-0.05588	0.00000	0.00185	0.08187
17			2PY	(O)	0.06673	0.00124	0.00000	0.24648	-0.00264
18			2PZ	(O)	0.00000	0.00000	-0.02986	0.00000	0.00000
19	3	C	1S		0.05290	-0.02151	0.00000	0.02115	0.01866
20			2S	(I)	-0.05526	0.02628	0.00000	-0.02498	-0.01765
21			2PX	(I)	0.13456	0.18082	0.00000	-0.11830	0.02910
22			2PY	(I)	-0.00772	-0.11310	0.00000	0.05427	-0.11941
23			2PZ	(I)	0.00000	0.00000	-0.07508	0.00000	0.00000
24			2S	(O)	-0.16154	0.03777	0.00000	-0.03629	-0.07721
25			2PX	(O)	0.13329	0.13731	0.00000	-0.07821	0.05239
26			2PY	(O)	-0.04986	-0.09020	0.00000	0.03136	-0.07097
27			2PZ	(O)	0.00000	0.00000	-0.06826	0.00000	0.00000
28	4	C	1S		-0.05121	-0.01752	0.00000	-0.01855	-0.01053
29			2S	(I)	0.05343	0.02207	0.00000	0.02190	0.01013
30			2PX	(I)	-0.13134	0.19653	0.00000	0.10198	-0.07774
31			2PY	(I)	-0.09653	0.11529	0.00000	-0.05467	0.09712
32			2PZ	(I)	0.00000	0.00000	-0.04399	0.00000	0.00000
33			2S	(O)	0.15645	0.02764	0.00000	0.02913	0.04921
34			2PX	(O)	-0.13844	0.15940	0.00000	0.05071	-0.06624
35			2PY	(O)	-0.09638	0.08492	0.00000	-0.03822	0.06224
36			2PZ	(O)	0.00000	0.00000	-0.03738	0.00000	0.00000
37	5	C	1S		0.05216	0.02055	0.00000	0.02034	-0.01656
38			2S	(I)	-0.05442	-0.02529	0.00000	-0.02408	0.01483
39			2PX	(I)	-0.11350	0.18572	0.00000	0.11431	0.01297
40			2PY	(I)	-0.04071	0.11368	0.00000	0.05888	0.12126
41			2PZ	(I)	0.00000	0.00000	-0.07643	0.00000	0.00000
42			2S	(O)	-0.16112	-0.03403	0.00000	-0.03606	0.06274
43			2PX	(O)	-0.11985	0.14322	0.00000	0.07874	0.03206
44			2PY	(O)	-0.06990	0.08906	0.00000	0.03146	0.09420
45			2PZ	(O)	0.00000	0.00000	-0.07324	0.00000	0.00000
46	6	C	1S		-0.05074	0.01825	0.00000	-0.01830	0.00930
47			2S	(I)	0.05294	-0.02273	0.00000	0.02158	-0.01042
48			2PX	(I)	0.14949	0.19249	0.00000	-0.10388	-0.07054
49			2PY	(I)	-0.06313	-0.11735	0.00000	-0.05886	-0.10475
50			2PZ	(I)	0.00000	0.00000	-0.04539	0.00000	0.00000
51			2S	(O)	0.15419	-0.03117	0.00000	0.02841	-0.02588
52			2PX	(O)	0.14738	0.15522	0.00000	-0.05343	-0.05596
53			2PY	(O)	-0.07847	-0.08664	0.00000	-0.04214	-0.05707
54			2PZ	(O)	0.00000	0.00000	-0.03734	0.00000	0.00000
55	7	C	1S		0.00491	-0.00033	0.00000	0.00409	0.00025
56			2S	(I)	-0.00177	0.00028	0.00000	0.00215	-0.00037
57			2PX	(I)	-0.00782	0.03073	0.00000	-0.01354	-0.33017
58			2PY	(I)	-0.11342	0.00103	0.00000	-0.22274	0.01500
59			2PZ	(I)	0.00000	0.00000	-0.34138	0.00000	0.00000
60			2S	(O)	-0.05741	0.00171	0.00000	-0.06592	0.00380
61			2PX	(O)	-0.00736	0.03421	0.00000	-0.00962	-0.29601
62			2PY	(O)	-0.05359	0.00075	0.00000	-0.14640	0.00979
63			2PZ	(O)	0.00000	0.00000	-0.28270	0.00000	0.00000
64	8	H	1S	(I)	-0.07241	-0.00064	0.00000	-0.17732	-0.00090
65			1S	(O)	-0.03192	-0.00062	0.00000	-0.13437	-0.00093
66	9	H	1S	(I)	0.15487	-0.13690	0.00000	-0.02314	0.02686
67			1S	(O)	0.09293	-0.10668	0.00000	-0.02680	0.01756

68	10	H	1S	(I)	-0.13049	-0.12384	0.00000	0.06753	-0.07456
69			1S	(O)	-0.07543	-0.10049	0.00000	0.06039	-0.04759
70	11	H	1S	(I)	0.15399	0.13452	0.00000	-0.02239	-0.01755
71			1S	(O)	0.09258	0.10525	0.00000	-0.02590	-0.00980
72	12	H	1S	(I)	-0.12865	0.12768	0.00000	0.06762	0.06456
73			1S	(O)	-0.07477	0.10244	0.00000	0.05867	0.04386
74	13	H	1S	(I)	-0.02975	-0.02382	0.00000	-0.04909	0.23179
75			1S	(O)	-0.03207	-0.02245	0.00000	-0.04290	0.20819
76	14	H	1S	(I)	-0.03110	0.01225	-0.19473	-0.05935	-0.11248
77			1S	(O)	-0.03098	0.01152	-0.16890	-0.05550	-0.10130
78	15	H	1S	(I)	-0.03110	0.01225	0.19473	-0.05935	-0.11248
79			1S	(O)	-0.03098	0.01152	0.16890	-0.05550	-0.10130
					21	22	23	24	25
					(A")	(A')	(A')	(A")	(A")
	EIGENVALUES --				-0.49368	-0.48358	-0.48163	-0.33690	-0.32624
1	1	C	1S		0.00000	0.00086	0.00567	0.00000	0.00000
2			2S	(I)	0.00000	0.00009	-0.00311	0.00000	0.00000
3			2PX	(I)	0.00000	0.23793	-0.03931	0.00000	0.00000
4			2PY	(I)	0.00000	-0.04069	-0.22557	0.00000	0.00000
5			2PZ	(I)	-0.12671	0.00000	0.00000	0.01582	0.26248
6			2S	(O)	0.00000	-0.00685	-0.01079	0.00000	0.00000
7			2PX	(O)	0.00000	0.19106	-0.04153	0.00000	0.00000
8			2PY	(O)	0.00000	-0.04941	-0.28664	0.00000	0.00000
9			2PZ	(O)	-0.13432	0.00000	0.00000	0.01628	0.32302
10	2	C	1S		0.00000	0.00007	-0.00284	0.00000	0.00000
11			2S	(I)	0.00000	0.00020	0.00430	0.00000	0.00000
12			2PX	(I)	0.00000	-0.20600	0.03216	0.00000	0.00000
13			2PY	(I)	0.00000	0.02482	0.16219	0.00000	0.00000
14			2PZ	(I)	-0.19058	0.00000	0.00000	-0.01168	-0.26292
15			2S	(O)	0.00000	0.00012	0.00831	0.00000	0.00000
16			2PX	(O)	0.00000	-0.13997	0.02385	0.00000	0.00000
17			2PY	(O)	0.00000	0.02891	0.19342	0.00000	0.00000
18			2PZ	(O)	-0.18599	0.00000	0.00000	-0.01366	-0.32311
19	3	C	1S		0.00000	0.00883	-0.00211	0.00000	0.00000
20			2S	(I)	0.00000	-0.01068	0.00286	0.00000	0.00000
21			2PX	(I)	0.00000	-0.19286	0.05714	0.00000	0.00000
22			2PY	(I)	0.00000	-0.00352	0.20841	0.00000	0.00000
23			2PZ	(I)	-0.16132	0.00000	0.00000	0.23969	0.13558
24			2S	(O)	0.00000	-0.02898	-0.02349	0.00000	0.00000
25			2PX	(O)	0.00000	-0.20185	-0.00899	0.00000	0.00000
26			2PY	(O)	0.00000	0.06461	0.17496	0.00000	0.00000
27			2PZ	(O)	-0.15595	0.00000	0.00000	0.29139	0.16594
28	4	C	1S		0.00000	-0.00508	0.00531	0.00000	0.00000
29			2S	(I)	0.00000	0.00560	-0.00778	0.00000	0.00000
30			2PX	(I)	0.00000	0.18617	-0.02191	0.00000	0.00000
31			2PY	(I)	0.00000	-0.03608	-0.20330	0.00000	0.00000
32			2PZ	(I)	-0.18261	0.00000	0.00000	0.22404	-0.13702
33			2S	(O)	0.00000	0.03240	-0.00023	0.00000	0.00000
34			2PX	(O)	0.00000	0.19205	-0.06050	0.00000	0.00000
35			2PY	(O)	0.00000	0.02287	-0.15766	0.00000	0.00000
36			2PZ	(O)	-0.17965	0.00000	0.00000	0.26909	-0.16662
37	5	C	1S		0.00000	-0.00874	0.00098	0.00000	0.00000
38			2S	(I)	0.00000	0.01034	-0.00139	0.00000	0.00000
39			2PX	(I)	0.00000	-0.20598	0.00591	0.00000	0.00000
40			2PY	(I)	0.00000	0.06792	0.19258	0.00000	0.00000
41			2PZ	(I)	-0.16042	0.00000	0.00000	-0.22778	0.15642
42			2S	(O)	0.00000	0.02000	-0.02413	0.00000	0.00000
43			2PX	(O)	0.00000	-0.19957	0.06446	0.00000	0.00000
44			2PY	(O)	0.00000	0.00039	0.18884	0.00000	0.00000
45			2PZ	(O)	-0.15287	0.00000	0.00000	-0.27580	0.18845
46	6	C	1S		0.00000	0.00633	0.00282	0.00000	0.00000
47			2S	(I)	0.00000	-0.00793	-0.00512	0.00000	0.00000
48			2PX	(I)	0.00000	0.18616	-0.03929	0.00000	0.00000
49			2PY	(I)	0.00000	-0.03054	-0.20020	0.00000	0.00000
50			2PZ	(I)	-0.18185	0.00000	0.00000	-0.23887	-0.10930
51			2S	(O)	0.00000	-0.02558	0.01424	0.00000	0.00000

52			2PX (O)	0.00000	0.20519	-0.00130	0.00000	0.00000
53			2PY (O)	0.00000	-0.06893	-0.13711	0.00000	0.00000
54			2PZ (O)	-0.17979	0.00000	0.00000	-0.28779	-0.13132
55	7	C	1S	0.00000	0.00389	0.02140	0.00000	0.00000
56			2S (I)	0.00000	-0.00446	-0.02498	0.00000	0.00000
57			2PX (I)	0.00000	-0.08671	0.02879	0.00000	0.00000
58			2PY (I)	0.00000	0.03952	0.22727	0.00000	0.00000
59			2PZ (I)	0.14075	0.00000	0.00000	-0.00034	-0.07772
60			2S (O)	0.00000	-0.00464	-0.01956	0.00000	0.00000
61			2PX (O)	0.00000	-0.09578	0.03227	0.00000	0.00000
62			2PY (O)	0.00000	0.02646	0.15162	0.00000	0.00000
63			2PZ (O)	0.13696	0.00000	0.00000	0.01291	-0.08247
64	8	H	1S (I)	0.00000	-0.02013	-0.13219	0.00000	0.00000
65			1S (O)	0.00000	-0.01660	-0.10919	0.00000	0.00000
66	9	H	1S (I)	0.00000	-0.11403	0.09249	0.00000	0.00000
67			1S (O)	0.00000	-0.09256	0.07972	0.00000	0.00000
68	10	H	1S (I)	0.00000	0.13069	0.04944	0.00000	0.00000
69			1S (O)	0.00000	0.11143	0.03451	0.00000	0.00000
70	11	H	1S (I)	0.00000	0.13894	0.05145	0.00000	0.00000
71			1S (O)	0.00000	0.11421	0.04532	0.00000	0.00000
72	12	H	1S (I)	0.00000	-0.11276	0.08446	0.00000	0.00000
73			1S (O)	0.00000	-0.09625	0.06725	0.00000	0.00000
74	13	H	1S (I)	0.00000	0.07935	0.02643	0.00000	0.00000
75			1S (O)	0.00000	0.08760	0.04295	0.00000	0.00000
76	14	H	1S (I)	0.09158	-0.02847	0.05076	-0.00273	-0.06795
77			1S (O)	0.08790	-0.02918	0.06602	-0.01528	-0.08683
78	15	H	1S (I)	-0.09158	-0.02847	0.05076	0.00273	0.06795
79			1S (O)	-0.08790	-0.02918	0.06602	0.01528	0.08683
				26 (A")	27 (A")	28 (A')	29 (A')	30 (A')
	EIGENVALUES --			0.15039	0.15653	0.26219	0.29909	0.31404
1	1	C	1S	0.00000	0.00000	0.02711	0.00490	-0.00355
2			2S (I)	0.00000	0.00000	-0.00912	-0.00820	-0.01508
3			2PX (I)	0.00000	0.00000	0.00428	-0.00432	-0.03963
4			2PY (I)	0.00000	0.00000	-0.03659	-0.00514	0.01135
5			2PZ (I)	0.16729	0.22514	0.00000	0.00000	0.00000
6			2S (O)	0.00000	0.00000	-0.42280	0.33138	0.12194
7			2PX (O)	0.00000	0.00000	-0.05927	0.04611	0.00460
8			2PY (O)	0.00000	0.00000	-0.00387	-0.37344	0.01076
9			2PZ (O)	0.33214	0.48472	0.00000	0.00000	0.00000
10	2	C	1S	0.00000	0.00000	0.04464	0.01548	0.00312
11			2S (I)	0.00000	0.00000	-0.02392	0.00815	0.00096
12			2PX (I)	0.00000	0.00000	0.00336	-0.00711	-0.02914
13			2PY (I)	0.00000	0.00000	0.09163	0.08563	0.02229
14			2PZ (I)	0.15719	0.20959	0.00000	0.00000	0.00000
15			2S (O)	0.00000	0.00000	-0.49889	-0.48884	-0.07684
16			2PX (O)	0.00000	0.00000	0.01487	-0.01859	0.02355
17			2PY (O)	0.00000	0.00000	0.38632	0.17679	0.06563
18			2PZ (O)	0.35439	0.47612	0.00000	0.00000	0.00000
19	3	C	1S	0.00000	0.00000	0.04783	-0.01782	-0.00900
20			2S (I)	0.00000	0.00000	-0.02662	0.01764	-0.01321
21			2PX (I)	0.00000	0.00000	0.08889	-0.04550	-0.15232
22			2PY (I)	0.00000	0.00000	-0.04677	0.03576	0.03533
23			2PZ (I)	0.09840	-0.24410	0.00000	0.00000	0.00000
24			2S (O)	0.00000	0.00000	-0.53573	0.12821	0.34669
25			2PX (O)	0.00000	0.00000	0.41327	-0.48271	-0.51544
26			2PY (O)	0.00000	0.00000	-0.24369	0.07380	0.26131
27			2PZ (O)	0.23473	-0.55392	0.00000	0.00000	0.00000
28	4	C	1S	0.00000	0.00000	0.04034	0.03462	-0.02659
29			2S (I)	0.00000	0.00000	-0.01243	-0.02458	0.00284
30			2PX (I)	0.00000	0.00000	0.08128	0.03954	-0.09446
31			2PY (I)	0.00000	0.00000	0.05866	-0.00089	-0.02711
32			2PZ (I)	-0.26177	0.03331	0.00000	0.00000	0.00000
33			2S (O)	0.00000	0.00000	-0.59901	-0.34411	0.51378
34			2PX (O)	0.00000	0.00000	0.24214	0.33990	-0.29490
35			2PY (O)	0.00000	0.00000	0.14437	0.06088	-0.12423

36			2PZ	(O)	-0.59160	0.07531	0.00000	0.00000	0.00000
37	5	C	1S		0.00000	0.00000	0.04984	-0.00942	0.01204
38			2S	(I)	0.00000	0.00000	-0.03390	0.02481	0.00246
39			2PX	(I)	0.00000	0.00000	-0.06389	-0.01094	-0.13149
40			2PY	(I)	0.00000	0.00000	-0.04916	0.02532	-0.03705
41			2PZ	(I)	-0.25861	0.04358	0.00000	0.00000	0.00000
42			2S	(O)	0.00000	0.00000	-0.47187	-0.08448	-0.37900
43			2PX	(O)	0.00000	0.00000	-0.37711	0.31741	-0.40636
44			2PY	(O)	0.00000	0.00000	-0.16544	-0.07664	-0.25803
45			2PZ	(O)	-0.58601	0.09204	0.00000	0.00000	0.00000
46	6	C	1S		0.00000	0.00000	0.03669	0.04082	0.03789
47			2S	(I)	0.00000	0.00000	-0.01109	-0.02306	-0.00759
48			2PX	(I)	0.00000	0.00000	-0.07351	-0.06974	-0.11657
49			2PY	(I)	0.00000	0.00000	0.06018	0.01409	0.04313
50			2PZ	(I)	0.10860	-0.24923	0.00000	0.00000	0.00000
51			2S	(O)	0.00000	0.00000	-0.53329	-0.49446	-0.67020
52			2PX	(O)	0.00000	0.00000	-0.19840	-0.44572	-0.40002
53			2PY	(O)	0.00000	0.00000	0.16941	0.08487	0.18488
54			2PZ	(O)	0.24407	-0.56234	0.00000	0.00000	0.00000
55	7	C	1S		0.00000	0.00000	0.01967	-0.14075	0.04338
56			2S	(I)	0.00000	0.00000	0.00150	0.03150	-0.01096
57			2PX	(I)	0.00000	0.00000	0.03279	-0.02792	-0.16878
58			2PY	(I)	0.00000	0.00000	-0.10236	0.09638	-0.02570
59			2PZ	(I)	0.01707	-0.00435	0.00000	0.00000	0.00000
60			2S	(O)	0.00000	0.00000	-0.39354	2.05263	-0.61656
61			2PX	(O)	0.00000	0.00000	0.20462	-0.13836	-0.77251
62			2PY	(O)	0.00000	0.00000	-0.41538	0.42952	-0.11442
63			2PZ	(O)	0.16054	0.01110	0.00000	0.00000	0.00000
64	8	H	1S	(I)	0.00000	0.00000	0.04331	0.00470	0.00218
65			1S	(O)	0.00000	0.00000	0.79554	0.46159	0.12340
66	9	H	1S	(I)	0.00000	0.00000	0.03802	0.01445	-0.01774
67			1S	(O)	0.00000	0.00000	0.73740	0.50608	-0.66113
68	10	H	1S	(I)	0.00000	0.00000	0.03193	0.03000	-0.01476
69			1S	(O)	0.00000	0.00000	0.85384	-0.43551	-0.84416
70	11	H	1S	(I)	0.00000	0.00000	0.03294	0.02297	0.02084
71			1S	(O)	0.00000	0.00000	0.67298	0.71447	0.87714
72	12	H	1S	(I)	0.00000	0.00000	0.02761	0.04122	0.01046
73			1S	(O)	0.00000	0.00000	0.76332	-0.11745	0.78527
74	13	H	1S	(I)	0.00000	0.00000	0.01269	-0.00922	-0.03248
75			1S	(O)	0.00000	0.00000	0.51377	-1.09957	-0.63463
76	14	H	1S	(I)	-0.03582	-0.04547	-0.00453	0.00237	0.01277
77			1S	(O)	-0.23134	-0.12803	0.17235	-0.85555	0.75662
78	15	H	1S	(I)	0.03582	0.04547	-0.00453	0.00237	0.01277
79			1S	(O)	0.23134	0.12803	0.17235	-0.85555	0.75662

APPENDIX B:

MOLECULAR ORBITALS AND EIGENVALUES FOR THE TRIPLET STATE TOLUENE MOLECULE

THE ELECTRONIC STATE IS 3-A'.

ALPHA MOLECULAR ORBITAL COEFFICIENTS

					1 (A')	2 (A')	3 (A')	4 (A')	5 (A')
			EIGENVALUES --		-11.18862	-11.18229	-11.13158	-11.17968	-11.16395
1	1	C	1S		-0.98658	0.00412	-0.03101	-0.00966	-0.00211
2			2S	(I)	-0.10063	-0.00015	-0.00039	-0.00107	-0.00101
3			2PX	(I)	0.00013	-0.00010	0.00027	-0.00064	0.00042
4			2PY	(I)	0.00034	0.00040	-0.00103	-0.00073	-0.00049
5			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
6			2S	(O)	0.08756	0.00772	-0.02305	0.01126	0.01415
7			2PX	(O)	-0.00531	-0.00195	-0.00845	-0.00142	0.00017
8			2PY	(O)	-0.00812	-0.00741	0.02309	-0.00469	-0.00798
9			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
10	2	C	1S		0.00853	0.97673	-0.10021	-0.09944	-0.01201
11			2S	(I)	0.00159	0.09901	-0.01038	-0.00698	0.00320
12			2PX	(I)	-0.00007	0.00016	0.00083	0.00009	0.00099
13			2PY	(I)	0.00027	0.00132	0.00045	0.00056	0.00128
14			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
15			2S	(O)	-0.00870	-0.08450	0.02121	-0.01762	-0.03492
16			2PX	(O)	-0.00021	-0.00402	0.00031	0.00651	-0.01212
17			2PY	(O)	-0.00531	-0.02174	0.01091	-0.01520	-0.01996
18			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
19	3	C	1S		0.00774	-0.00072	0.00261	0.01340	0.02339
20			2S	(I)	0.00489	0.00070	-0.00007	0.00593	0.00336
21			2PX	(I)	0.00175	0.00002	0.00088	0.00048	0.00034
22			2PY	(I)	0.00062	0.00069	0.00029	-0.00195	-0.00025
23			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
24			2S	(O)	-0.03165	-0.01544	0.01395	-0.03559	-0.01400
25			2PX	(O)	-0.01907	-0.00810	0.00722	-0.00956	-0.00691
26			2PY	(O)	-0.00446	0.00568	-0.00909	0.01361	0.00588
27			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
28	4	C	1S		0.00752	-0.03579	0.05013	-0.98094	-0.00341
29			2S	(I)	0.00074	-0.01267	0.00635	-0.09883	-0.00102
30			2PX	(I)	0.00012	-0.00066	0.00046	-0.00106	0.00074
31			2PY	(I)	0.00075	-0.00031	0.00011	-0.00047	-0.00044
32			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
33			2S	(O)	0.00534	0.03393	-0.01803	0.07981	0.01353
34			2PX	(O)	0.00631	0.01973	-0.00893	0.01566	0.00762
35			2PY	(O)	0.00028	0.00206	-0.00465	0.01161	0.00564
36			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
37	5	C	1S		0.03158	-0.10474	-0.98007	-0.03918	-0.01299
38			2S	(I)	0.00572	-0.01041	-0.09927	-0.00309	0.00313
39			2PX	(I)	-0.00044	0.00032	0.00106	-0.00039	-0.00075
40			2PY	(I)	-0.00002	0.00102	0.00047	-0.00016	-0.00149
41			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
42			2S	(O)	-0.02346	-0.00310	0.08638	-0.00466	-0.03574
43			2PX	(O)	0.01372	0.00613	-0.01993	0.00433	0.01395
44			2PY	(O)	-0.00225	0.00215	-0.01246	0.00268	0.01815
45			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
46	6	C	1S		0.00151	-0.01099	0.01516	0.00531	-0.98664
47			2S	(I)	-0.00016	-0.00511	0.00646	0.00086	-0.09901

48			2PX	(I)	-0.00004	0.00175	-0.00065	-0.00109	0.00106
49			2PY	(I)	0.00059	0.00045	0.00176	-0.00021	-0.00071
50			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
51			2S	(O)	0.00843	0.03387	-0.04130	0.00696	0.09329
52			2PX	(O)	-0.00591	-0.02204	0.01368	-0.00345	-0.02030
53			2PY	(O)	0.00256	0.00055	-0.02068	0.00423	0.01358
54			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
55	7	C	1S		0.00505	-0.00022	0.00474	0.00401	0.02775
56			2S	(I)	0.00216	-0.00017	0.00144	0.00118	0.00356
57			2PX	(I)	-0.00045	0.00000	0.00016	-0.00013	0.00022
58			2PY	(I)	-0.00058	-0.00016	-0.00008	-0.00026	-0.00036
59			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
60			2S	(O)	-0.01300	0.00310	-0.00916	-0.00132	-0.00185
61			2PX	(O)	0.00401	0.00001	0.00227	0.00095	-0.00175
62			2PY	(O)	0.00899	-0.00121	0.00441	0.00119	0.00087
63			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
64	8	H	1S	(I)	-0.00012	-0.00262	0.00075	0.00021	-0.00004
65			1S	(O)	-0.00136	0.00634	0.00056	-0.00528	-0.00548
66	9	H	1S	(I)	0.00048	0.00032	-0.00032	0.00268	0.00055
67			1S	(O)	0.00094	0.00379	-0.00214	-0.00721	0.00155
68	10	H	1S	(I)	0.00058	-0.00045	0.00069	0.00014	-0.00038
69			1S	(O)	-0.00260	-0.00173	0.00226	-0.00444	-0.00216
70	11	H	1S	(I)	0.00041	0.00002	-0.00004	0.00045	0.00233
71			1S	(O)	0.00099	0.00459	-0.00572	0.00048	-0.00616
72	12	H	1S	(I)	0.00023	-0.00024	0.00278	-0.00006	-0.00003
73			1S	(O)	-0.00188	-0.00207	-0.00616	-0.00211	-0.00510
74	13	H	1S	(I)	0.00088	-0.00003	0.00050	0.00038	-0.00011
75			1S	(O)	0.00127	-0.00016	0.00024	-0.00022	-0.00053
76	14	H	1S	(I)	0.00106	-0.00009	0.00030	0.00008	0.00029
77			1S	(O)	-0.00251	-0.00009	-0.00032	-0.00013	0.00059
78	15	H	1S	(I)	0.00106	-0.00009	0.00030	0.00008	0.00029
79			1S	(O)	-0.00251	-0.00009	-0.00032	-0.00013	0.00059

					6	7	8	9	10
					(A')	(A')	(A')	(A')	(A')
	EIGENVALUES	--			-11.16146	-11.16068	-1.14642	-1.04889	-1.01671
1	1	C	1S		0.00380	-0.00790	0.11371	0.12280	0.00251
2			2S	(I)	-0.00073	0.00352	-0.12175	-0.12622	-0.00194
3			2PX	(I)	-0.00011	-0.00146	0.01429	0.01343	0.09116
4			2PY	(I)	-0.00105	-0.00152	0.03515	-0.04655	0.00505
5			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
6			2S	(O)	0.01258	-0.03657	-0.25474	-0.31928	-0.02883
7			2PX	(O)	0.00242	0.01682	0.00580	0.00549	0.01600
8			2PY	(O)	0.02116	0.02179	-0.00915	0.00285	0.02288
9			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
10	2	C	1S		0.00092	-0.00310	0.08932	-0.12219	-0.00124
11			2S	(I)	-0.00021	-0.00080	-0.03753	0.12797	0.00046
12			2PX	(I)	-0.00015	-0.00062	-0.01512	0.02431	0.03771
13			2PY	(I)	-0.00010	0.00058	-0.04544	0.02669	-0.00136
14			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
15			2S	(O)	0.00197	0.01235	-0.19886	0.31688	0.02479
16			2PX	(O)	0.00113	0.00106	-0.00680	0.01208	0.00936
17			2PY	(O)	0.00053	0.00909	-0.01643	0.01518	0.01895
18			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
19	3	C	1S		-0.14233	-0.97681	0.09286	0.03401	0.10882
20			2S	(I)	-0.01496	-0.09818	-0.10522	-0.03736	-0.11966
21			2PX	(I)	-0.00041	-0.00095	-0.05010	-0.04551	0.00815
22			2PY	(I)	-0.00048	0.00087	0.02188	-0.06893	0.06285
23			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
24			2S	(O)	0.01473	0.09652	-0.14731	-0.06148	-0.19287
25			2PX	(O)	0.00503	0.02234	-0.00473	0.00738	0.01076

26			2PY	(O)	-0.00262	-0.01299	0.01061	0.00599	-0.00935
27			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
28	4	C	1S		0.00179	-0.01268	0.08998	-0.06546	0.13111
29			2S	(I)	0.00013	0.00322	-0.09932	0.06786	-0.13485
30			2PX	(I)	-0.00012	0.00092	-0.03664	0.03072	0.00900
31			2PY	(I)	-0.00014	0.00130	-0.03226	-0.03257	-0.06135
32			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
33			2S	(O)	-0.00388	-0.03528	-0.18572	0.16592	-0.36919
34			2PX	(O)	-0.00030	-0.01504	-0.00517	0.00189	-0.02069
35			2PY	(O)	-0.00146	-0.01845	-0.00492	0.00756	-0.02562
36			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
37	5	C	1S		0.00437	-0.00409	0.09890	0.01432	-0.12777
38			2S	(I)	-0.00024	-0.00064	-0.10745	-0.01499	0.13131
39			2PX	(I)	0.00017	-0.00073	0.04033	0.02110	0.01110
40			2PY	(I)	-0.00073	0.00044	0.02430	-0.07081	-0.05733
41			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
42			2S	(O)	0.00158	0.01092	-0.22548	-0.03166	0.36019
43			2PX	(O)	-0.00412	-0.00720	0.01536	-0.00858	-0.01822
44			2PY	(O)	0.00218	-0.00724	0.02008	0.00139	-0.02517
45			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
46	6	C	1S		0.02387	-0.02659	0.08620	-0.07831	-0.10402
47			2S	(I)	0.00177	-0.00143	-0.09907	0.08538	0.11438
48			2PX	(I)	0.00004	-0.00025	0.04317	-0.05488	0.00955
49			2PY	(I)	-0.00032	0.00019	-0.03181	-0.03003	0.06127
50			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
51			2S	(O)	-0.00041	-0.01259	-0.11744	0.14900	0.18733
52			2PX	(O)	0.00103	0.00693	-0.00329	0.00504	0.00874
53			2PY	(O)	0.00255	-0.00594	0.00737	0.01086	-0.00956
54			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
55	7	C	1S		0.97698	-0.14144	0.04583	0.11407	-0.00754
56			2S	(I)	0.10115	-0.01361	-0.04872	-0.11028	0.00753
57			2PX	(I)	0.00018	-0.00022	0.00399	0.00642	0.01216
58			2PY	(I)	0.00008	-0.00001	0.03133	0.04339	-0.00273
59			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
60			2S	(O)	-0.08606	0.00267	-0.08421	-0.29637	0.01503
61			2PX	(O)	0.00026	-0.00151	-0.00558	-0.00378	0.00431
62			2PY	(O)	0.00711	0.00372	-0.01081	0.00766	0.00163
63			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
64	8	H	1S	(I)	-0.00010	0.00063	-0.03215	0.05759	-0.00111
65			1S	(O)	0.00019	0.00150	0.00560	0.00410	0.00398
66	9	H	1S	(I)	0.00005	-0.00010	-0.03201	0.03140	-0.06785
67			1S	(O)	0.00035	-0.00580	0.00846	0.00218	-0.01322
68	10	H	1S	(I)	0.00055	0.00229	-0.03549	-0.02105	-0.05727
69			1S	(O)	-0.00067	-0.00572	0.00148	-0.00668	-0.00581
70	11	H	1S	(I)	-0.00012	-0.00021	-0.03163	0.03696	0.05521
71			1S	(O)	0.00078	-0.00281	0.00825	0.00387	0.00632
72	12	H	1S	(I)	-0.00006	0.00074	-0.03704	-0.01302	0.06729
73			1S	(O)	0.00132	0.00211	0.00292	-0.00316	0.01330
74	13	H	1S	(I)	0.00025	0.00005	-0.02048	-0.05596	-0.00091
75			1S	(O)	0.01419	-0.00229	0.00144	-0.00341	-0.00338
76	14	H	1S	(I)	0.00046	0.00035	-0.02031	-0.05576	0.00689
77			1S	(O)	0.01434	-0.00188	0.00554	0.00263	0.00249
78	15	H	1S	(I)	0.00046	0.00035	-0.02031	-0.05576	0.00689
79			1S	(O)	0.01434	-0.00188	0.00554	0.00263	0.00249
					11 (A')	12 (A')	13 (A')	14 (A')	15 (A')
EIGENVALUES --					-0.93732	-0.84091	-0.78934	-0.69388	-0.64268
1	1	C	1S		0.02029	0.08161	0.07556	0.00736	0.07729
2			2S	(I)	-0.02055	-0.08085	-0.07185	-0.00432	-0.07438
3			2PX	(I)	0.01705	0.13895	-0.10824	0.01564	-0.00696

4			2PY	(I)	0.13151	0.04605	0.03033	-0.08867	-0.07957
5			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
6			2S	(O)	-0.06913	-0.29189	-0.27720	-0.03794	-0.29718
7			2PX	(O)	0.01287	0.06354	-0.05751	0.01638	-0.02370
8			2PY	(O)	0.01840	0.02382	0.02045	-0.05875	-0.09825
9			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
10	2	C	1S		-0.11072	0.05702	0.06539	0.02575	-0.05327
11			2S	(I)	0.11153	-0.05668	-0.06223	-0.02119	0.05442
12			2PX	(I)	0.02576	-0.11312	0.11799	0.02564	-0.00395
13			2PY	(I)	-0.02186	0.02800	0.04696	0.21645	-0.03552
14			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
15			2S	(O)	0.34090	-0.20694	-0.24304	-0.12021	0.18887
16			2PX	(O)	0.01076	-0.04486	0.05180	0.01437	-0.01214
17			2PY	(O)	0.00980	-0.00343	0.00844	0.15177	-0.05949
18			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
19	3	C	1S		0.06852	0.05433	-0.08019	0.02961	-0.06361
20			2S	(I)	-0.07341	-0.05606	0.08149	-0.02749	0.06735
21			2PX	(I)	-0.02070	-0.10071	-0.09359	0.11602	-0.08509
22			2PY	(I)	0.01854	-0.14075	-0.00866	-0.12218	-0.01727
23			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
24			2S	(O)	-0.15310	-0.15205	0.24655	-0.10475	0.18537
25			2PX	(O)	-0.00480	-0.03096	-0.02814	0.07760	-0.08248
26			2PY	(O)	0.01369	-0.02119	-0.00013	-0.06772	0.02657
27			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
28	4	C	1S		0.00692	-0.11554	0.01031	-0.01388	0.05023
29			2S	(I)	-0.00605	0.11316	-0.00869	0.01717	-0.04825
30			2PX	(I)	0.03018	-0.07146	-0.05756	0.12447	0.14816
31			2PY	(I)	-0.08340	-0.01587	0.13357	0.06766	0.12829
32			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
33			2S	(O)	-0.03401	0.40866	-0.03259	0.03751	-0.19117
34			2PX	(O)	-0.00941	-0.01549	-0.02951	0.08527	0.13893
35			2PY	(O)	-0.02587	0.00440	0.05714	0.04224	0.11164
36			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
37	5	C	1S		0.08886	-0.08392	0.03311	0.02469	-0.05014
38			2S	(I)	-0.08948	0.08202	-0.03098	-0.02025	0.04958
39			2PX	(I)	0.00338	0.07784	0.06164	-0.15881	0.09256
40			2PY	(I)	0.01286	-0.00089	-0.16554	-0.10227	0.04449
41			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
42			2S	(O)	-0.26551	0.29890	-0.11580	-0.11042	0.19090
43			2PX	(O)	0.01193	0.02200	0.03196	-0.11566	0.09058
44			2PY	(O)	0.00815	-0.00452	-0.06369	-0.06978	0.06651
45			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
46	6	C	1S		-0.01491	0.02633	-0.10953	-0.01509	0.05992
47			2S	(I)	0.01717	-0.02708	0.11202	0.01963	-0.06248
48			2PX	(I)	-0.06282	0.07158	0.07697	-0.12920	-0.11907
49			2PY	(I)	-0.10170	0.10686	-0.00424	0.03900	0.06522
50			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
51			2S	(O)	0.02290	-0.07588	0.34170	0.02857	-0.18123
52			2PX	(O)	-0.00048	0.02300	0.02006	-0.07387	-0.10674
53			2PY	(O)	-0.02067	0.02245	0.00443	0.04928	0.06943
54			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
55	7	C	1S		-0.14670	-0.06066	-0.04491	-0.02120	-0.01195
56			2S	(I)	0.13615	0.05514	0.03993	0.01706	0.00686
57			2PX	(I)	0.00220	0.03783	-0.02569	0.02140	0.02169
58			2PY	(I)	0.01826	0.05491	0.07885	0.07101	0.14425
59			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
60			2S	(O)	0.45775	0.21495	0.16809	0.09119	0.09531
61			2PX	(O)	-0.00019	0.01966	-0.01527	0.01072	0.01534
62			2PY	(O)	-0.00300	0.01748	0.03169	0.04190	0.06670
63			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000

64	8	H	1S	(I)	0.07639	-0.04701	-0.07628	-0.14037	0.06980
65			1S	(O)	0.02321	-0.02056	-0.03793	-0.08255	0.02811
66	9	H	1S	(I)	0.00010	0.11126	-0.01255	-0.06560	-0.15832
67			1S	(O)	-0.00437	0.04661	-0.00756	-0.04388	-0.08878
68	10	H	1S	(I)	-0.03477	-0.03914	0.10376	-0.12522	0.10435
69			1S	(O)	-0.00756	-0.01831	0.06116	-0.08478	0.06080
70	11	H	1S	(I)	0.01245	-0.02005	0.12384	-0.07880	-0.14800
71			1S	(O)	0.00134	-0.01100	0.06977	-0.06018	-0.09511
72	12	H	1S	(I)	-0.04394	0.03965	-0.03497	-0.12312	0.10752
73			1S	(O)	-0.01187	0.03941	-0.01670	-0.07022	0.05564
74	13	H	1S	(I)	0.08930	0.03533	0.06450	0.02166	0.04289
75			1S	(O)	0.01586	0.00744	0.03555	0.00808	0.04025
76	14	H	1S	(I)	0.08935	0.05829	0.03524	0.03472	0.04407
77			1S	(O)	0.01670	0.02545	0.01598	0.02079	0.03986
78	15	H	1S	(I)	0.08995	0.05829	0.03524	0.03472	0.04407
79			1S	(O)	0.01670	0.02545	0.01598	0.02079	0.03986
					16	17	18	19	20
					(A')	(A")	(A')	(A')	(A')
	EIGENVALUES --				-0.62535	-0.59551	-0.59171	-0.55956	-0.53467
1	1	C	1S		-0.00890	0.00000	0.00342	0.00055	-0.00239
2			2S	(I)	0.00341	0.00000	-0.00698	-0.00028	0.00277
3			2PX	(I)	0.19303	0.00000	0.11249	0.02446	0.06274
4			2PY	(I)	0.01610	0.00000	0.08954	-0.20129	-0.09424
5			2PZ	(I)	0.00000	-0.21747	0.00000	0.00000	0.00000
6			2S	(O)	0.03888	0.00000	-0.00451	-0.02559	-0.01492
7			2PX	(O)	0.15493	0.00000	0.08587	0.02420	0.06514
8			2PY	(O)	0.01586	0.00000	0.07169	-0.16805	-0.08528
9			2PZ	(O)	0.00000	-0.18657	0.00000	0.00000	0.00000
10	2	C	1S		0.00549	0.00000	-0.01183	0.01622	0.00836
11			2S	(I)	-0.00146	0.00000	0.01491	-0.01733	-0.00422
12			2PX	(I)	0.18931	0.00000	0.11970	-0.02349	0.16266
13			2PY	(I)	0.00726	0.00000	0.08640	-0.24277	-0.08149
14			2PZ	(I)	0.00000	-0.06042	0.00000	0.00000	0.00000
15			2S	(O)	-0.02471	0.00000	0.03385	-0.03473	-0.02862
16			2PX	(O)	0.11862	0.00000	0.07154	-0.01570	0.11599
17			2PY	(O)	0.00803	0.00000	0.07345	-0.22547	-0.07998
18			2PZ	(O)	0.00000	-0.05521	0.00000	0.00000	0.00000
19	3	C	1S		-0.01256	0.00000	0.01249	-0.01567	0.01486
20			2S	(I)	0.01142	0.00000	-0.01711	0.01613	-0.01465
21			2PX	(I)	-0.09161	0.00000	-0.22034	0.02653	0.02354
22			2PY	(I)	-0.17324	0.00000	0.12885	0.00681	-0.11522
23			2PZ	(I)	0.00000	-0.07783	0.00000	0.00000	0.00000
24			2S	(O)	0.05848	0.00000	0.01363	0.04649	-0.05806
25			2PX	(O)	-0.03490	0.00000	-0.15275	0.01413	0.05248
26			2PY	(O)	-0.09382	0.00000	0.09970	0.01480	-0.06272
27			2PZ	(O)	0.00000	-0.05962	0.00000	0.00000	0.00000
28	4	C	1S		-0.00111	0.00000	0.01753	0.02227	-0.00134
29			2S	(I)	0.00672	0.00000	-0.01913	-0.02242	0.00411
30			2PX	(I)	-0.04179	0.00000	-0.14483	-0.13593	-0.14479
31			2PY	(I)	0.20467	0.00000	-0.09482	0.00443	0.10511
32			2PZ	(I)	0.00000	-0.07127	0.00000	0.00000	0.00000
33			2S	(O)	-0.01177	0.00000	-0.04664	-0.05586	0.02578
34			2PX	(O)	-0.02958	0.00000	-0.12839	-0.10071	-0.13181
35			2PY	(O)	0.12711	0.00000	-0.06715	0.00513	0.07159
36			2PZ	(O)	0.00000	-0.06195	0.00000	0.00000	0.00000
37	5	C	1S		0.02006	0.00000	-0.01648	-0.01523	-0.02203
38			2S	(I)	-0.02325	0.00000	0.01810	0.01804	0.01818
39			2PX	(I)	-0.04735	0.00000	-0.12289	-0.19835	-0.06066
40			2PY	(I)	0.20397	0.00000	-0.05731	-0.11096	0.11293
41			2PZ	(I)	0.00000	-0.11679	0.00000	0.00000	0.00000

42			2S	(O)	-0.07460	0.00000	0.03995	0.01846	0.07497
43			2PX	(O)	-0.02403	0.00000	-0.09980	-0.17420	-0.03491
44			2PY	(O)	0.11494	0.00000	-0.04831	-0.08502	0.08860
45			2PZ	(O)	0.00000	-0.10652	0.00000	0.00000	0.00000
46	6	C	1S		-0.00959	0.00000	-0.01171	0.00224	0.00807
47			2S	(I)	0.00924	0.00000	0.01540	-0.00320	-0.00933
48			2PX	(I)	-0.05734	0.00000	-0.21930	0.07265	-0.08157
49			2PY	(I)	-0.21115	0.00000	0.09144	0.10077	-0.08931
50			2PZ	(I)	0.00000	-0.04755	0.00000	0.00000	0.00000
51			2S	(O)	0.03639	0.00000	-0.00551	0.00495	-0.01971
52			2PX	(O)	-0.02062	0.00000	-0.15811	0.03811	-0.06554
53			2PY	(O)	-0.12418	0.00000	0.07165	0.06777	-0.03960
54			2PZ	(O)	0.00000	-0.03429	0.00000	0.00000	0.00000
55	7	C	1S		0.00436	0.00000	0.00406	-0.00057	0.00024
56			2S	(I)	-0.00387	0.00000	-0.00173	-0.00350	-0.00117
57			2PX	(I)	0.17005	0.00000	-0.00411	0.14151	-0.27371
58			2PY	(I)	-0.06243	0.00000	-0.07458	0.14768	0.10761
59			2PZ	(I)	0.00000	-0.30048	0.00000	0.00000	0.00000
60			2S	(O)	-0.02941	0.00000	-0.03378	0.03905	0.01856
61			2PX	(O)	0.12203	0.00000	-0.01129	0.11091	-0.25617
62			2PY	(O)	-0.03805	0.00000	-0.04662	0.09629	0.08215
63			2PZ	(O)	0.00000	-0.23879	0.00000	0.00000	0.00000
64	8	H	1S	(I)	-0.02019	0.00000	-0.04936	0.14956	0.03870
65			1S	(O)	-0.01371	0.00000	-0.03600	0.11042	0.02839
66	9	H	1S	(I)	-0.03275	0.00000	-0.09213	0.05851	0.05949
67			1S	(O)	-0.02629	0.00000	0.06623	0.05246	0.04191
68	10	H	1S	(I)	-0.00506	0.00000	0.16451	0.00214	-0.07450
69			1S	(O)	-0.00610	0.00000	0.13662	-0.00427	-0.05185
70	11	H	1S	(I)	0.05670	0.00000	-0.15055	0.00031	-0.02392
71			1S	(O)	0.04212	0.00000	-0.12362	0.00288	-0.01495
72	12	H	1S	(I)	0.01546	0.00000	-0.07029	-0.13649	0.01575
73			1S	(O)	0.01773	0.00000	-0.05319	-0.10220	0.00256
74	13	H	1S	(I)	-0.12482	0.00000	-0.02024	-0.04150	0.21863
75			1S	(O)	-0.10271	0.00000	-0.01403	-0.03599	0.19656
76	14	H	1S	(I)	0.04435	-0.17176	-0.02089	0.08361	-0.08511
77			1S	(O)	0.03715	-0.14863	-0.01877	0.07752	-0.07648
78	15	H	1S	(I)	0.04435	0.17176	-0.02089	0.08361	-0.08511
79			1S	(O)	0.03715	0.14863	-0.01877	0.07752	-0.07648
					21 (A")	22 (A')	23 (A')	24 (A")	25 (A")
	EIGENVALUES --				-0.52254	-0.50142	-0.46118	-0.42028	-0.38359
1	1	C	1S		0.00000	-0.00386	-0.00319	0.00000	0.00000
2			2S	(I)	0.00000	0.00065	0.00872	0.00000	0.00000
3			2PX	(I)	0.00000	0.14662	-0.19483	0.00000	0.00000
4			2PY	(I)	0.00000	0.20022	0.12345	0.00000	0.00000
5			2PZ	(I)	0.08477	0.00000	0.00000	-0.18323	-0.24727
6			2S	(O)	0.00000	0.01603	0.00409	0.00000	0.00000
7			2PX	(O)	0.00000	0.13569	-0.17281	0.00000	0.00000
8			2PY	(O)	0.00000	0.23707	0.16463	0.00000	0.00000
9			2PZ	(O)	0.09153	0.00000	0.00000	-0.20373	-0.30081
10	2	C	1S		0.00000	0.00266	0.00047	0.00000	0.00000
11			2S	(I)	0.00000	-0.00502	0.00522	0.00000	0.00000
12			2PX	(I)	0.00000	-0.11185	0.17058	0.00000	0.00000
13			2PY	(I)	0.00000	-0.13112	-0.09170	0.00000	0.00000
14			2PZ	(I)	0.24280	0.00000	0.00000	0.18184	0.25070
15			2S	(O)	0.00000	-0.00076	-0.01671	0.00000	0.00000
16			2PX	(O)	0.00000	-0.08420	0.12986	0.00000	0.00000
17			2PY	(O)	0.00000	-0.15306	-0.12274	0.00000	0.00000
18			2PZ	(O)	0.23882	0.00000	0.00000	0.20156	0.30838
19	3	C	1S		0.00000	0.00649	-0.01115	0.00000	0.00000

20			2S	(I)	0.00000	-0.00778	0.01093	0.00000	0.00000
21			2PX	(I)	0.00000	-0.13453	0.14546	0.00000	0.00000
22			2PY	(I)	0.00000	-0.18401	-0.08264	0.00000	0.00000
23			2PZ	(I)	0.09818	0.00000	0.00000	0.02845	-0.19064
24			2S	(O)	0.00000	0.00507	0.04026	0.00000	0.00000
25			2PX	(O)	0.00000	-0.06915	0.17965	0.00000	0.00000
26			2PY	(O)	0.00000	-0.12377	-0.14220	0.00000	0.00000
27			2PZ	(O)	0.08051	0.00000	0.00000	0.02646	-0.19078
28	4	C	1S		0.00000	-0.00835	0.00152	0.00000	0.00000
29			2S	(I)	0.00000	0.01174	0.00524	0.00000	0.00000
30			2PX	(I)	0.00000	0.10438	-0.14917	0.00000	0.00000
31			2PY	(I)	0.00000	0.18277	0.12315	0.00000	0.00000
32			2PZ	(I)	0.22628	0.00000	0.00000	0.25931	-0.17438
33			2S	(O)	0.00000	0.01162	-0.03750	0.00000	0.00000
34			2PX	(O)	0.00000	0.13317	-0.16313	0.00000	0.00000
35			2PY	(O)	0.00000	0.15622	0.05950	0.00000	0.00000
36			2PZ	(O)	0.22370	0.00000	0.00000	0.29066	-0.21892
37	5	C	1S		0.00000	-0.00518	0.00697	0.00000	0.00000
38			2S	(I)	0.00000	0.00685	-0.00076	0.00000	0.00000
39			2PX	(I)	0.00000	-0.08474	0.17605	0.00000	0.00000
40			2PY	(I)	0.00000	-0.14584	-0.15239	0.00000	0.00000
41			2PZ	(I)	0.16812	0.00000	0.00000	-0.31872	0.12723
42			2S	(O)	0.00000	0.02055	-0.03099	0.00000	0.00000
43			2PX	(O)	0.00000	-0.12552	0.17928	0.00000	0.00000
44			2PY	(O)	0.00000	-0.15734	-0.09333	0.00000	0.00000
45			2PZ	(O)	0.16468	0.00000	0.00000	-0.36012	0.16494
46	6	C	1S		0.00000	0.00028	-0.00965	0.00000	0.00000
47			2S	(I)	0.00000	0.00084	0.00977	0.00000	0.00000
48			2PX	(I)	0.00000	0.10296	-0.13920	0.00000	0.00000
49			2PY	(I)	0.00000	0.14990	0.11040	0.00000	0.00000
50			2PZ	(I)	0.12909	0.00000	0.00000	-0.05352	0.17065
51			2S	(O)	0.00000	-0.01999	0.02980	0.00000	0.00000
52			2PX	(O)	0.00000	0.06833	-0.18102	0.00000	0.00000
53			2PY	(O)	0.00000	0.08351	0.13354	0.00000	0.00000
54			2PZ	(O)	0.10928	0.00000	0.00000	-0.05142	0.16800
55	7	C	1S		0.00000	-0.01607	-0.01204	0.00000	0.00000
56			2S	(I)	0.00000	0.01942	0.01316	0.00000	0.00000
57			2PX	(I)	0.00000	-0.09935	0.05822	0.00000	0.00000
58			2PY	(I)	0.00000	-0.18559	-0.11253	0.00000	0.00000
59			2PZ	(I)	-0.17771	0.00000	0.00000	0.03368	0.07491
60			2S	(O)	0.00000	0.00102	0.01280	0.00000	0.00000
61			2PX	(O)	0.00000	-0.09535	0.07582	0.00000	0.00000
62			2PY	(O)	0.00000	-0.11301	-0.07634	0.00000	0.00000
63			2PZ	(O)	-0.16068	0.00000	0.00000	0.09510	0.06759
64	8	H	1S	(I)	0.00000	0.10296	0.06333	0.00000	0.00000
65			1S	(O)	0.00000	0.07629	0.04629	0.00000	0.00000
66	9	H	1S	(I)	0.00000	-0.12271	0.06273	0.00000	0.00000
67			1S	(O)	0.00000	-0.09475	0.04457	0.00000	0.00000
68	10	H	1S	(I)	0.00000	0.00026	-0.13915	0.00000	0.00000
69			1S	(O)	0.00000	0.00763	-0.12314	0.00000	0.00000
70	11	H	1S	(I)	0.00000	0.00135	-0.14642	0.00000	0.00000
71			1S	(O)	0.00000	-0.00059	-0.12800	0.00000	0.00000
72	12	H	1S	(I)	0.00000	-0.10386	0.06602	0.00000	0.00000
73			1S	(O)	0.00000	-0.07658	0.05249	0.00000	0.00000
74	13	H	1S	(I)	0.00000	0.01686	-0.03156	0.00000	0.00000
75			1S	(O)	0.00000	0.00435	-0.09816	0.00000	0.00000
76	14	H	1S	(I)	-0.11428	-0.06857	0.01272	0.07061	0.06703
77			1S	(O)	-0.11127	-0.08110	0.00691	0.07771	0.09733
78	15	H	1S	(I)	0.11428	-0.06857	0.01272	-0.07061	-0.06703
79			1S	(O)	0.11127	-0.08110	0.00691	-0.07771	-0.09733

				26	27	28	29	30
				(A")	(A")	(A")	(A")	(A")
	EIGENVALUES --			-0.22300	0.19084	0.26471	0.29072	0.29757
1	1	C	1S	0.00000	0.00000	-0.02345	0.00000	0.00752
2			2S (I)	0.00000	0.00000	0.00862	0.00000	-0.00652
3			2PX (I)	0.00000	0.00000	-0.01719	0.00000	-0.00595
4			2PY (I)	0.00000	0.00000	0.03396	0.00000	-0.00401
5			2PZ (I)	-0.28939	0.12744	0.00000	0.17285	0.00000
6			2S (O)	0.00000	0.00000	0.36182	0.00000	0.19861
7			2PX (O)	0.00000	0.00000	0.02474	0.00000	-0.03103
8			2PY (O)	0.00000	0.00000	0.03224	0.00000	-0.34879
9			2PZ (O)	-0.43834	0.29801	0.00000	0.33346	0.00000
10	2	C	1S	0.00000	0.00000	-0.04718	0.00000	0.00987
11			2S (I)	0.00000	0.00000	0.02557	0.00000	0.00896
12			2PX (I)	0.00000	0.00000	-0.00291	0.00000	-0.01352
13			2PY (I)	0.00000	0.00000	-0.08878	0.00000	0.08283
14			2PZ (I)	-0.26227	0.12181	0.00000	0.17830	0.00000
15			2S (O)	0.00000	0.00000	0.55135	0.00000	-0.37998
16			2PX (O)	0.00000	0.00000	-0.03581	0.00000	-0.06621
17			2PY (O)	0.00000	0.00000	-0.39276	0.00000	0.18317
18			2PZ (O)	-0.41088	0.29781	0.00000	0.44777	0.00000
19	3	C	1S	0.00000	0.00000	-0.03986	0.00000	-0.02107
20			2S (I)	0.00000	0.00000	0.02459	0.00000	0.02196
21			2PX (I)	0.00000	0.00000	-0.07828	0.00000	-0.02246
22			2PY (I)	0.00000	0.00000	0.05556	0.00000	0.02327
23			2PZ (I)	-0.01363	-0.25864	0.00000	-0.23852	0.00000
24			2S (O)	0.00000	0.00000	0.44478	0.00000	0.12113
25			2PX (O)	0.00000	0.00000	-0.37129	0.00000	-0.40064
26			2PY (O)	0.00000	0.00000	0.27268	0.00000	0.02237
27			2PZ (O)	-0.02209	-0.63956	0.00000	-0.62064	0.00000
28	4	C	1S	0.00000	0.00000	-0.04383	0.00000	0.04565
29			2S (I)	0.00000	0.00000	0.01466	0.00000	-0.02749
30			2PX (I)	0.00000	0.00000	-0.07918	0.00000	0.03421
31			2PY (I)	0.00000	0.00000	-0.04432	0.00000	0.00567
32			2PZ (I)	0.27723	0.10616	0.00000	0.18662	0.00000
33			2S (O)	0.00000	0.00000	0.63543	0.00000	-0.53737
34			2PX (O)	0.00000	0.00000	-0.24963	0.00000	0.31481
35			2PY (O)	0.00000	0.00000	-0.12410	0.00000	0.07235
36			2PZ (O)	0.43377	0.26450	0.00000	0.44966	0.00000
37	5	C	1S	0.00000	0.00000	-0.05995	0.00000	-0.01192
38			2S (I)	0.00000	0.00000	0.03816	0.00000	0.02171
39			2PX (I)	0.00000	0.00000	0.06309	0.00000	0.00481
40			2PY (I)	0.00000	0.00000	0.04708	0.00000	0.03881
41			2PZ (I)	0.26283	0.11554	0.00000	-0.14987	0.00000
42			2S (O)	0.00000	0.00000	0.64847	0.00000	0.05828
43			2PX (O)	0.00000	0.00000	0.37293	0.00000	0.29889
44			2PY (O)	0.00000	0.00000	0.16533	0.00000	-0.03967
45			2PZ (O)	0.41953	0.28021	0.00000	-0.40660	0.00000
46	6	C	1S	0.00000	0.00000	-0.02674	0.00000	0.03555
47			2S (I)	0.00000	0.00000	0.00635	0.00000	-0.02362
48			2PX (I)	0.00000	0.00000	0.07286	0.00000	-0.05312
49			2PY (I)	0.00000	0.00000	-0.06945	0.00000	0.00964
50			2PZ (I)	-0.00411	-0.27042	0.00000	0.22414	0.00000
51			2S (O)	0.00000	0.00000	0.42750	0.00000	-0.38802
52			2PX (O)	0.00000	0.00000	0.19175	0.00000	-0.38766
53			2PY (O)	0.00000	0.00000	-0.19923	0.00000	0.08194
54			2PZ (O)	-0.00945	-0.66366	0.00000	0.62401	0.00000
55	7	C	1S	0.00000	0.00000	-0.02004	0.00000	-0.14634
56			2S (I)	0.00000	0.00000	-0.00063	0.00000	0.03357
57			2PX (I)	0.00000	0.00000	-0.01459	0.00000	0.00260

58			2PY	(I)	0.00000	0.00000	0.10149	0.00000	0.03334
59			2PZ	(I)	0.03286	-0.00623	0.00000	0.10959	0.00000
60			2S	(O)	0.00000	0.00000	0.38333	0.00000	2.11384
61			2PX	(O)	0.00000	0.00000	-0.13416	0.00000	0.00853
62			2PY	(O)	0.00000	0.00000	0.42913	0.00000	0.42730
63			2PZ	(O)	0.01496	-0.04429	0.00000	0.49613	0.00000
64	8	H	1S	(I)	0.00000	0.00000	-0.04732	0.00000	0.00410
65			1S	(O)	0.00000	0.00000	-0.83130	0.00000	0.41181
66	9	H	1S	(I)	0.00000	0.00000	-0.04021	0.00000	0.01973
67			1S	(O)	0.00000	0.00000	-0.74754	0.00000	0.59064
68	10	H	1S	(I)	0.00000	0.00000	-0.02721	0.00000	0.02936
69			1S	(O)	0.00000	0.00000	-0.78630	0.00000	-0.33285
70	11	H	1S	(I)	0.00000	0.00000	-0.02682	0.00000	0.02261
71			1S	(O)	0.00000	0.00000	-0.62518	0.00000	0.60045
72	12	H	1S	(I)	0.00000	0.00000	-0.03605	0.00000	0.03983
73			1S	(O)	0.00000	0.00000	-0.85323	0.00000	-0.20899
74	13	H	1S	(I)	0.00000	0.00000	-0.01420	0.00000	-0.00459
75			1S	(O)	0.00000	0.00000	-0.49604	0.00000	-1.01771
76	14	H	1S	(I)	0.05348	-0.02618	0.00656	-0.04394	0.00051
77			1S	(O)	0.12200	-0.02765	-0.17931	-0.57918	-0.92807
78	15	H	1S	(I)	-0.05348	0.02618	-0.00656	0.04394	0.00051
79			1S	(O)	-0.12200	0.02765	-0.17931	0.57918	-0.92807

31
(A')

EIGENVALUES --					0.30969
1	1	C	1S		0.01236
2			2S	(I)	-0.02417
3			2PX	(I)	-0.07339
4			2PY	(I)	0.05300
5			2PZ	(I)	0.00000
6			2S	(O)	-0.00976
7			2PX	(O)	-0.12486
8			2PY	(O)	0.05917
9			2PZ	(O)	0.00000
10	2	C	1S		0.01561
11			2S	(I)	-0.00067
12			2PX	(I)	-0.03755
13			2PY	(I)	0.05434
14			2PZ	(I)	0.00000
15			2S	(O)	-0.31198
16			2PX	(O)	-0.03219
17			2PY	(O)	0.13682
18			2PZ	(O)	0.00000
19	3	C	1S		-0.01550
20			2S	(I)	-0.00610
21			2PX	(I)	-0.14133
22			2PY	(I)	0.06323
23			2PZ	(I)	0.00000
24			2S	(O)	0.34829
25			2PX	(O)	-0.51777
26			2PY	(O)	0.35363
27			2PZ	(O)	0.00000
28	4	C	1S		-0.02611
29			2S	(I)	0.00115
30			2PX	(I)	-0.08868
31			2PY	(I)	-0.00423
32			2PZ	(I)	0.00000
33			2S	(O)	0.50183
34			2PX	(O)	-0.22435
35			2PY	(O)	-0.04022

36			2PZ	(O)	0.00000
37	5	C	1S		-0.01007
38			2S	(I)	0.01168
39			2PX	(I)	-0.13951
40			2PY	(I)	0.01358
41			2PZ	(I)	0.00000
42			2S	(O)	-0.08564
43			2PX	(O)	-0.38173
44			2PY	(O)	-0.05492
45			2PZ	(O)	0.00000
46	6	C	1S		0.03892
47			2S	(I)	-0.01317
48			2PX	(I)	-0.11475
49			2PY	(I)	0.04664
50			2PZ	(I)	0.00000
51			2S	(O)	-0.58132
52			2PX	(O)	-0.45771
53			2PY	(O)	0.18938
54			2PZ	(O)	0.00000
55	7	C	1S		0.03322
56			2S	(I)	-0.00973
57			2PX	(I)	-0.16512
58			2PY	(I)	0.00999
59			2PZ	(I)	0.00000
60			2S	(O)	-0.44053
61			2PX	(O)	-0.75014
62			2PY	(O)	0.03717
63			2PZ	(O)	0.00000
64	8	H	1S	(I)	0.00888
65			1S	(O)	0.33571
66	9	H	1S	(I)	-0.01944
67			1S	(O)	-0.56050
68	10	H	1S	(I)	-0.02139
69			1S	(O)	-0.92803
70	11	H	1S	(I)	0.03217
71			1S	(O)	0.92001
72	12	H	1S	(I)	0.00962
73			1S	(O)	0.53387
74	13	H	1S	(I)	-0.03787
75			1S	(O)	-0.72372
76	14	H	1S	(I)	0.01534
77			1S	(O)	0.66139
78	15	H	1S	(I)	0.01534
79			1S	(O)	0.66139

BETA MOLECULAR ORBITAL COEFFICIENTS.

					1 (A")	2 (A")	3 (A")	4 (A")	5 (A")
	EIGENVALUES --				-11.17801	-11.17466	-11.17027	-11.16434	-11.16426
1	1	C	1S		0.00412	-0.04831	-0.98581	-0.01601	0.01008
2			2S	(I)	-0.00040	-0.00891	-0.09896	-0.00020	0.00007
3			2PX	(I)	0.00040	0.00151	0.00002	-0.00013	-0.00010
4			2PY	(I)	-0.00043	0.00167	0.00026	0.00100	0.00034
5			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
6			2S	(O)	0.01357	0.03853	0.08872	-0.01368	0.01097
7			2PX	(O)	0.00056	-0.01699	-0.00457	0.00068	-0.00196
8			2PY	(O)	-0.00875	-0.02450	-0.00727	-0.02064	-0.00594
9			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
10	2	C	1S		0.01652	-0.00351	0.01086	0.14616	0.97053
11			2S	(I)	0.00600	0.00030	0.00187	0.01463	0.09684
12			2PX	(I)	0.00105	0.00062	-0.00012	-0.00005	0.00008

13			2PY (I)	0.00132	-0.00053	0.00031	0.00028	0.00130
14			2PZ (I)	0.00000	0.00000	0.00000	0.00000	0.00000
15			2S (O)	-0.03666	-0.01281	-0.00930	-0.01271	-0.08590
16			2PX (O)	-0.01207	-0.00098	-0.00028	-0.00140	-0.00373
17			2PY (O)	-0.02008	-0.00940	-0.00557	-0.00242	-0.02245
18			2PZ (O)	0.00000	0.00000	0.00000	0.00000	0.00000
19	3	C	1S	0.02087	0.98558	-0.04694	-0.00913	0.00353
20			2S (I)	0.00307	0.10055	-0.00064	-0.00024	0.00106
21			2PX (I)	0.00030	0.00109	0.00155	0.00018	-0.00002
22			2PY (I)	-0.00021	-0.00080	0.00055	0.00074	0.00063
23			2PZ (I)	0.00000	0.00000	0.00000	0.00000	0.00000
24			2S (O)	-0.01354	-0.09862	-0.02771	-0.00257	-0.01647
25			2PX (O)	-0.00684	-0.02353	-0.01872	-0.00336	-0.00862
26			2PY (O)	0.00592	0.01315	-0.00508	0.00161	0.00601
27			2PZ (O)	0.00000	0.00000	0.00000	0.00000	0.00000
28	4	C	1S	0.00192	-0.01759	0.00692	0.00931	-0.09026
29			2S (I)	-0.00054	-0.00613	0.00086	0.00109	-0.01225
30			2PX (I)	0.00072	-0.00090	0.00016	0.00014	-0.00069
31			2PY (I)	-0.00044	-0.00132	0.00083	0.00031	-0.00041
32			2PZ (I)	0.00000	0.00000	0.00000	0.00000	0.00000
33			2S (O)	0.01357	0.03726	0.00409	0.00240	0.03518
34			2PX (O)	0.00782	0.01521	0.00618	0.00121	0.02100
35			2PY (O)	0.00543	0.01839	-0.00054	-0.00106	0.00242
36			2PZ (O)	0.00000	0.00000	0.00000	0.00000	0.00000
37	5	C	1S	0.01607	-0.00383	0.03140	0.07732	-0.07618
38			2S (I)	0.00601	0.00010	0.00581	0.00827	-0.00758
39			2PX (I)	-0.00077	0.00066	-0.00044	-0.00031	0.00035
40			2PY (I)	-0.00154	-0.00032	-0.00009	0.00092	0.00094
41			2PZ (I)	0.00000	0.00000	0.00000	0.00000	0.00000
42			2S (O)	-0.03758	-0.01152	-0.02442	-0.00815	-0.00492
43			2PX (O)	0.01425	0.00822	0.01439	0.00557	0.00633
44			2PY (O)	0.01806	0.00646	-0.00227	-0.00227	0.00268
45			2PZ (O)	0.00000	0.00000	0.00000	0.00000	0.00000
46	6	C	1S	-0.98661	0.02005	-0.00468	-0.00124	0.01478
47			2S (I)	-0.10029	0.00099	-0.00084	-0.00039	-0.00276
48			2PX (I)	0.00111	0.00019	-0.00001	0.00021	0.00160
49			2PY (I)	-0.00074	-0.00011	0.00060	0.00027	0.00026
50			2PZ (I)	0.00000	0.00000	0.00000	0.00000	0.00000
51			2S (O)	0.09364	0.01253	0.00934	0.00467	0.03407
52			2PX (O)	-0.02066	-0.00708	-0.00649	-0.00389	-0.02265
53			2PY (O)	0.01374	0.00544	0.00280	-0.00169	0.00138
54			2PZ (O)	0.00000	0.00000	0.00000	0.00000	0.00000
55	7	C	1S	0.00477	-0.00969	0.02118	-0.97340	0.13854
56			2S (I)	0.00113	-0.00188	0.00398	-0.10095	0.01414
57			2PX (I)	0.00021	0.00017	-0.00044	-0.00023	0.00001
58			2PY (I)	-0.00034	-0.00003	-0.00047	-0.00006	-0.00015
59			2PZ (I)	0.00000	0.00000	0.00000	0.00000	0.00000
60			2S (O)	0.00042	0.00941	-0.01543	0.08550	-0.00841
61			2PX (O)	-0.00183	0.00166	0.00400	-0.00064	0.00007
62			2PY (O)	0.00054	-0.00403	0.00949	-0.00696	-0.00059
63			2PZ (O)	0.00000	0.00000	0.00000	0.00000	0.00000
64	8	H	1S (I)	-0.00010	-0.00057	-0.00012	-0.00021	-0.00240
65			1S (O)	-0.00512	-0.00170	-0.00144	0.00112	0.00623
66	9	H	1S (I)	0.00052	0.00018	0.00053	-0.00008	0.00033
67			1S (O)	0.00164	0.00532	0.00083	-0.00023	0.00432
68	10	H	1S (I)	-0.00041	-0.00244	0.00070	-0.00032	-0.00050
69			1S (O)	-0.00214	0.00560	-0.00311	-0.00058	-0.00188
70	11	H	1S (I)	0.00246	0.00026	0.00047	0.00002	-0.00003
71			1S (O)	-0.00601	0.00257	0.00109	0.00023	0.00521
72	12	H	1S (I)	-0.00009	-0.00066	0.00023	-0.00012	-0.00040

					6 (A')	7 (A')	8 (A')	9 (A')	10 (A')
73			1S	(O)	-0.00477	-0.00240	-0.00205	-0.00054	-0.00177
74	13	H	1S	(I)	-0.00013	-0.00002	0.00093	-0.00027	-0.00002
75			1S	(O)	-0.00086	0.00011	0.00159	-0.01416	0.00190
76	14	H	1S	(I)	0.00026	-0.00034	0.00110	-0.00041	-0.00006
77			1S	(O)	0.00028	-0.00047	-0.00220	-0.01427	0.00196
78	15	H	1S	(I)	0.00026	-0.00034	0.00110	-0.00041	-0.00006
79			1S	(O)	0.00028	-0.00047	-0.00220	-0.01427	0.00196
	EIGENVALUES	--			-11.16324	-11.16138	-1.11195	-1.03079	-0.98627
1	1	C	1S		0.03211	-0.00920	-0.09677	0.08280	-0.05164
2			2S	(I)	0.00016	-0.00084	0.10773	-0.09274	0.05477
3			2PX	(I)	-0.00022	-0.00071	-0.02666	0.05844	0.07200
4			2PY	(I)	0.00098	-0.00075	-0.03784	-0.02871	0.08551
5			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
6			2S	(O)	0.02541	0.01001	0.15151	-0.11794	0.11045
7			2PX	(O)	0.00885	-0.00085	0.01359	-0.00270	0.01628
8			2PY	(O)	-0.02245	-0.00501	0.00662	-0.02557	-0.01484
9			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
10	2	C	1S		0.05926	-0.09000	-0.07814	-0.07882	0.02554
11			2S	(I)	0.00607	-0.00570	0.08789	0.08956	-0.02698
12			2PX	(I)	-0.00089	0.00016	0.02543	0.07254	0.04788
13			2PY	(I)	-0.00055	0.00060	0.04944	0.02654	-0.01377
14			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
15			2S	(O)	-0.01771	-0.01941	0.12721	0.11261	-0.06487
16			2PX	(O)	0.00041	0.00665	-0.00451	-0.00088	0.00575
17			2PY	(O)	-0.01038	-0.01623	0.01018	-0.02111	-0.01382
18			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
19	3	C	1S		0.00548	-0.01780	-0.11738	0.10400	-0.09973
20			2S	(I)	0.00089	0.00274	0.12803	-0.10947	-0.10494
21			2PX	(I)	-0.00089	0.00049	0.04902	-0.02693	0.02272
22			2PY	(I)	-0.00041	-0.00174	-0.02285	-0.01833	0.08184
23			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
24			2S	(O)	-0.01490	-0.03395	0.29077	-0.29762	-0.28062
25			2PX	(O)	-0.00742	-0.00935	0.02750	-0.03085	-0.00890
26			2PY	(O)	0.00971	0.01907	-0.01667	0.01356	0.03871
27			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
28	4	C	1S		-0.05514	-0.98168	-0.07926	0.02350	0.10250
29			2S	(I)	-0.00681	-0.09730	0.09004	-0.02892	-0.11218
30			2PX	(I)	-0.00051	-0.00110	0.03643	0.02150	-0.00636
31			2PY	(I)	-0.00011	-0.00041	0.04416	-0.05995	-0.05719
32			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
33			2S	(O)	0.01854	0.08137	0.11694	-0.00740	-0.19136
34			2PX	(O)	0.00889	0.01608	0.00238	0.02585	-0.00279
35			2PY	(O)	0.00515	0.01152	-0.00521	0.01142	-0.00076
36			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
37	5	C	1S		0.97990	-0.04663	-0.03298	-0.05177	-0.06348
38			2S	(I)	0.09764	-0.00365	0.09353	0.05948	0.07080
39			2PX	(I)	-0.00109	-0.00042	-0.03836	0.01480	-0.00148
40			2PY	(I)	-0.00054	-0.00012	-0.03640	-0.09173	-0.00043
41			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
42			2S	(O)	-0.08769	-0.00488	0.13582	0.05722	0.11680
43			2PX	(O)	0.02001	0.00468	-0.01109	0.02126	0.00977
44			2PY	(O)	0.01267	0.00275	-0.00707	0.01260	0.00432
45			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
46	6	C	1S		0.01655	-0.00499	-0.10892	-0.14401	-0.04363
47			2S	(I)	-0.00321	-0.00021	0.12016	0.15151	0.04652
48			2PX	(I)	0.00057	-0.00107	-0.04368	-0.03315	0.02186
49			2PY	(I)	-0.00163	-0.00022	0.03054	0.00905	0.03353
50			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000

					11 (A')	12 (A')	13 (A')	14 (A')	15 (A')
			EIGENVALUES --		-0.89425	-0.79817	-0.77408	-0.68353	-0.62428
1	1	C	1S		-0.05730	-0.02291	0.10524	-0.01881	0.07931
2			2S	(I)	0.06194	0.02635	-0.10929	0.01605	-0.08336
3			2PX	(I)	-0.00008	-0.16188	-0.02410	0.00999	0.03012
4			2PY	(I)	-0.09945	0.00678	0.05350	0.08231	-0.05189
5			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
6			2S	(O)	0.13782	0.04534	-0.30946	0.07107	-0.22418
7			2PX	(O)	0.01281	-0.06933	-0.01789	0.00799	0.01453
8			2PY	(O)	-0.01521	0.00939	0.03312	0.04222	-0.09048
9			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
10	2	C	1S		0.12150	-0.01491	0.09005	-0.03294	-0.05567
11			2S	(I)	-0.13056	0.01773	-0.09423	0.03122	0.06193
12			2PX	(I)	0.01265	0.14862	0.03307	-0.03484	0.03616
13			2PY	(I)	0.00553	-0.02513	0.02823	-0.20179	-0.02632
14			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
15			2S	(O)	-0.28671	0.02393	-0.26592	0.11711	0.13579
16			2PX	(O)	0.01177	0.05652	0.01313	-0.01634	0.02146
17			2PY	(O)	-0.00310	-0.01700	0.00206	-0.12852	-0.07138
18			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
19	3	C	1S		-0.04131	-0.06719	-0.04643	-0.01487	-0.04827
20			2S	(I)	0.04317	0.06922	0.04550	0.01120	0.05062
21			2PX	(I)	0.05019	0.03888	-0.16675	-0.10949	-0.14178
22			2PY	(I)	0.05313	0.15752	-0.07682	0.13267	-0.00871
23			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
24			2S	(O)	0.13019	0.22501	0.16666	0.06508	0.14802
25			2PX	(O)	0.02936	0.01962	-0.07957	-0.09042	-0.14072
26			2PY	(O)	0.01369	0.06592	-0.02941	0.09003	0.04509
27			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
28	4	C	1S		0.07231	0.11362	-0.03599	0.01123	0.05443
51			2S	(O)	-0.03888	0.00823	-0.25111	-0.40798	-0.12380
52			2PX	(O)	-0.01282	-0.00411	-0.01691	-0.03794	-0.00075
53			2PY	(O)	0.02143	0.00451	0.00743	0.02731	0.00989
54			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
55	7	C	1S		0.08538	-0.02624	-0.04598	0.09096	-0.14507
56			2S	(I)	0.00784	-0.00191	0.04659	-0.08743	0.13733
57			2PX	(I)	-0.00015	-0.00014	-0.00507	0.01131	0.00726
58			2PY	(I)	0.00007	-0.00029	-0.02775	0.02887	-0.02194
59			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
60			2S	(O)	0.00182	0.00120	0.10915	-0.24996	0.44337
61			2PX	(O)	-0.00235	0.00085	-0.00187	-0.00040	0.00559
62			2PY	(O)	-0.00401	0.00110	0.00195	0.00801	-0.01739
63			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
64	8	H	1S	(I)	-0.00069	0.00014	0.03031	0.03821	-0.01417
65			1S	(O)	-0.00090	-0.00550	-0.00043	-0.00013	-0.00659
66	9	H	1S	(I)	0.00032	0.00243	0.03036	-0.01153	-0.05712
67			1S	(O)	0.00219	-0.00726	-0.00337	0.00584	-0.01540
68	10	H	1S	(I)	-0.00074	0.00019	0.04547	-0.05574	-0.04954
69			1S	(O)	-0.00238	-0.00482	0.00165	-0.01636	-0.00976
70	11	H	1S	(I)	-0.00001	0.00053	0.04106	0.07113	0.02635
71			1S	(O)	0.00606	0.00054	-0.00346	0.01694	0.00590
72	12	H	1S	(I)	-0.00253	-0.00005	0.03368	0.02133	0.04404
73			1S	(O)	0.00623	-0.00231	0.00256	-0.00574	0.01205
74	13	H	1S	(I)	-0.00051	0.00038	0.02084	-0.04830	0.07424
75			1S	(O)	0.00105	-0.00072	-0.00233	-0.00538	0.00504
76	14	H	1S	(I)	-0.00028	0.00008	0.02026	-0.04263	0.07828
77			1S	(O)	0.00164	-0.00056	-0.00519	0.00369	0.00403
78	15	H	1S	(I)	-0.00028	0.00008	0.02026	-0.04263	0.07828
79			1S	(O)	0.00164	-0.00056	-0.00519	0.00369	0.00403

29			2S	(I)	-0.07746	-0.11902	0.03911	-0.01546	-0.05804
30			2PX	(I)	-0.02537	0.02684	-0.10256	-0.10636	0.11588
31			2PY	(I)	0.06292	0.04628	0.10180	-0.08710	0.10930
32			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
33			2S	(O)	-0.17681	-0.32218	0.09039	-0.01643	-0.14397
34			2PX	(O)	-0.01190	0.00250	-0.05124	-0.05976	0.12817
35			2PY	(O)	0.01908	0.01564	0.03778	-0.04822	0.08986
36			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
37	5	C	1S		-0.11044	0.09962	0.00239	-0.02954	-0.05111
38			2S	(I)	0.11875	-0.10438	-0.00133	0.02762	0.05582
39			2PX	(I)	-0.00919	-0.02671	0.10395	0.13497	0.08084
40			2PY	(I)	-0.01047	-0.05269	-0.12501	0.11710	0.03248
41			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
42			2S	(O)	0.25626	-0.28410	-0.02143	0.10496	0.12827
43			2PX	(O)	-0.01297	-0.00465	0.05046	0.09149	0.10182
44			2PY	(O)	-0.00149	-0.01742	-0.03997	0.06563	0.05109
45			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
46	6	C	1S		-0.00253	-0.06432	-0.07173	0.01952	0.04109
47			2S	(I)	0.00213	0.06576	0.07224	-0.02552	-0.04253
48			2PX	(I)	0.08326	-0.02460	0.13967	0.12982	-0.15904
49			2PY	(I)	0.12871	-0.13428	0.04195	-0.10003	0.06723
50			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
51			2S	(O)	0.00829	0.22071	0.25708	-0.04908	-0.12441
52			2PX	(O)	0.02957	-0.01466	0.06921	0.08885	-0.16150
53			2PY	(O)	0.05411	-0.05703	0.02025	-0.06762	0.09067
54			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
55	7	C	1S		0.09935	0.01128	-0.04711	0.02295	-0.00756
56			2S	(I)	-0.09301	-0.00957	0.04402	-0.01874	0.00361
57			2PX	(I)	-0.00104	-0.04965	-0.00314	-0.00919	0.03695
58			2PY	(I)	-0.03960	-0.01286	0.03398	-0.09070	0.13917
59			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
60			2S	(O)	-0.32510	-0.04289	0.16679	-0.09267	0.06421
61			2PX	(O)	-0.00326	-0.03133	-0.00376	-0.00358	0.02512
62			2PY	(O)	-0.01001	-0.00369	0.04887	-0.05891	0.07492
63			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
64	8	H	1S	(I)	-0.09563	0.01839	-0.09575	0.15812	0.07626
65			1S	(O)	-0.04155	0.00776	-0.05666	0.11206	0.03786
66	9	H	1S	(I)	-0.05825	-0.11983	0.05554	0.07120	-0.16273
67			1S	(O)	-0.02528	-0.06770	0.03000	0.05734	-0.10958
68	10	H	1S	(I)	0.02197	0.07730	0.08344	0.10563	0.11619
69			1S	(O)	0.00651	0.03653	0.04472	0.06155	0.06031
70	11	H	1S	(I)	0.00034	0.07407	0.10099	0.07512	-0.14445
71			1S	(O)	0.00180	0.03512	0.04926	0.05111	-0.07996
72	12	H	1S	(I)	0.07745	-0.11053	0.01691	0.13593	0.11594
73			1S	(O)	0.03296	-0.06311	0.01035	0.09501	0.07310
74	13	H	1S	(I)	-0.06909	0.01369	0.05972	-0.03582	0.02983
75			1S	(O)	-0.01892	0.01039	0.03132	-0.01850	0.03102
76	14	H	1S	(I)	-0.06323	-0.02281	0.04387	-0.03348	0.04234
77			1S	(O)	-0.01429	-0.01255	0.02254	-0.01959	0.03959
78	15	H	1S	(I)	-0.06323	-0.02281	0.04387	-0.03348	0.04234
79			1S	(O)	-0.01429	-0.01255	0.02254	-0.01959	0.03959
					16	17	18	19	20
					(A')	(A')	(A')	(A')	(A')
	EIGENVALUES --				-0.61726	-0.59272	-0.55982	-0.54586	-0.52598
1	1	C	1S		0.01567	0.01186	0.00000	-0.00055	-0.00807
2			2S	(I)	-0.01312	-0.00918	0.00000	0.00083	0.00889
3			2PX	(I)	-0.16758	-0.11893	0.00000	0.00792	0.03089
4			2PY	(I)	-0.00826	-0.10536	0.00000	-0.14742	-0.13887
5			2PZ	(I)	0.00000	0.00000	0.07707	0.00000	0.00000
6			2S	(O)	-0.05334	-0.06459	0.00000	-0.00226	0.01883

7			2PX	(O)	-0.12134	-0.08269	0.00000	0.00511	0.08358
8			2PY	(O)	-0.02018	-0.06721	0.00000	-0.11013	-0.11575
9			2PZ	(O)	0.00000	0.00000	0.04460	0.00000	0.00000
10	2	C	1S		-0.01242	0.00248	0.00000	0.01409	0.01822
11			2S	(I)	0.01113	-0.00447	0.00000	-0.01585	-0.01660
12			2PX	(I)	-0.16186	-0.12159	0.00000	-0.06256	0.15836
13			2PY	(I)	-0.00560	-0.09897	0.00000	-0.19625	-0.15085
14			2PZ	(I)	0.00000	0.00000	0.00884	0.00000	0.00000
15			2S	(O)	0.04416	0.01962	0.00000	-0.03292	-0.06604
16			2PX	(O)	-0.09388	-0.06448	0.00000	-0.03597	0.10702
17			2PY	(O)	-0.01601	-0.06943	0.00000	-0.17049	-0.13679
18			2PZ	(O)	0.00000	0.00000	0.00854	0.00000	0.00000
19	3	C	1S		0.01184	-0.02101	0.00000	-0.01692	0.00828
20			2S	(I)	-0.01118	0.02764	0.00000	0.01687	-0.00714
21			2PX	(I)	0.06036	0.22197	0.00000	0.01625	0.00546
22			2PY	(I)	0.19235	-0.12496	0.00000	0.05167	-0.11402
23			2PZ	(I)	0.00000	0.00000	0.06201	0.00000	0.00000
24			2S	(O)	-0.06167	0.03901	0.00000	0.06128	-0.03792
25			2PX	(O)	0.01342	0.17316	0.00000	-0.00404	0.03065
26			2PY	(O)	0.12934	-0.10463	0.00000	0.03621	-0.06734
27			2PZ	(O)	0.00000	0.00000	0.06466	0.00000	0.00000
28	4	C	1S		0.00118	-0.00966	0.00000	0.02518	0.01168
29			2S	(I)	-0.00544	0.01098	0.00000	-0.02713	-0.01099
30			2PX	(I)	0.02534	0.14549	0.00000	-0.08520	-0.13846
31			2PY	(I)	-0.19262	0.08919	0.00000	-0.02754	0.10810
32			2PZ	(I)	0.00000	0.00000	0.01848	0.00000	0.00000
33			2S	(O)	0.03323	0.00834	0.00000	-0.06933	-0.02745
34			2PX	(O)	0.02349	0.10946	0.00000	-0.05178	-0.15273
35			2PY	(O)	-0.10539	0.05357	0.00000	-0.01787	0.07185
36			2PZ	(O)	0.00000	0.00000	0.01326	0.00000	0.00000
37	5	C	1S		-0.02384	0.00643	0.00000	-0.00868	-0.03110
38			2S	(I)	0.02689	-0.00771	0.00000	0.01255	0.03066
39			2PX	(I)	0.04287	0.12352	0.00000	-0.16559	-0.12802
40			2PY	(I)	-0.19233	0.03542	0.00000	-0.14009	0.07629
41			2PZ	(I)	0.00000	0.00000	0.01798	0.00000	0.00000
42			2S	(O)	0.04997	0.00277	0.00000	0.00059	0.09135
43			2PX	(O)	0.03081	0.08329	0.00000	-0.14055	-0.08742
44			2PY	(O)	-0.09472	0.02932	0.00000	-0.09790	0.05515
45			2PZ	(O)	0.00000	0.00000	0.02073	0.00000	0.00000
46	6	C	1S		0.00807	0.02112	0.00000	-0.00145	0.00577
47			2S	(I)	-0.00732	-0.02639	0.00000	0.00108	-0.00676
48			2PX	(I)	0.03192	0.21545	0.00000	0.09605	-0.06410
49			2PY	(I)	0.23404	-0.06201	0.00000	0.14493	-0.05559
50			2PZ	(I)	0.00000	0.00000	0.02031	0.00000	0.00000
51			2S	(O)	-0.02642	-0.05049	0.00000	0.01215	-0.01092
52			2PX	(O)	-0.00397	0.16975	0.00000	0.05812	-0.06117
53			2PY	(O)	0.16260	-0.05674	0.00000	0.09721	-0.02330
54			2PZ	(O)	0.00000	0.00000	0.01846	0.00000	0.00000
55	7	C	1S		-0.00262	-0.00534	0.00000	-0.00011	0.00427
56			2S	(I)	0.00225	0.00192	0.00000	-0.00361	-0.00668
57			2PX	(I)	-0.18420	-0.01769	0.00000	0.22160	-0.21178
58			2PY	(I)	0.06826	0.11967	0.00000	0.10771	0.13778
59			2PZ	(I)	0.00000	0.00000	0.37030	0.00000	0.00000
60			2S	(O)	0.01905	0.03644	0.00000	0.02077	0.00025
61			2PX	(O)	-0.14300	-0.00875	0.00000	0.13970	-0.20520
62			2PY	(O)	0.04469	0.08118	0.00000	0.07636	0.10676
63			2PZ	(O)	0.00000	0.00000	0.32176	0.00000	0.00000
64	8	H	1S	(I)	0.02772	0.07465	0.00000	0.13896	0.08649
65			1S	(O)	0.01933	0.06192	0.00000	0.12124	0.07630
66	9	H	1S	(I)	0.04305	-0.10953	0.00000	0.03782	0.08084

67			1S	(O)	0.04061	-0.09099	0.00000	0.04266	0.07274
68	10	H	1S	(I)	0.02884	-0.14372	0.00000	0.02463	-0.05284
69			1S	(O)	0.02112	-0.10814	0.00000	0.01038	-0.03323
70	11	H	1S	(I)	-0.07339	0.11808	0.00000	0.00074	-0.02308
71			1S	(O)	-0.04713	0.08909	0.00000	0.00149	-0.01298
72	12	H	1S	(I)	-0.01165	0.08210	0.00000	-0.14879	-0.02929
73			1S	(O)	-0.01904	0.07036	0.00000	-0.12854	-0.03622
74	13	H	1S	(I)	0.13341	0.04926	0.00000	-0.10674	0.18424
75			1S	(O)	0.10837	0.03864	0.00000	-0.09371	0.16846
76	14	H	1S	(I)	-0.04759	0.02096	0.20750	0.10000	-0.05592
77			1S	(O)	-0.03699	0.01939	0.18159	0.08937	-0.04727
78	15	H	1S	(I)	-0.04759	0.02096	-0.20750	0.10000	-0.05592
79			1S	(O)	-0.03699	0.01939	-0.18159	0.08937	-0.04727
					21 (A')	22 (A')	23 (A")	24 (A")	25 (A")
	EIGENVALUES --				-0.49627	-0.44909	-0.43294	-0.37161	0.04957
1	1	C	1S		0.00624	-0.00212	0.00000	0.00000	0.00000
2			2S	(I)	-0.00428	-0.00146	0.00000	0.00000	0.00000
3			2PX	(I)	-0.13567	0.19598	0.00000	0.00000	0.00000
4			2PY	(I)	-0.19397	-0.12775	0.00000	0.00000	0.00000
5			2PZ	(I)	0.00000	0.00000	-0.09372	0.09432	0.19250
6			2S	(O)	-0.02327	0.03210	0.00000	0.00000	0.00000
7			2PX	(O)	-0.10976	0.16396	0.00000	0.00000	0.00000
8			2PY	(O)	-0.20561	-0.16575	0.00000	0.00000	0.00000
9			2PZ	(O)	0.00000	0.00000	-0.09144	0.08585	0.30878
10	2	C	1S		-0.00044	-0.00487	0.00000	0.00000	0.00000
11			2S	(I)	0.00201	0.00096	0.00000	0.00000	0.00000
12			2PX	(I)	0.10729	-0.17193	0.00000	0.00000	0.00000
13			2PY	(I)	0.11509	0.09517	0.00000	0.00000	0.00000
14			2PZ	(I)	0.00000	0.00000	-0.12081	-0.08837	-0.19798
15			2S	(O)	-0.01029	0.04118	0.00000	0.00000	0.00000
16			2PX	(O)	0.06812	-0.12634	0.00000	0.00000	0.00000
17			2PY	(O)	0.12243	0.12114	0.00000	0.00000	0.00000
18			2PZ	(O)	0.00000	0.00000	-0.10927	-0.08182	-0.33264
19	3	C	1S		-0.00644	0.01524	0.00000	0.00000	0.00000
20			2S	(I)	0.00783	-0.01809	0.00000	0.00000	0.00000
21			2PX	(I)	0.14264	-0.14940	0.00000	0.00000	0.00000
22			2PY	(I)	0.19356	0.08420	0.00000	0.00000	0.00000
23			2PZ	(I)	0.00000	0.00000	-0.24882	0.32653	0.01046
24			2S	(O)	-0.00121	-0.06797	0.00000	0.00000	0.00000
25			2PX	(O)	0.08626	-0.18711	0.00000	0.00000	0.00000
26			2PY	(O)	0.14256	0.14205	0.00000	0.00000	0.00000
27			2PZ	(O)	0.00000	0.00000	-0.28873	0.39548	0.01896
28	4	C	1S		0.00791	-0.00564	0.00000	0.00000	0.00000
29			2S	(I)	-0.01045	0.00057	0.00000	0.00000	0.00000
30			2PX	(I)	-0.10411	0.15266	0.00000	0.00000	0.00000
31			2PY	(I)	-0.16801	-0.12217	0.00000	0.00000	0.00000
32			2PZ	(I)	0.00000	0.00000	-0.10961	0.10339	-0.19262
33			2S	(O)	-0.00557	0.06147	0.00000	0.00000	0.00000
34			2PX	(O)	-0.12032	0.16262	0.00000	0.00000	0.00000
35			2PY	(O)	-0.12541	-0.05584	0.00000	0.00000	0.00000
36			2PZ	(O)	0.00000	0.00000	-0.10171	0.09752	-0.32304
37	5	C	1S		0.00294	-0.01207	0.00000	0.00000	0.00000
38			2S	(I)	-0.00364	0.00827	0.00000	0.00000	0.00000
39			2PX	(I)	0.07539	-0.17984	0.00000	0.00000	0.00000
40			2PY	(I)	0.13241	0.14787	0.00000	0.00000	0.00000
41			2PZ	(I)	0.00000	0.00000	-0.11535	-0.08986	0.13564
42			2S	(O)	-0.01021	0.05631	0.00000	0.00000	0.00000
43			2PX	(O)	0.10592	-0.17523	0.00000	0.00000	0.00000
44			2PY	(O)	0.12725	0.08821	0.00000	0.00000	0.00000

45			2PZ	(O)	0.00000	0.00000	-0.10242	-0.08454	0.32604
46	6	C	1S		-0.00029	0.01370	0.00000	0.00000	0.00000
47			2S	(I)	-0.00071	-0.01733	0.00000	0.00000	0.00000
48			2PX	(I)	-0.10911	0.14134	0.00000	0.00000	0.00000
49			2PY	(I)	-0.15524	-0.10966	0.00000	0.00000	0.00000
50			2PZ	(I)	0.00000	0.00000	-0.28801	-0.29718	0.00473
51			2S	(O)	0.01833	-0.05029	0.00000	0.00000	0.00000
52			2PX	(O)	-0.08137	0.18219	0.00000	0.00000	0.00000
53			2PY	(O)	-0.09871	-0.13301	0.00000	0.00000	0.00000
54			2PZ	(O)	0.00000	0.00000	-0.33631	-0.35827	0.01013
55	7	C	1S		0.01703	0.01428	0.00000	0.00000	0.00000
56			2S	(I)	-0.02119	-0.01666	0.00000	0.00000	0.00000
57			2PX	(I)	0.10163	-0.05007	0.00000	0.00000	0.00000
58			2PY	(I)	0.20493	0.12124	0.00000	0.00000	0.00000
59			2PZ	(I)	0.00000	0.00000	0.07290	-0.03960	-0.03319
60			2S	(O)	-0.02093	-0.02723	0.00000	0.00000	0.00000
61			2PX	(O)	0.09833	-0.06432	0.00000	0.00000	0.00000
62			2PY	(O)	0.14065	0.08645	0.00000	0.00000	0.00000
63			2PZ	(O)	0.00000	0.00000	0.07442	-0.02827	-0.01043
64	8	H	1S	(I)	-0.10527	-0.06932	0.00000	0.00000	0.00000
65			1S	(O)	-0.09235	-0.06044	0.00000	0.00000	0.00000
66	9	H	1S	(I)	0.13314	-0.06928	0.00000	0.00000	0.00000
67			1S	(O)	0.12103	-0.05852	0.00000	0.00000	0.00000
68	10	H	1S	(I)	-0.00138	0.13081	0.00000	0.00000	0.00000
69			1S	(O)	-0.00790	0.11328	0.00000	0.00000	0.00000
70	11	H	1S	(I)	-0.00291	0.13541	0.00000	0.00000	0.00000
71			1S	(O)	-0.00055	0.11591	0.00000	0.00000	0.00000
72	12	H	1S	(I)	0.10824	-0.07279	0.00000	0.00000	0.00000
73			1S	(O)	0.09546	-0.06825	0.00000	0.00000	0.00000
74	13	H	1S	(I)	-0.01196	0.07688	0.00000	0.00000	0.00000
75			1S	(O)	-0.00035	0.09645	0.00000	0.00000	0.00000
76	14	H	1S	(I)	0.06752	-0.00985	0.04890	-0.03129	-0.04924
77			1S	(O)	0.07838	-0.00371	0.04944	-0.04408	-0.09575
78	15	H	1S	(I)	0.06752	-0.00985	-0.04890	0.03129	0.04924
79			1S	(O)	0.07838	-0.00371	-0.04944	0.04408	0.09575
					26	27	28	29	30
					(A**)	(A**)	(A**)	(A**)	(A**)
	EIGENVALUES		--		0.20431	0.22854	0.26914	0.29893	0.31131
1	1	C	1S		0.00000	0.00000	-0.02300	-0.00604	-0.00140
2			2S	(I)	0.00000	0.00000	0.00897	0.01235	0.01740
3			2PX	(I)	0.00000	0.00000	-0.00209	0.02091	0.05571
4			2PY	(I)	0.00000	0.00000	0.03233	-0.00529	-0.04234
5			2PZ	(I)	0.13215	0.22329	0.00000	0.00000	0.00000
6			2S	(O)	0.00000	0.00000	0.34781	-0.24739	-0.04185
7			2PX	(O)	0.00000	0.00000	0.07060	0.02707	0.05797
8			2PY	(O)	0.00000	0.00000	0.00156	0.31716	-0.11473
9			2PZ	(O)	0.34997	0.47371	0.00000	0.00000	0.00000
10	2	C	1S		0.00000	0.00000	-0.04241	-0.01373	-0.00057
11			2S	(I)	0.00000	0.00000	0.02475	-0.00743	-0.00127
12			2PX	(I)	0.00000	0.00000	-0.01284	0.01217	0.03632
13			2PY	(I)	0.00000	0.00000	-0.08200	-0.09046	-0.02172
14			2PZ	(I)	0.12571	0.20099	0.00000	0.00000	0.00000
15			2S	(O)	0.00000	0.00000	0.44008	0.41765	0.04190
16			2PX	(O)	0.00000	0.00000	-0.03461	0.00272	0.02964
17			2PY	(O)	0.00000	0.00000	-0.36969	-0.20063	-0.03279
18			2PZ	(O)	0.33778	0.49428	0.00000	0.00000	0.00000
19	3	C	1S		0.00000	0.00000	-0.05119	0.01669	0.01457
20			2S	(I)	0.00000	0.00000	0.02881	-0.01368	0.00928
21			2PX	(I)	0.00000	0.00000	-0.08691	0.06134	0.13848
22			2PY	(I)	0.00000	0.00000	0.05777	-0.04345	-0.04753

23			2PZ	(I)	-0.22301	-0.02919	0.00000	0.00000	0.00000
24			2S	(O)	0.00000	0.00000	0.62763	-0.14615	-0.37557
25			2PX	(O)	0.00000	0.00000	-0.42745	0.49986	0.43495
26			2PY	(O)	0.00000	0.00000	0.27382	-0.12384	-0.31941
27			2PZ	(O)	-0.51061	-0.04384	0.00000	0.00000	0.00000
28	4	C	1S		0.00000	0.00000	-0.03646	-0.03278	0.02946
29			2S	(I)	0.00000	0.00000	0.01183	0.02572	-0.00536
30			2PX	(I)	0.00000	0.00000	-0.07364	-0.00687	0.09652
31			2PY	(I)	0.00000	0.00000	-0.05207	-0.00124	0.00375
32			2PZ	(I)	0.15254	-0.17613	0.00000	0.00000	0.00000
33			2S	(O)	0.00000	0.00000	0.50852	0.29039	-0.51120
34			2PX	(O)	0.00000	0.00000	-0.20844	-0.23333	0.29071
35			2PY	(O)	0.00000	0.00000	-0.16414	-0.05172	0.05023
36			2PZ	(O)	0.40205	-0.43755	0.00000	0.00000	0.00000
37	5	C	1S		0.00000	0.00000	-0.05272	0.00796	0.00002
38			2S	(I)	0.00000	0.00000	0.03688	-0.02155	-0.00517
39			2PX	(I)	0.00000	0.00000	0.05893	0.03960	0.12242
40			2PY	(I)	0.00000	0.00000	0.05214	-0.02138	0.00704
41			2PZ	(I)	0.16677	-0.18471	0.00000	0.00000	0.00000
42			2S	(O)	0.00000	0.00000	0.51035	0.06039	0.19747
43			2PX	(O)	0.00000	0.00000	0.36471	-0.16257	0.39265
44			2PY	(O)	0.00000	0.00000	0.18643	0.13441	0.06679
45			2PZ	(O)	0.42914	-0.46558	0.00000	0.00000	0.00000
46	6	C	1S		0.00000	0.00000	-0.03788	-0.05328	-0.02756
47			2S	(I)	0.00000	0.00000	0.01025	0.02708	0.00691
48			2PX	(I)	0.00000	0.00000	0.07216	0.09467	0.08902
49			2PY	(I)	0.00000	0.00000	-0.06815	-0.03425	-0.04770
50			2PZ	(I)	-0.23167	-0.01003	0.00000	0.00000	0.00000
51			2S	(O)	0.00000	0.00000	0.60440	0.71344	0.45184
52			2PX	(O)	0.00000	0.00000	0.19037	0.52524	0.31551
53			2PY	(O)	0.00000	0.00000	-0.19885	-0.17937	-0.19495
54			2PZ	(O)	-0.52301	-0.02164	0.00000	0.00000	0.00000
55	7	C	1S		0.00000	0.00000	-0.02967	0.12692	-0.07754
56			2S	(I)	0.00000	0.00000	0.00044	-0.03051	0.02052
57			2PX	(I)	0.00000	0.00000	-0.01920	0.04032	0.16111
58			2PY	(I)	0.00000	0.00000	0.10439	-0.09087	0.01954
59			2PZ	(I)	-0.01601	0.04955	0.00000	0.00000	0.00000
60			2S	(O)	0.00000	0.00000	0.52275	-1.84582	1.08703
61			2PX	(O)	0.00000	0.00000	-0.13422	0.19062	0.73552
62			2PY	(O)	0.00000	0.00000	0.43978	-0.42053	0.09306
63			2PZ	(O)	-0.06960	0.32435	0.00000	0.00000	0.00000
64	8	H	1S	(I)	0.00000	0.00000	-0.03801	-0.00437	-0.00200
65			1S	(O)	0.00000	0.00000	-0.74448	-0.46558	-0.07524
66	9	H	1S	(I)	0.00000	0.00000	-0.03156	-0.01039	0.01593
67			1S	(O)	0.00000	0.00000	-0.66054	-0.36596	0.62465
68	10	H	1S	(I)	0.00000	0.00000	-0.03325	-0.02315	0.03600
69			1S	(O)	0.00000	0.00000	-0.91747	0.51753	0.87301
70	11	H	1S	(I)	0.00000	0.00000	-0.03396	-0.03624	-0.02731
71			1S	(O)	0.00000	0.00000	-0.70738	-0.96841	-0.71909
72	12	H	1S	(I)	0.00000	0.00000	-0.02150	-0.04356	0.00842
73			1S	(O)	0.00000	0.00000	-0.77120	-0.05050	-0.55848
74	13	H	1S	(I)	0.00000	0.00000	-0.00774	0.01501	0.03315
75			1S	(O)	0.00000	0.00000	-0.54379	1.13997	0.37768
76	14	H	1S	(I)	-0.03463	-0.06027	0.00162	-0.00452	-0.01282
77			1S	(O)	-0.02686	-0.44399	-0.24230	0.69749	-0.93585
78	15	H	1S	(I)	0.03463	0.06027	0.00162	-0.00452	-0.01282
79			1S	(O)	0.02686	0.44399	-0.24230	0.69749	-0.93585

	31
	(A")
EIGENVALUES --	0.34648

1	1	C	1S		0.00000
2			2S	(I)	0.00000
3			2PX	(I)	0.00000
4			2PY	(I)	0.00000
5			2PZ	(I)	-0.03007
6			2S	(O)	0.00000
7			2PX	(O)	0.00000
8			2PY	(O)	0.00000
9			2PZ	(O)	0.07233
10	2	C	1S		0.00000
11			2S	(I)	0.00000
12			2PX	(I)	0.00000
13			2PY	(I)	0.00000
14			2PZ	(I)	0.15287
15			2S	(O)	0.00000
16			2PX	(O)	0.00000
17			2PY	(O)	0.00000
18			2PZ	(O)	0.46349
19	3	C	1S		0.00000
20			2S	(I)	0.00000
21			2PX	(I)	0.00000
22			2PY	(I)	0.00000
23			2PZ	(I)	0.11773
24			2S	(O)	0.00000
25			2PX	(O)	0.00000
26			2PY	(O)	0.00000
27			2PZ	(O)	0.23090
28	4	C	1S		0.00000
29			2S	(I)	0.00000
30			2PX	(I)	0.00000
31			2PY	(I)	0.00000
32			2PZ	(I)	-0.17113
33			2S	(O)	0.00000
34			2PX	(O)	0.00000
35			2PY	(O)	0.00000
36			2PZ	(O)	-0.46579
37	5	C	1S		0.00000
38			2S	(I)	0.00000
39			2PX	(I)	0.00000
40			2PY	(I)	0.00000
41			2PZ	(I)	0.02813
42			2S	(O)	0.00000
43			2PX	(O)	0.00000
44			2PY	(O)	0.00000
45			2PZ	(O)	0.15291
46	6	C	1S		0.00000
47			2S	(I)	0.00000
48			2PX	(I)	0.00000
49			2PY	(I)	0.00000
50			2PZ	(I)	-0.10425
51			2S	(O)	0.00000
52			2PX	(O)	0.00000
53			2PY	(O)	0.00000
54			2PZ	(O)	-0.29613
55	7	C	1S		0.00000
56			2S	(I)	0.00000
57			2PX	(I)	0.00000
58			2PY	(I)	0.00000
59			2PZ	(I)	-0.23926
60			2S	(O)	0.00000

61			2PX	(0)	0.00000
62			2PY	(0)	0.00000
63			2PZ	(0)	-1.14340
64	8	H	1S	(I)	0.00000
65			1S	(0)	0.00000
66	9	H	1S	(I)	0.00000
67			1S	(0)	0.00000
68	10	H	1S	(I)	0.00000
69			1S	(0)	0.00000
70	11	H	1S	(I)	0.00000
71			1S	(0)	0.00000
72	12	H	1S	(I)	0.00000
73			1S	(0)	0.00000
74	13	H	1S	(I)	0.00000
75			1S	(0)	0.00000
76	14	H	1S	(I)	0.04626
77			1S	(0)	1.19015
78	15	H	1S	(I)	-0.04626
79			1S	(0)	-1.19015

ORBITAL SYMMETRIES.

ALPHA ORBITALS

OCCUPIED (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A") (A') (A') (A')
(A") (A') (A') (A") (A") (A")

VIRTUAL (A") (A') (A") (A') (A') (A') (A') (A') (A") (A')
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BETA ORBITALS

OCCUPIED (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
(A') (A') (A') (A') (A') (A') (A') (A") (A') (A')
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VIRTUAL (A") (A") (A") (A') (A') (A') (A") (A') (A') (A')
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APPENDIX C:

MOLECULAR ORBITALS AND EIGENVALUES FOR THE BENZYL RADICAL

```
ORBITAL SYMMETRIES.
  ALPHA ORBITALS
      OCCUPIED  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                (A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
                (A') (A') (A") (A") (A")
      VIRTUAL   (A") (A") (A') (A') (A') (A') (A') (A") (A') (A')
                (A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
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                (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                (A') (A')
  BETA ORBITALS
      OCCUPIED  (A') (A') (A') (A') (A') (A') (A') (A') (A') (A')
                (A') (A') (A') (A') (A') (A') (A') (A') (A') (A")
                (A') (A') (A") (A")
      VIRTUAL   (A") (A") (A") (A') (A') (A') (A') (A') (A') (A')
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                (A') (A') (A')
 THE ELECTRONIC STATE IS 2-A".
    ALPHA MOLECULAR ORBITAL COEFFICIENTS
                                    1          2          3          4          5
                                  (A')       (A')       (A')       (A')       (A')
    EIGENVALUES --            -11.18100  -11.18091  -11.18058  -11.17694  -11.17587
  1  1    C  1S               -0.01218   -0.07636   -0.03803   -0.96637   -0.18457
  2          2S   (I)         -0.00198   -0.01234   -0.00584   -0.09772   -0.01552
  3          2PX  (I)         -0.00167    0.00027    0.00001    0.00000    0.00000
  4          2PY  (I)          0.00033    0.00202    0.00107   -0.00023    0.00187
  5          2PZ  (I)          0.00000    0.00000    0.00000    0.00000    0.00000
  6          2S   (O)          0.00758    0.04655    0.02435    0.09252   -0.00527
  7          2PX  (O)          0.02063   -0.00329   -0.00016    0.00000   -0.00001
  8          2PY  (O)         -0.00564   -0.03443   -0.02002   -0.00408   -0.01126
  9          2PZ  (O)          0.00000    0.00000    0.00000    0.00000    0.00000
 10  2    C  1S               -0.02804   -0.22381    0.96051   -0.01838   -0.00484
 11          2S   (I)         -0.00275   -0.02215    0.09782   -0.00110   -0.00049
 12          2PX  (I)         -0.00114    0.00018    0.00001    0.00000    0.00000
 13          2PY  (I)         -0.00017   -0.00109    0.00111    0.00027    0.00018
 14          2PZ  (I)          0.00000    0.00000    0.00000    0.00000    0.00000
 15          2S   (O)         -0.00081   -0.00034   -0.09539   -0.00745    0.00320
 16          2PX  (O)          0.00044   -0.00007    0.00000    0.00000    0.00000
 17          2PY  (O)         -0.00155   -0.00834   -0.02832   -0.00527    0.00274
 18          2PZ  (O)          0.00000    0.00000    0.00000    0.00000    0.00000
 19  3    C  1S                0.79698    0.55871    0.15227   -0.05420   -0.02699
 20          2S   (I)          0.08118    0.05723    0.01604   -0.00213   -0.00176
 21          2PX  (I)         -0.00139   -0.00007    0.00007   -0.00106   -0.00037
 22          2PY  (I)         -0.00046   -0.00085    0.00076    0.00017    0.00097
 23          2PZ  (I)          0.00000    0.00000    0.00000    0.00000    0.00000
 24          2S   (O)         -0.07016   -0.06268   -0.03269   -0.02326    0.00133
 25          2PX  (O)          0.01486    0.01845    0.01455    0.01572    0.00120
 26          2PY  (O)          0.00524    0.01192    0.00764   -0.00349   -0.00537
 27          2PZ  (O)          0.00000    0.00000    0.00000    0.00000    0.00000
 28  4    C  1S               -0.00900   -0.00911   -0.01964    0.00458    0.00797
 29          2S   (I)         -0.00384   -0.00333   -0.00701    0.00047    0.00176
 30          2PX  (I)          0.00033    0.00023    0.00163   -0.00012   -0.00017
 31          2PY  (I)         -0.00113   -0.00099   -0.00001    0.00077    0.00036
 32          2PZ  (I)          0.00000    0.00000    0.00000    0.00000    0.00000
 33          2S   (O)          0.02260    0.02573    0.04640    0.00599   -0.00703
 34          2PX  (O)         -0.00700   -0.00922   -0.02681   -0.00597    0.00252
```

35			2PY	(O)	0.01300	0.01483	0.00618	0.00113	-0.00408
36			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
37	5	C	1S		-0.58138	0.77835	0.16320	-0.05458	-0.02716
38			2S	(I)	-0.05912	0.07958	0.01716	-0.00216	-0.00178
39			2PX	(I)	-0.00130	0.00050	-0.00005	0.00106	0.00037
40			2PY	(I)	0.00019	-0.00095	0.00075	0.00017	0.00097
41			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
42			2S	(O)	0.04671	-0.08130	-0.03362	-0.02324	0.00133
43			2PX	(O)	0.00818	-0.02212	-0.01474	-0.01572	-0.00120
44			2PY	(O)	-0.00115	0.01293	0.00769	-0.00349	-0.00539
45			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
46	6	C	1S		0.00542	-0.01139	-0.01970	0.00457	0.00794
47			2S	(I)	0.00250	-0.00434	-0.00705	0.00047	0.00176
48			2PX	(I)	0.00021	-0.00032	-0.00163	0.00012	0.00017
49			2PY	(I)	0.00077	-0.00130	-0.00002	0.00077	0.00036
50			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
51			2S	(O)	-0.01277	0.03137	0.04668	0.00599	-0.00703
52			2PX	(O)	-0.00337	0.01088	0.02689	0.00597	-0.00251
53			2PY	(O)	-0.00765	0.01812	0.00634	0.00113	-0.00409
54			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
55	7	C	1S		-0.00351	-0.02211	-0.00676	0.18741	-0.96823
56			2S	(I)	-0.00049	-0.00305	-0.00099	0.02149	-0.09492
57			2PX	(I)	-0.00026	0.00004	0.00000	0.00000	0.00000
58			2PY	(I)	0.00000	0.00001	-0.00019	-0.00126	-0.00004
59			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
60			2S	(O)	0.00217	0.01321	0.00780	-0.03174	0.06006
61			2PX	(O)	-0.00395	0.00063	0.00003	0.00000	0.00000
62			2PY	(O)	-0.00096	-0.00585	-0.00332	0.01148	-0.00453
63			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
64	8	H	1S	(I)	-0.00004	-0.00011	-0.00273	-0.00008	0.00025
65			1S	(O)	-0.00052	-0.00350	0.00501	-0.00172	0.00041
66	9	H	1S	(I)	0.00000	0.00029	0.00018	0.00049	-0.00005
67			1S	(O)	0.00298	0.00378	0.00630	0.00090	-0.00140
68	10	H	1S	(I)	-0.00172	-0.00183	-0.00103	0.00053	0.00046
69			1S	(O)	0.00567	0.00159	-0.00125	-0.00309	0.00054
70	11	H	1S	(I)	0.00009	0.00028	0.00018	0.00049	-0.00005
71			1S	(O)	-0.00156	0.00450	0.00634	0.00089	-0.00140
72	12	H	1S	(I)	0.00105	-0.00227	-0.00105	0.00053	0.00046
73			1S	(O)	-0.00491	0.00328	-0.00117	-0.00310	0.00054
74	13	H	1S	(I)	0.00046	-0.00026	-0.00011	0.00056	0.00184
75			1S	(O)	0.00077	-0.00009	-0.00005	0.00242	-0.01216
76	14	H	1S	(I)	-0.00052	-0.00011	-0.00010	0.00056	0.00184
77			1S	(O)	-0.00076	0.00016	-0.00004	0.00242	-0.01216
					6	7	8	9	10
					(A')	(A')	(A')	(A')	(A')
	EIGENVALUES			--	-11.16602	-11.16588	-1.15369	-1.05111	-1.01716
1	1	C	1S		0.00093	0.00660	-0.10472	0.11325	0.00003
2			2S	(I)	0.00017	0.00125	0.11827	-0.12264	-0.00003
3			2PX	(I)	-0.00058	0.00008	-0.00003	0.00005	-0.10791
4			2PY	(I)	0.00012	0.00089	-0.03421	-0.06305	0.00000
5			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
6			2S	(O)	-0.00276	-0.01987	0.14542	-0.21521	-0.00004
7			2PX	(O)	-0.00414	0.00058	0.00000	0.00002	-0.00556
8			2PY	(O)	0.00154	0.01105	0.03989	-0.00307	-0.00004
9			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
10	2	C	1S		0.00315	0.02245	-0.09290	-0.12685	-0.00002
11			2S	(I)	-0.00051	-0.00371	0.10054	0.13475	0.00002
12			2PX	(I)	-0.00111	0.00015	-0.00001	-0.00001	-0.08486
13			2PY	(I)	-0.00023	-0.00164	0.05268	0.03419	0.00000
14			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000

15			2S	(O)	0.00679	0.04893	0.23400	0.32466	0.00002
16			2PX	(O)	0.01445	-0.00201	-0.00001	0.00000	-0.01288
17			2PY	(O)	0.00405	0.02920	0.04262	0.02065	-0.00002
18			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
19	3	C	1S		0.00881	0.01323	-0.10281	0.02864	0.13252
20			2S	(I)	-0.00220	-0.00219	0.11124	-0.03036	-0.13948
21			2PX	(I)	0.00022	0.00067	-0.04804	0.02915	-0.00758
22			2PY	(I)	0.00115	0.00108	-0.02111	-0.07136	0.04916
23			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
24			2S	(O)	0.02477	0.03093	0.26055	-0.07533	-0.35505
25			2PX	(O)	-0.00746	-0.01306	-0.03970	0.00347	0.01177
26			2PY	(O)	-0.01173	-0.01512	-0.02772	-0.00345	0.01556
27			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
28	4	C	1S		0.78747	0.59536	-0.08455	-0.06843	0.10286
29			2S	(I)	0.07892	0.05985	0.09864	0.07419	-0.11210
30			2PX	(I)	-0.00152	0.00013	-0.04574	-0.05203	-0.00586
31			2PY	(I)	0.00029	0.00070	0.03096	-0.03630	-0.06423
32			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
33			2S	(O)	-0.06577	-0.06640	0.09105	0.13326	-0.20117
34			2PX	(O)	0.01328	0.01826	0.01914	-0.00375	0.00027
35			2PY	(O)	-0.00678	-0.01194	-0.01474	0.00884	-0.00193
36			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
37	5	C	1S		-0.00484	0.01513	-0.10284	0.02869	-0.13247
38			2S	(I)	0.00152	-0.00271	0.11128	-0.03042	0.13944
39			2PX	(I)	0.00003	-0.00070	0.04805	-0.02916	-0.00759
40			2PY	(I)	-0.00081	0.00135	-0.02111	-0.07138	-0.04918
41			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
42			2S	(O)	-0.01541	0.03651	0.26060	-0.07544	0.35485
43			2PX	(O)	-0.00362	0.01460	0.03970	-0.00347	0.01171
44			2PY	(O)	0.00717	-0.01774	-0.02768	-0.00345	-0.01551
45			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
46	6	C	1S		-0.59555	0.78733	-0.08457	-0.06842	-0.10286
47			2S	(I)	-0.05964	0.07909	0.09867	0.07418	0.11210
48			2PX	(I)	-0.00150	0.00029	0.04575	0.05204	-0.00586
49			2PY	(I)	-0.00009	0.00075	0.03097	-0.03633	0.06420
50			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
51			2S	(O)	0.04520	-0.08181	0.09111	0.13325	0.20127
52			2PX	(O)	0.00781	-0.02118	-0.01914	0.00374	0.00030
53			2PY	(O)	0.00327	-0.01333	-0.01471	0.00883	0.00197
54			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
55	7	C	1S		0.00125	0.00887	-0.04992	0.12665	0.00001
56			2S	(I)	-0.00001	-0.00010	0.05754	-0.13533	-0.00001
57			2PX	(I)	-0.00037	0.00005	0.00000	-0.00001	-0.01952
58			2PY	(I)	0.00006	0.00044	-0.03945	0.06209	0.00000
59			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
60			2S	(O)	-0.00015	-0.00102	0.08465	-0.32823	-0.00001
61			2PX	(O)	0.00377	-0.00053	-0.00001	0.00000	-0.00995
62			2PY	(O)	-0.00023	-0.00165	0.00861	0.02012	-0.00001
63			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
64	8	H	1S	(I)	0.00001	0.00004	0.03268	0.05898	0.00001
65			1S	(O)	0.00106	0.00767	0.00143	0.00648	-0.00001
66	9	H	1S	(I)	-0.00168	-0.00183	0.02965	0.03218	-0.05532
67			1S	(O)	0.00534	0.00275	-0.01231	0.00574	-0.01061
68	10	H	1S	(I)	-0.00020	0.00021	0.03792	-0.02009	-0.07008
69			1S	(O)	0.00275	0.00485	0.00450	-0.00658	-0.01199
70	11	H	1S	(I)	0.00112	-0.00222	0.02967	0.03218	0.05534
71			1S	(O)	-0.00439	0.00410	-0.01231	0.00574	0.01063
72	12	H	1S	(I)	0.00025	0.00015	0.03793	-0.02011	0.07005
73			1S	(O)	-0.00132	0.00542	0.00449	-0.00658	0.01196
74	13	H	1S	(I)	-0.00053	-0.00011	0.01985	-0.05869	-0.00591

75			1S	(O)	-0.00117	0.00104	-0.00419	-0.00015	-0.00366
76	14	H	1S	(I)	0.00048	-0.00025	0.01985	-0.05870	0.00590
77			1S	(O)	0.00141	0.00068	-0.00420	-0.00015	0.00366
					11	12	13	14	15
					(A')	(A')	(A')	(A')	(A')
	EIGENVALUES		--		-0.94319	-0.82281	-0.79097	-0.70396	-0.64537
1	1	C	1S		0.00687	0.00000	-0.10860	-0.01343	0.00001
2			2S	(I)	-0.00773	-0.00001	0.11292	0.01148	-0.00002
3			2PX	(I)	-0.00001	0.16153	-0.00001	-0.00003	0.18347
4			2PY	(I)	0.15132	0.00003	-0.06686	0.08819	0.00001
5			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
6			2S	(O)	-0.01322	0.00003	0.32976	0.05559	0.00000
7			2PX	(O)	-0.00006	0.05480	0.00001	-0.00001	0.11651
8			2PY	(O)	0.00812	-0.00001	-0.04328	0.04694	-0.00012
9			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
10	2	C	1S		-0.11380	0.00001	-0.06961	-0.02976	-0.00002
11			2S	(I)	0.11748	-0.00001	0.07051	0.02476	0.00002
12			2PX	(I)	0.00000	-0.19408	-0.00003	0.00001	0.20044
13			2PY	(I)	-0.01580	0.00000	-0.03869	-0.21876	-0.00003
14			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
15			2S	(O)	0.34017	-0.00007	0.25358	0.12876	0.00006
16			2PX	(O)	0.00002	-0.08425	-0.00002	0.00000	0.12078
17			2PY	(O)	0.00895	-0.00002	-0.00576	-0.15369	-0.00006
18			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
19	3	C	1S		0.08508	-0.07619	0.02128	-0.02535	0.01902
20			2S	(I)	-0.08783	0.07670	-0.02010	0.02135	-0.01856
21			2PX	(I)	0.01174	-0.00340	-0.14279	0.13351	-0.08583
22			2PY	(I)	0.01970	0.11800	0.12009	0.11867	0.17581
23			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
24			2S	(O)	-0.25352	0.26953	-0.08615	0.10442	-0.07599
25			2PX	(O)	0.01701	-0.00989	-0.06463	0.10173	-0.04657
26			2PY	(O)	0.01479	0.04445	0.04880	0.07600	0.10261
27			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
28	4	C	1S		-0.00680	0.10385	0.06477	0.01557	-0.00789
29			2S	(I)	0.00830	-0.10822	-0.06696	-0.01974	0.00740
30			2PX	(I)	-0.05134	0.00204	-0.10493	0.11686	-0.06592
31			2PY	(I)	-0.09952	0.08393	-0.06850	-0.08161	-0.18850
32			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
33			2S	(O)	0.00870	-0.30043	-0.19668	-0.03074	0.03307
34			2PX	(O)	0.00025	0.00779	-0.03882	0.06724	-0.03012
35			2PY	(O)	-0.01939	0.01850	-0.02042	-0.04595	-0.10027
36			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
37	5	C	1S		0.08509	0.07618	0.02129	-0.02535	-0.01904
38			2S	(I)	-0.08785	-0.07669	-0.02011	0.02135	0.01860
39			2PX	(I)	-0.01174	-0.00344	0.14282	-0.13351	-0.08588
40			2PY	(I)	0.01974	-0.11799	0.12010	0.11868	-0.17581
41			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
42			2S	(O)	-0.25359	-0.26952	-0.08618	0.10446	0.07593
43			2PX	(O)	-0.01704	-0.00995	0.06467	-0.10173	-0.04674
44			2PY	(O)	0.01472	-0.04445	0.04881	0.07600	-0.10250
45			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
46	6	C	1S		-0.00678	-0.10384	0.06475	0.01558	0.00793
47			2S	(I)	0.00828	0.10821	-0.06694	-0.01976	-0.00745
48			2PX	(I)	0.05136	0.00201	0.10497	-0.11689	-0.06583
49			2PY	(I)	-0.09955	-0.08394	-0.06853	-0.08162	0.18856
50			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
51			2S	(O)	0.00862	0.30045	-0.19662	-0.03080	-0.03309
52			2PX	(O)	-0.00023	0.00780	0.03883	-0.06726	-0.02998
53			2PY	(O)	-0.01945	-0.01851	-0.02043	-0.04596	0.10039
54			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000

55	7	C	1S		-0.14823	-0.00002	0.07158	0.03018	-0.00001
56			2S	(I)	0.15287	0.00002	-0.07001	-0.02604	0.00000
57			2PX	(I)	0.00000	0.05746	0.00004	0.00001	0.22108
58			2PY	(I)	-0.00273	0.00003	-0.11908	-0.10740	0.00009
59			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
60			2S	(O)	0.45180	0.00008	-0.25456	-0.12631	0.00011
61			2PX	(O)	0.00002	0.03764	0.00001	0.00000	0.16541
62			2PY	(O)	-0.01257	0.00001	-0.05455	-0.06161	0.00002
63			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
64	8	H	1S	(I)	0.07748	-0.00001	0.07084	0.14459	0.00004
65			1S	(O)	0.02323	-0.00001	0.03402	0.08242	0.00001
66	9	H	1S	(I)	0.00731	-0.10313	-0.08337	0.06931	0.03245
67			1S	(O)	-0.00009	-0.05437	-0.04531	0.05157	0.02396
68	10	H	1S	(I)	-0.04423	0.08116	-0.04763	0.11653	-0.00548
69			1S	(O)	-0.00989	0.03648	-0.02702	0.06405	0.00051
70	11	H	1S	(I)	0.00730	0.10316	-0.08336	0.06932	-0.03256
71			1S	(O)	-0.00009	0.05438	-0.04530	0.05156	-0.02401
72	12	H	1S	(I)	-0.04423	-0.08112	-0.04767	0.11653	0.00556
73			1S	(O)	-0.00988	-0.03646	-0.02704	0.06405	-0.00052
74	13	H	1S	(I)	0.08947	0.02336	-0.08199	-0.05166	0.11342
75			1S	(O)	0.01533	0.01226	-0.03818	-0.02736	0.07800
76	14	H	1S	(I)	0.08948	-0.02333	-0.08202	-0.05166	-0.11338
77			1S	(O)	0.01535	-0.01224	-0.03819	-0.02736	-0.07796
					16	17	18	19	20
					(A')	(A')	(A')	(A')	(A")
	EIGENVALUES		--		-0.64003	-0.59014	-0.58356	-0.55761	-0.52603
1	1	C	1S		-0.07224	0.00001	-0.01321	0.00002	0.00000
2			2S	(I)	0.07503	-0.00001	0.01396	-0.00002	0.00000
3			2PX	(I)	0.00003	-0.10479	0.00002	-0.07882	0.00000
4			2PY	(I)	0.10841	0.00008	-0.24732	-0.00007	0.00000
5			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	-0.16709
6			2S	(O)	0.23599	-0.00002	0.01690	-0.00013	0.00000
7			2PX	(O)	-0.00007	-0.07664	0.00010	-0.10477	0.00000
8			2PY	(O)	0.12121	0.00002	-0.17334	0.00000	0.00000
9			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	-0.13431
10	2	C	1S		0.05312	-0.00001	0.02331	0.00000	0.00000
11			2S	(I)	-0.05625	0.00001	-0.02803	0.00000	0.00000
12			2PX	(I)	0.00003	-0.10745	0.00002	-0.17448	0.00000
13			2PY	(I)	0.05408	0.00012	-0.24652	-0.00015	0.00000
14			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	-0.17851
15			2S	(O)	-0.17379	-0.00001	-0.05485	0.00003	0.00000
16			2PX	(O)	0.00004	-0.06086	-0.00001	-0.11310	0.00000
17			2PY	(O)	0.08204	0.00007	-0.20987	-0.00015	0.00000
18			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	-0.18162
19	3	C	1S		0.05053	0.02002	-0.00800	0.01815	0.00000
20			2S	(I)	-0.05238	-0.02482	0.00971	-0.01732	0.00000
21			2PX	(I)	-0.08282	0.19738	-0.14843	0.00884	0.00000
22			2PY	(I)	-0.03542	0.11341	-0.02126	-0.15244	0.00000
23			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	-0.21531
24			2S	(O)	-0.16516	-0.03714	0.01064	-0.05302	0.00000
25			2PX	(O)	-0.09382	0.16099	-0.12223	-0.02934	0.00000
26			2PY	(O)	-0.06419	0.09657	-0.01917	-0.09807	0.00000
27			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	-0.22016
28	4	C	1S		-0.05751	0.01682	0.00714	-0.00950	0.00000
29			2S	(I)	0.06057	-0.02020	-0.00948	0.01035	0.00000
30			2PX	(I)	0.11805	0.18329	0.12855	0.09908	0.00000
31			2PY	(I)	-0.06570	-0.10984	0.00089	0.12393	0.00000
32			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	-0.12106
33			2S	(O)	0.16745	-0.01997	0.00412	0.03337	0.00000
34			2PX	(O)	0.11497	0.13912	0.09018	0.08024	0.00000

35			2PY	(O)	-0.07254	-0.07616	-0.00583	0.06955	0.00000
36			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	-0.09841
37	5	C	1S		0.05052	-0.02001	-0.00801	-0.01820	0.00000
38			2S	(I)	-0.05237	0.02482	0.00973	0.01736	0.00000
39			2PX	(I)	0.08278	0.19725	0.14857	0.00885	0.00000
40			2PY	(I)	-0.03544	-0.11335	-0.02145	0.15232	0.00000
41			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	-0.21534
42			2S	(O)	-0.16521	0.03702	0.01070	0.05328	0.00000
43			2PX	(O)	0.09374	0.16084	0.12240	-0.02926	0.00000
44			2PY	(O)	-0.06425	-0.09646	-0.01923	0.09796	0.00000
45			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	-0.22018
46	6	C	1S		-0.05750	-0.01684	0.00712	0.00954	0.00000
47			2S	(I)	0.06056	0.02022	-0.00946	-0.01039	0.00000
48			2PX	(I)	-0.11807	0.18336	-0.12848	0.09905	0.00000
49			2PY	(I)	-0.06566	0.10981	0.00107	-0.12377	0.00000
50			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	-0.12109
51			2S	(O)	0.16743	0.02010	0.00416	-0.03353	0.00000
52			2PX	(O)	-0.11494	0.13920	-0.09014	0.08023	0.00000
53			2PY	(O)	-0.07254	0.07619	-0.00568	-0.06945	0.00000
54			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	-0.09843
55	7	C	1S		0.00921	0.00000	0.00065	0.00000	0.00000
56			2S	(I)	-0.00160	0.00001	-0.00943	0.00000	0.00000
57			2PX	(I)	0.00021	-0.00147	-0.00014	0.30810	0.00000
58			2PY	(I)	-0.21440	-0.00007	0.22934	0.00015	0.00000
59			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	-0.15822
60			2S	(O)	-0.10241	0.00001	0.04992	-0.00001	0.00000
61			2PX	(O)	0.00017	0.01151	-0.00013	0.30237	0.00000
62			2PY	(O)	-0.10718	-0.00005	0.14741	0.00013	0.00000
63			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	-0.16091
64	8	H	1S	(I)	-0.08227	-0.00007	0.13901	0.00011	0.00000
65			1S	(O)	-0.03617	-0.00005	0.10284	0.00008	0.00000
66	9	H	1S	(I)	0.14783	0.13305	0.07137	0.02903	0.00000
67			1S	(O)	0.09400	0.11051	0.06001	0.01879	0.00000
68	10	H	1S	(I)	-0.10218	0.12883	-0.08350	-0.05963	0.00000
69			1S	(O)	-0.05152	0.09583	-0.05895	-0.03389	0.00000
70	11	H	1S	(I)	0.14783	-0.13307	0.07128	-0.02912	0.00000
71			1S	(O)	0.09399	-0.11050	0.05992	-0.01885	0.00000
72	12	H	1S	(I)	-0.10216	-0.12875	-0.08362	0.05960	0.00000
73			1S	(O)	-0.05152	-0.09580	-0.05904	0.03389	0.00000
74	13	H	1S	(I)	-0.07508	0.00330	0.07241	0.17899	0.00000
75			1S	(O)	-0.06225	0.00326	0.05829	0.12863	0.00000
76	14	H	1S	(I)	-0.07526	-0.00334	0.07252	-0.17893	0.00000
77			1S	(O)	-0.06236	-0.00329	0.05834	-0.12856	0.00000
					21	22	23	24	25
					(A')	(A')	(A")	(A")	(A")
	EIGENVALUES		--		-0.50286	-0.47986	-0.42242	-0.37435	-0.31532
1	1	C	1S		0.00613	0.00001	0.00000	0.00000	0.00000
2			2S	(I)	-0.00476	-0.00001	0.00000	0.00000	0.00000
3			2PX	(I)	-0.00007	-0.23350	0.00000	0.00000	0.00000
4			2PY	(I)	0.17636	-0.00009	0.00000	0.00000	0.00000
5			2PZ	(I)	0.00000	0.00000	0.13555	-0.00001	-0.04929
6			2S	(O)	-0.02669	-0.00006	0.00000	0.00000	0.00000
7			2PX	(O)	-0.00015	-0.21443	0.00000	0.00000	0.00000
8			2PY	(O)	0.20842	-0.00009	0.00000	0.00000	0.00000
9			2PZ	(O)	0.00000	0.00000	0.12368	-0.00002	-0.05479
10	2	C	1S		0.00315	0.00000	0.00000	0.00000	0.00000
11			2S	(I)	-0.00423	0.00000	0.00000	0.00000	0.00000
12			2PX	(I)	0.00009	0.21211	0.00000	0.00000	0.00000
13			2PY	(I)	-0.20542	0.00005	0.00000	0.00000	0.00000
14			2PZ	(I)	0.00000	0.00000	-0.28844	0.00005	0.27060

15			2S	(O)	-0.01652	-0.00001	0.00000	0.00000	0.00000
16			2PX	(O)	0.00004	0.15430	0.00000	0.00000	0.00000
17			2PY	(O)	-0.24578	0.00004	0.00000	0.00000	0.00000
18			2PZ	(O)	0.00000	0.00000	-0.33200	0.00006	0.35811
19	3	C	1S		-0.00757	0.01013	0.00000	0.00000	0.00000
20			2S	(I)	0.00973	-0.01148	0.00000	0.00000	0.00000
21			2PX	(I)	0.01649	0.20531	0.00000	0.00000	0.00000
22			2PY	(I)	-0.22045	-0.04779	0.00000	0.00000	0.00000
23			2PZ	(I)	0.00000	0.00000	0.01406	-0.31501	-0.21365
24			2S	(O)	0.03394	-0.02505	0.00000	0.00000	0.00000
25			2PX	(O)	-0.02805	0.20911	0.00000	0.00000	0.00000
26			2PY	(O)	-0.19156	0.02662	0.00000	0.00000	0.00000
27			2PZ	(O)	0.00000	0.00000	0.01664	-0.38227	-0.27815
28	4	C	1S		0.00218	-0.00654	0.00000	0.00000	0.00000
29			2S	(I)	-0.00076	0.00667	0.00000	0.00000	0.00000
30			2PX	(I)	0.01109	-0.18232	0.00000	0.00000	0.00000
31			2PY	(I)	0.21234	0.00650	0.00000	0.00000	0.00000
32			2PZ	(I)	0.00000	0.00000	-0.10445	-0.14368	0.02252
33			2S	(O)	-0.02059	0.03064	0.00000	0.00000	0.00000
34			2PX	(O)	-0.03864	-0.19194	0.00000	0.00000	0.00000
35			2PY	(O)	0.15289	0.05343	0.00000	0.00000	0.00000
36			2PZ	(O)	0.00000	0.00000	-0.10062	-0.14620	0.01791
37	5	C	1S		-0.00756	-0.01013	0.00000	0.00000	0.00000
38			2S	(I)	0.00973	0.01150	0.00000	0.00000	0.00000
39			2PX	(I)	-0.01632	0.20532	0.00000	0.00000	0.00000
40			2PY	(I)	-0.22053	0.04794	0.00000	0.00000	0.00000
41			2PZ	(I)	0.00000	0.00000	0.01411	0.31491	-0.21374
42			2S	(O)	0.03370	0.02501	0.00000	0.00000	0.00000
43			2PX	(O)	0.02817	0.20909	0.00000	0.00000	0.00000
44			2PY	(O)	-0.19167	-0.02644	0.00000	0.00000	0.00000
45			2PZ	(O)	0.00000	0.00000	0.01671	0.38215	-0.27827
46	6	C	1S		0.00216	0.00653	0.00000	0.00000	0.00000
47			2S	(I)	-0.00075	-0.00668	0.00000	0.00000	0.00000
48			2PX	(I)	-0.01123	-0.18231	0.00000	0.00000	0.00000
49			2PY	(I)	0.21242	-0.00662	0.00000	0.00000	0.00000
50			2PZ	(I)	0.00000	0.00000	-0.10445	0.14370	0.02247
51			2S	(O)	-0.02052	-0.03054	0.00000	0.00000	0.00000
52			2PX	(O)	0.03854	-0.19193	0.00000	0.00000	0.00000
53			2PY	(O)	0.15297	-0.05348	0.00000	0.00000	0.00000
54			2PZ	(O)	0.00000	0.00000	-0.10062	0.14621	0.01786
55	7	C	1S		-0.02436	0.00001	0.00000	0.00000	0.00000
56			2S	(I)	0.03150	-0.00001	0.00000	0.00000	0.00000
57			2PX	(I)	-0.00004	0.08542	0.00000	0.00000	0.00000
58			2PY	(I)	-0.18627	0.00010	0.00000	0.00000	0.00000
59			2PZ	(I)	0.00000	0.00000	0.32918	0.00001	0.31133
60			2S	(O)	0.02681	-0.00001	0.00000	0.00000	0.00000
61			2PX	(O)	-0.00002	0.11163	0.00000	0.00000	0.00000
62			2PY	(O)	-0.10789	0.00008	0.00000	0.00000	0.00000
63			2PZ	(O)	0.00000	0.00000	0.38970	0.00001	0.41658
64	8	H	1S	(I)	0.15439	-0.00005	0.00000	0.00000	0.00000
65			1S	(O)	0.11382	-0.00004	0.00000	0.00000	0.00000
66	9	H	1S	(I)	-0.08351	-0.13271	0.00000	0.00000	0.00000
67			1S	(O)	-0.06984	-0.11558	0.00000	0.00000	0.00000
68	10	H	1S	(I)	-0.06509	0.11470	0.00000	0.00000	0.00000
69			1S	(O)	-0.04952	0.09210	0.00000	0.00000	0.00000
70	11	H	1S	(I)	-0.08343	0.13276	0.00000	0.00000	0.00000
71			1S	(O)	-0.06974	0.11563	0.00000	0.00000	0.00000
72	12	H	1S	(I)	-0.06522	-0.11466	0.00000	0.00000	0.00000
73			1S	(O)	-0.04963	-0.09208	0.00000	0.00000	0.00000
74	13	H	1S	(I)	-0.04649	0.06264	0.00000	0.00000	0.00000

75			1S	(O)	-0.05649	0.05613	0.00000	0.00000	0.00000
76	14	H	1S	(I)	-0.04640	-0.06259	0.00000	0.00000	0.00000
77			1S	(O)	-0.05639	-0.05607	0.00000	0.00000	0.00000
					26	27	28	29	30
					(A")	(A")	(A')	(A')	(A')
	EIGENVALUES		--		0.17016	0.19832	0.26220	0.30002	0.30917
1	1	C	1S		0.00000	0.00000	-0.01543	0.01368	-0.00004
2			2S	(I)	0.00000	0.00000	-0.00230	-0.03845	-0.00001
3			2PX	(I)	0.00000	0.00000	0.00001	-0.00006	0.05923
4			2PY	(I)	0.00000	0.00000	0.00961	-0.02814	-0.00004
5			2PZ	(I)	-0.00001	0.30502	0.00000	0.00000	0.00000
6			2S	(O)	0.00000	0.00000	0.36584	0.36946	0.00075
7			2PX	(O)	0.00000	0.00000	0.00009	-0.00016	-0.05977
8			2PY	(O)	0.00000	0.00000	-0.00981	-0.35960	-0.00048
9			2PZ	(O)	-0.00006	0.71067	0.00000	0.00000	0.00000
10	2	C	1S		0.00000	0.00000	-0.04884	0.02109	-0.00001
11			2S	(I)	0.00000	0.00000	0.02672	0.00775	0.00001
12			2PX	(I)	0.00000	0.00000	-0.00001	-0.00002	0.04030
13			2PY	(I)	0.00000	0.00000	-0.09327	0.09962	0.00003
14			2PZ	(I)	-0.00003	0.20103	0.00000	0.00000	0.00000
15			2S	(O)	0.00000	0.00000	0.55713	-0.59484	0.00004
16			2PX	(O)	0.00000	0.00000	0.00003	-0.00003	0.03033
17			2PY	(O)	0.00000	0.00000	-0.40928	0.23352	-0.00001
18			2PZ	(O)	-0.00004	0.48823	0.00000	0.00000	0.00000
19	3	C	1S		0.00000	0.00000	-0.05312	-0.01564	-0.01516
20			2S	(I)	0.00000	0.00000	0.03222	0.01604	-0.00999
21			2PX	(I)	0.00000	0.00000	0.07357	0.02487	0.16393
22			2PY	(I)	0.00000	0.00000	0.04692	0.03293	0.03493
23			2PZ	(I)	-0.17576	-0.05114	0.00000	0.00000	0.00000
24			2S	(O)	0.00000	0.00000	0.57549	0.08888	0.48540
25			2PX	(O)	0.00000	0.00000	0.39521	0.42413	0.52828
26			2PY	(O)	0.00000	0.00000	0.19924	-0.02101	0.27512
27			2PZ	(O)	-0.41007	-0.14366	0.00000	0.00000	0.00000
28	4	C	1S		0.00000	0.00000	-0.03301	0.04150	-0.02907
29			2S	(I)	0.00000	0.00000	0.00866	-0.02579	0.00475
30			2PX	(I)	0.00000	0.00000	0.07641	-0.05905	0.10720
31			2PY	(I)	0.00000	0.00000	-0.06425	0.00247	-0.03435
32			2PZ	(I)	0.26138	-0.17050	0.00000	0.00000	0.00000
33			2S	(O)	0.00000	0.00000	0.49592	-0.47377	0.52836
34			2PX	(O)	0.00000	0.00000	0.20780	-0.42803	0.35021
35			2PY	(O)	0.00000	0.00000	-0.16917	0.04893	-0.15144
36			2PZ	(O)	0.60392	-0.40101	0.00000	0.00000	0.00000
37	5	C	1S		0.00000	0.00000	-0.05313	-0.01562	0.01519
38			2S	(I)	0.00000	0.00000	0.03221	0.01601	0.01002
39			2PX	(I)	0.00000	0.00000	-0.07362	-0.02508	0.16389
40			2PY	(I)	0.00000	0.00000	0.04691	0.03295	-0.03494
41			2PZ	(I)	0.17575	-0.05110	0.00000	0.00000	0.00000
42			2S	(O)	0.00000	0.00000	0.57571	0.08891	-0.48611
43			2PX	(O)	0.00000	0.00000	-0.39535	-0.42484	0.52754
44			2PY	(O)	0.00000	0.00000	0.19930	-0.02086	-0.27520
45			2PZ	(O)	0.41009	-0.14360	0.00000	0.00000	0.00000
46	6	C	1S		0.00000	0.00000	-0.03302	0.04145	0.02912
47			2S	(I)	0.00000	0.00000	0.00865	-0.02577	-0.00479
48			2PX	(I)	0.00000	0.00000	-0.07641	0.05891	0.10723
49			2PY	(I)	0.00000	0.00000	-0.06424	0.00244	0.03431
50			2PZ	(I)	-0.26132	-0.17056	0.00000	0.00000	0.00000
51			2S	(O)	0.00000	0.00000	0.49609	-0.47306	-0.52889
52			2PX	(O)	0.00000	0.00000	-0.20782	0.42755	0.35059
53			2PY	(O)	0.00000	0.00000	-0.16923	0.04883	0.15168
54			2PZ	(O)	-0.60379	-0.40116	0.00000	0.00000	0.00000

55	7	C	1S		0.00000	0.00000	-0.02562	-0.12111	-0.00008
56			2S	(I)	0.00000	0.00000	0.00794	0.04792	0.00003
57			2PX	(I)	0.00000	0.00000	-0.00003	-0.00010	0.16500
58			2PY	(I)	0.00000	0.00000	0.09317	0.11553	0.00014
59			2PZ	(I)	-0.00001	-0.15291	0.00000	0.00000	0.00000
60			2S	(O)	0.00000	0.00000	0.41015	1.70503	0.00124
61			2PX	(O)	0.00000	0.00000	-0.00017	-0.00051	0.77722
62			2PY	(O)	0.00000	0.00000	0.42893	0.53515	0.00054
63			2PZ	(O)	0.00001	-0.38195	0.00000	0.00000	0.00000
64	8	H	1S	(I)	0.00000	0.00000	-0.05033	0.00741	-0.00001
65			1S	(O)	0.00000	0.00000	-0.85999	0.57512	0.00000
66	9	H	1S	(I)	0.00000	0.00000	-0.02919	0.01764	-0.02116
67			1S	(O)	0.00000	0.00000	-0.65879	0.65052	-0.75272
68	10	H	1S	(I)	0.00000	0.00000	-0.03349	0.03590	-0.01935
69			1S	(O)	0.00000	0.00000	-0.84024	-0.31210	-0.94939
70	11	H	1S	(I)	0.00000	0.00000	-0.02918	0.01760	0.02115
71			1S	(O)	0.00000	0.00000	-0.65892	0.64953	0.75338
72	12	H	1S	(I)	0.00000	0.00000	-0.03349	0.03587	0.01941
73			1S	(O)	0.00000	0.00000	-0.84043	-0.31298	0.94930
74	13	H	1S	(I)	0.00000	0.00000	-0.00552	-0.03502	-0.01121
75			1S	(O)	0.00000	0.00000	-0.42119	-1.11493	-0.80057
76	14	H	1S	(I)	0.00000	0.00000	-0.00552	-0.03506	0.01115
77			1S	(O)	0.00000	0.00000	-0.42135	-1.11594	0.79894

BETA MOLECULAR ORBITAL COEFFICIENTS.

					1	2	3	4	5
					(A')	(A')	(A')	(A')	(A')
	EIGENVALUES --				-11.19227	-11.18040	-11.18028	-11.16506	-11.16505
1	1	C	1S		-0.98711	0.00088	-0.00530	0.00246	0.00346
2			2S	(I)	-0.10086	0.00022	-0.00136	-0.00087	-0.00126
3			2PX	(I)	0.00000	-0.00053	-0.00009	-0.00144	0.00071
4			2PY	(I)	0.00033	0.00013	-0.00081	0.00040	0.00051
5			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
6			2S	(O)	0.09322	-0.00352	0.02155	0.00840	0.01129
7			2PX	(O)	-0.00001	-0.00459	-0.00076	0.01938	-0.00951
8			2PY	(O)	-0.00963	0.00199	-0.01217	-0.00684	-0.00859
9			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
10	2	C	1S		0.00248	-0.00365	0.02249	-0.34084	-0.76678
11			2S	(I)	0.00103	-0.00133	0.00817	-0.03405	-0.07666
12			2PX	(I)	0.00000	-0.00121	-0.00020	-0.00108	0.00053
13			2PY	(I)	0.00024	-0.00028	0.00170	-0.00070	-0.00141
14			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
15			2S	(O)	-0.01038	0.00857	-0.05248	0.02622	0.06254
16			2PX	(O)	0.00000	0.01409	0.00230	0.00072	-0.00036
17			2PY	(O)	-0.00634	0.00488	-0.02988	0.00481	0.01323
18			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
19	3	C	1S		0.00892	-0.00940	0.01320	0.82039	0.00810
20			2S	(I)	0.00441	-0.00411	0.00474	0.08236	0.00067
21			2PX	(I)	-0.00119	0.00025	-0.00064	-0.00134	0.00041
22			2PY	(I)	0.00035	0.00126	-0.00110	-0.00083	-0.00097
23			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
24			2S	(O)	-0.02972	0.02684	-0.03282	-0.07025	0.00276
25			2PX	(O)	0.01755	-0.00802	0.01357	0.01369	-0.00231
26			2PY	(O)	-0.00297	-0.01199	0.01516	0.00526	0.00196
27			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
28	4	C	1S		0.00370	0.80123	-0.57612	0.00458	-0.00867
29			2S	(I)	0.00012	0.08131	-0.05889	-0.00138	0.00176
30			2PX	(I)	-0.00007	-0.00151	-0.00008	-0.00008	-0.00093
31			2PY	(I)	0.00071	0.00033	-0.00071	-0.00116	-0.00026
32			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
33			2S	(O)	0.00881	-0.06711	0.06651	0.01297	-0.01916

34			2PX	(O)	-0.00709	0.01378	-0.01897	-0.00080	0.01365
35			2PY	(O)	0.00200	-0.00726	0.01213	0.01380	0.00190
36			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
37	5	C	1S		0.00891	0.00473	0.01549	-0.43102	0.62195
38			2S	(I)	0.00441	0.00239	0.00580	-0.04336	0.06234
39			2PX	(I)	0.00119	0.00003	0.00068	-0.00114	0.00080
40			2PY	(I)	0.00035	-0.00085	-0.00144	-0.00027	-0.00125
41			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
42			2S	(O)	-0.02973	-0.01500	-0.03967	0.03727	-0.04999
43			2PX	(O)	-0.01756	-0.00328	-0.01542	0.00764	-0.00815
44			2PY	(O)	-0.00297	0.00654	0.01818	-0.00011	0.00460
45			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
46	6	C	1S		0.00369	-0.57621	-0.80117	-0.00752	-0.00275
47			2S	(I)	0.00012	-0.05834	-0.08170	0.00183	0.00018
48			2PX	(I)	0.00007	-0.00146	-0.00041	0.00054	0.00070
49			2PY	(I)	0.00071	-0.00009	-0.00078	0.00041	-0.00103
50			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
51			2S	(O)	0.00881	0.04246	0.08441	-0.01763	-0.00415
52			2PX	(O)	0.00710	0.00703	0.02237	-0.00851	-0.00908
53			2PY	(O)	0.00200	0.00302	0.01381	-0.00520	0.01122
54			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
55	7	C	1S		0.00500	-0.00056	0.00345	-0.00311	-0.00471
56			2S	(I)	0.00345	-0.00020	0.00123	-0.00058	-0.00086
57			2PX	(I)	0.00000	-0.00036	-0.00006	-0.00024	0.00012
58			2PY	(I)	-0.00134	0.00007	-0.00041	0.00007	0.00015
59			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
60			2S	(O)	-0.01841	-0.00013	0.00079	0.00285	0.00349
61			2PX	(O)	0.00000	0.00380	0.00062	-0.00378	0.00185
62			2PY	(O)	0.00964	-0.00023	0.00140	-0.00139	-0.00176
63			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
64	8	H	1S	(I)	-0.00015	0.00003	-0.00016	0.00063	0.00156
65			1S	(O)	-0.00163	0.00118	-0.00721	-0.00261	-0.00551
66	9	H	1S	(I)	0.00047	-0.00187	0.00187	0.00000	0.00011
67			1S	(O)	0.00116	0.00532	-0.00231	0.00193	-0.00276
68	10	H	1S	(I)	0.00038	-0.00016	-0.00031	-0.00154	0.00000
69			1S	(O)	-0.00266	0.00267	-0.00460	0.00603	-0.00008
70	11	H	1S	(I)	0.00047	0.00118	0.00237	0.00011	0.00005
71			1S	(O)	0.00116	-0.00431	-0.00388	-0.00251	-0.00059
72	12	H	1S	(I)	0.00038	0.00025	-0.00024	0.00070	-0.00110
73			1S	(O)	-0.00266	-0.00106	-0.00520	-0.00363	0.00466
74	13	H	1S	(I)	0.00086	-0.00053	0.00006	0.00040	-0.00031
75			1S	(O)	0.00014	-0.00118	-0.00088	0.00083	-0.00028
76	14	H	1S	(I)	0.00086	0.00048	0.00022	-0.00052	0.00014
77			1S	(O)	0.00014	0.00140	-0.00046	-0.00071	0.00048
					6	7	8	9	10
					(A')	(A')	(A')	(A')	(A')
	EIGENVALUES		--		-11.16487	-11.15501	-1.14801	-1.03967	-1.01317
1	1	C	1S		0.01107	-0.00481	-0.11481	-0.14570	-0.00002
2			2S	(I)	-0.00369	0.00253	0.12378	0.15506	0.00002
3			2PX	(I)	0.00010	0.00000	-0.00003	-0.00005	0.08220
4			2PY	(I)	0.00220	0.00179	-0.03602	0.04829	0.00000
5			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
6			2S	(O)	0.04231	-0.02185	0.28855	0.38321	0.00006
7			2PX	(O)	-0.00131	-0.00001	-0.00002	-0.00002	0.03271
8			2PY	(O)	-0.03875	-0.01202	-0.01127	0.02991	0.00001
9			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
10	2	C	1S		0.52018	-0.00156	-0.08423	0.10605	0.00000
11			2S	(I)	0.05244	-0.00019	0.09754	-0.11734	-0.00001
12			2PX	(I)	0.00007	0.00000	-0.00001	0.00001	0.11075
13			2PY	(I)	-0.00011	0.00014	0.05581	-0.03854	0.00000

14			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
15			2S	(O)	-0.06571	0.00345	0.10737	-0.18538	0.00000
16			2PX	(O)	-0.00005	0.00000	0.00000	-0.00001	0.00251
17			2PY	(O)	-0.02482	0.00303	-0.01176	0.00691	0.00001
18			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
19	3	C	1S		0.54940	-0.00918	-0.09033	-0.03146	-0.10224
20			2S	(I)	0.05538	-0.00048	0.10381	0.03333	0.11220
21			2PX	(I)	0.00005	-0.00020	-0.04950	-0.04410	0.00640
22			2PY	(I)	-0.00007	0.00090	-0.02440	0.08169	-0.06498
23			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
24			2S	(O)	-0.06874	0.00396	0.11920	0.07406	0.18793
25			2PX	(O)	0.02277	-0.00090	0.00712	-0.01077	0.00530
26			2PY	(O)	0.01414	-0.00412	0.00011	-0.01082	-0.00593
27			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
28	4	C	1S		0.01909	-0.00243	-0.09831	0.08195	-0.13292
29			2S	(I)	-0.00358	0.00066	0.10744	-0.08602	0.14028
30			2PX	(I)	0.00131	-0.00014	-0.04597	0.04379	0.00679
31			2PY	(I)	-0.00077	0.00022	0.02961	0.03470	0.04928
32			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
33			2S	(O)	0.04898	-0.00642	0.23318	-0.23002	0.35659
34			2PX	(O)	-0.02507	0.00303	-0.02986	0.02345	-0.01454
35			2PY	(O)	0.01532	-0.00384	0.01541	-0.01023	0.01625
36			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
37	5	C	1S		0.63430	-0.00922	-0.09036	-0.03149	0.10221
38			2S	(I)	0.06391	-0.00048	0.10384	0.03337	-0.11217
39			2PX	(I)	0.00012	0.00020	0.04952	0.04411	0.00642
40			2PY	(I)	-0.00010	0.00090	-0.02440	0.08170	0.06500
41			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
42			2S	(O)	-0.07604	0.00396	0.11922	0.07410	-0.18786
43			2PX	(O)	-0.02422	0.00090	-0.00713	0.01077	0.00532
44			2PY	(O)	0.01450	-0.00413	0.00011	-0.01079	0.00591
45			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
46	6	C	1S		0.01994	-0.00244	-0.09834	0.08195	0.13292
47			2S	(I)	-0.00379	0.00066	0.10747	-0.08602	-0.14028
48			2PX	(I)	-0.00134	0.00014	0.04597	-0.04379	0.00680
49			2PY	(I)	-0.00088	0.00022	0.02962	0.03472	-0.04926
50			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
51			2S	(O)	0.05106	-0.00642	0.23325	-0.23000	-0.35659
52			2PX	(O)	0.02571	-0.00303	0.02987	-0.02345	-0.01455
53			2PY	(O)	0.01661	-0.00384	0.01541	-0.01020	-0.01625
54			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
55	7	C	1S		-0.01212	-0.98704	-0.03870	-0.09368	-0.00001
56			2S	(I)	-0.00238	-0.09556	0.04654	0.10462	0.00001
57			2PX	(I)	0.00002	0.00000	0.00001	0.00001	0.01329
58			2PY	(I)	0.00000	0.00018	-0.04085	-0.07424	0.00000
59			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
60			2S	(O)	0.01676	0.06693	0.04270	0.15295	0.00001
61			2PX	(O)	0.00026	0.00000	0.00000	-0.00001	-0.00620
62			2PY	(O)	-0.00781	-0.00714	0.01020	-0.00053	0.00000
63			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
64	8	H	1S	(I)	-0.00195	0.00026	0.03019	-0.05217	0.00000
65			1S	(O)	0.00140	0.00057	-0.00833	-0.00509	0.00000
66	9	H	1S	(I)	0.00020	-0.00010	0.03474	-0.03940	0.07071
67			1S	(O)	0.00770	-0.00152	-0.00083	-0.00830	0.01389
68	10	H	1S	(I)	-0.00210	0.00030	0.03382	0.02164	0.05603
69			1S	(O)	0.00083	0.00089	-0.00456	0.01238	0.01129
70	11	H	1S	(I)	0.00020	-0.00010	0.03475	-0.03941	-0.07072
71			1S	(O)	0.00800	-0.00152	-0.00083	-0.00829	-0.01389
72	12	H	1S	(I)	-0.00225	0.00030	0.03382	0.02165	-0.05602
73			1S	(O)	0.00148	0.00089	-0.00457	0.01238	-0.01128

74	13	H	1S	(I)	-0.00036	0.00141	0.01651	0.04631	0.00516
75			1S	(O)	0.00010	-0.01250	-0.00078	0.00832	0.00760
76	14	H	1S	(I)	-0.00030	0.00141	0.01651	0.04632	-0.00515
77			1S	(O)	0.00021	-0.01250	-0.00078	0.00831	-0.00760
					11	12	13	14	15
					(A')	(A')	(A')	(A')	(A')
	EIGENVALUES --				-0.87732	-0.82079	-0.78529	-0.69367	-0.63995
1	1	C	1S		-0.01010	-0.00002	-0.08227	0.03024	0.00007
2			2S	(I)	0.01033	0.00002	0.08561	-0.02865	-0.00008
3			2PX	(I)	-0.00003	0.20225	-0.00003	0.00003	0.20212
4			2PY	(I)	0.17699	0.00002	-0.11012	-0.07854	-0.00005
5			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
6			2S	(O)	0.04142	0.00010	0.29428	-0.12415	-0.00022
7			2PX	(O)	-0.00006	0.11506	-0.00001	0.00002	0.15595
8			2PY	(O)	0.09559	0.00000	-0.09553	-0.03582	-0.00018
9			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
10	2	C	1S		-0.10781	-0.00001	-0.08099	0.02339	-0.00008
11			2S	(I)	0.11347	0.00001	0.08517	-0.02079	0.00008
12			2PX	(I)	-0.00001	-0.15383	0.00000	-0.00001	0.19528
13			2PY	(I)	-0.02562	-0.00001	-0.01741	0.20141	-0.00010
14			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
15			2S	(O)	0.28429	0.00001	0.23722	-0.09476	0.00022
16			2PX	(O)	0.00001	-0.04525	0.00001	0.00000	0.09725
17			2PY	(O)	0.00484	-0.00001	0.00157	0.12633	-0.00014
18			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
19	3	C	1S		0.07837	-0.10027	0.02138	0.01730	0.01885
20			2S	(I)	-0.08490	0.10542	-0.02019	-0.01570	-0.01873
21			2PX	(I)	0.00619	-0.00076	-0.13297	-0.09802	-0.08489
22			2PY	(I)	0.03783	0.09403	0.08512	-0.10966	0.17672
23			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
24			2S	(O)	-0.18168	0.27697	-0.08197	-0.06052	-0.07004
25			2PX	(O)	-0.00378	-0.00041	-0.03815	-0.07644	-0.03609
26			2PY	(O)	0.00426	0.01916	0.02479	-0.06156	0.08634
27			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
28	4	C	1S		-0.00073	0.07870	0.05521	-0.00757	-0.00529
29			2S	(I)	0.00144	-0.07984	-0.05533	0.01326	0.00402
30			2PX	(I)	-0.05763	0.00472	-0.13089	-0.13649	-0.07507
31			2PY	(I)	-0.12245	0.10693	-0.06571	0.09894	-0.21114
32			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
33			2S	(O)	-0.01590	-0.27571	-0.19270	0.00472	0.02802
34			2PX	(O)	-0.00887	0.00870	-0.07118	-0.09200	-0.04393
35			2PY	(O)	-0.05442	0.04037	-0.02742	0.06614	-0.13282
36			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
37	5	C	1S		0.07836	0.10027	0.02135	0.01731	-0.01897
38			2S	(I)	-0.08490	-0.10542	-0.02016	-0.01571	0.01888
39			2PX	(I)	-0.00619	-0.00074	0.13300	0.09803	-0.08514
40			2PY	(I)	0.03787	-0.09397	0.08516	-0.10967	-0.17664
41			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
42			2S	(O)	-0.18169	-0.27697	-0.08189	-0.06055	0.07030
43			2PX	(O)	0.00376	-0.00042	0.03817	0.07645	-0.03644
44			2PY	(O)	0.00422	-0.01917	0.02479	-0.06155	-0.08615
45			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
46	6	C	1S		-0.00072	-0.07868	0.05522	-0.00758	0.00541
47			2S	(I)	0.00142	0.07981	-0.05534	0.01328	-0.00416
48			2PX	(I)	0.05765	0.00474	0.13092	0.13652	-0.07479
49			2PY	(I)	-0.12248	-0.10697	-0.06570	0.09894	0.21130
50			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
51			2S	(O)	-0.01596	0.27562	-0.19274	0.00479	-0.02834
52			2PX	(O)	0.00889	0.00872	0.07119	0.09202	-0.04359
53			2PY	(O)	-0.05446	-0.04041	-0.02743	0.06615	0.13305

54			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
55	7	C	1S		-0.13683	-0.00001	0.09194	-0.04742	-0.00002
56			2S	(I)	0.14826	0.00001	-0.09747	0.04662	0.00001
57			2PX	(I)	0.00000	0.05976	0.00002	-0.00002	0.18412
58			2PY	(I)	-0.01847	0.00001	-0.07682	0.12585	0.00021
59			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.00000
60			2S	(O)	0.31157	0.00002	-0.24414	0.15627	0.00018
61			2PX	(O)	0.00001	0.02337	0.00001	-0.00001	0.11559
62			2PY	(O)	0.00905	0.00000	-0.04113	0.06787	0.00006
63			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.00000
64	8	H	1S	(I)	0.09357	0.00001	0.07770	-0.14363	0.00014
65			1S	(O)	0.04431	0.00001	0.04303	-0.09851	0.00008
66	9	H	1S	(I)	0.00551	-0.07982	-0.08101	-0.08684	0.02968
67			1S	(O)	-0.00136	-0.03553	-0.03656	-0.05576	0.01998
68	10	H	1S	(I)	-0.04654	0.10531	-0.05799	-0.09960	-0.00611
69			1S	(O)	-0.01073	0.05599	-0.04234	-0.06297	-0.00081
70	11	H	1S	(I)	0.00550	0.07981	-0.08104	-0.08684	-0.02999
71			1S	(O)	-0.00137	0.03552	-0.03657	-0.05576	-0.02013
72	12	H	1S	(I)	-0.04653	-0.10529	-0.05799	-0.09960	0.00644
73			1S	(O)	-0.01072	-0.05597	-0.04234	-0.06297	0.00099
74	13	H	1S	(I)	0.10090	0.02756	-0.10178	0.08349	0.10642
75			1S	(O)	0.03954	0.02154	-0.05755	0.05688	0.08766
76	14	H	1S	(I)	0.10092	-0.02755	-0.10179	0.08350	-0.10626
77			1S	(O)	0.03955	-0.02153	-0.05756	0.05688	-0.08749
					16	17	18	19	20
					(A')	(A')	(A')	(A')	(A")
	EIGENVALUES --				-0.63808	-0.58957	-0.57784	-0.54689	-0.50543
1	1	C	1S		0.06829	0.00001	0.00833	-0.00002	0.00000
2			2S	(I)	-0.07279	-0.00001	-0.00770	0.00001	0.00000
3			2PX	(I)	-0.00022	-0.10164	-0.00005	0.06462	0.00000
4			2PY	(I)	-0.08226	0.00002	0.27996	0.00006	0.00000
5			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.23749
6			2S	(O)	-0.24552	-0.00003	-0.00581	0.00011	0.00000
7			2PX	(O)	-0.00009	-0.08645	-0.00012	0.09826	0.00000
8			2PY	(O)	-0.10859	0.00000	0.22095	0.00001	0.00000
9			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.25199
10	2	C	1S		-0.06109	0.00000	-0.01986	0.00000	0.00000
11			2S	(I)	0.06487	0.00000	0.02329	0.00000	0.00000
12			2PX	(I)	-0.00020	-0.11342	-0.00004	0.15467	0.00000
13			2PY	(I)	-0.07227	0.00005	0.22304	0.00016	0.00000
14			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.12975
15			2S	(O)	0.17792	-0.00001	0.03027	-0.00003	0.00000
16			2PX	(O)	-0.00012	-0.05677	0.00000	0.08941	0.00000
17			2PY	(O)	-0.09507	0.00003	0.17027	0.00015	0.00000
18			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.10684
19	3	C	1S		-0.05850	0.01844	0.00924	-0.02000	0.00000
20			2S	(I)	0.06131	-0.02245	-0.01075	0.02009	0.00000
21			2PX	(I)	0.10549	0.17477	0.13612	0.00904	0.00000
22			2PY	(I)	0.04295	0.10594	0.01705	0.13179	0.00000
23			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.13338
24			2S	(O)	0.17410	-0.01529	-0.00992	0.05604	0.00000
25			2PX	(O)	0.10625	0.12072	0.10084	0.04468	0.00000
26			2PY	(O)	0.06512	0.08121	0.01385	0.07243	0.00000
27			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.10817
28	4	C	1S		0.05180	0.01902	-0.01013	0.00845	0.00000
29			2S	(I)	-0.05403	-0.02363	0.01280	-0.00883	0.00000
30			2PX	(I)	-0.10983	0.20594	-0.12785	-0.10073	0.00000
31			2PY	(I)	0.06294	-0.11517	-0.00236	-0.11710	0.00000
32			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.21241
33			2S	(O)	-0.16483	-0.04138	0.01632	-0.03584	0.00000

34			2PX	(O)	-0.11834	0.17769	-0.09929	-0.09077	0.00000
35			2PY	(O)	0.07358	-0.09091	0.00829	-0.07601	0.00000
36			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.22432
37	5	C	1S		-0.05845	-0.01843	0.00924	0.02005	0.00000
38			2S	(I)	0.06126	0.02245	-0.01075	-0.02013	0.00000
39			2PX	(I)	-0.10530	0.17472	-0.13616	0.00903	0.00000
40			2PY	(I)	0.04330	-0.10589	0.01718	-0.13164	0.00000
41			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.13341
42			2S	(O)	0.17402	0.01522	-0.00995	-0.05626	0.00000
43			2PX	(O)	-0.10612	0.12065	-0.10094	0.04461	0.00000
44			2PY	(O)	0.06534	-0.08114	0.01385	-0.07232	0.00000
45			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.10818
46	6	C	1S		0.05179	-0.01904	-0.01012	-0.00849	0.00000
47			2S	(I)	-0.05402	0.02364	0.01279	0.00886	0.00000
48			2PX	(I)	0.10999	0.20595	0.12786	-0.10068	0.00000
49			2PY	(I)	0.06251	0.11514	-0.00248	0.11690	0.00000
50			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.21242
51			2S	(O)	-0.16476	0.04147	0.01628	0.03599	0.00000
52			2PX	(O)	0.11839	0.17771	0.09931	-0.09074	0.00000
53			2PY	(O)	0.07332	0.09093	0.00816	0.07588	0.00000
54			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.22433
55	7	C	1S		-0.01012	0.00000	0.00228	0.00000	0.00000
56			2S	(I)	0.00537	0.00000	0.00505	0.00000	0.00000
57			2PX	(I)	-0.00033	0.00098	0.00015	-0.29845	0.00000
58			2PY	(I)	0.16097	-0.00002	-0.23498	-0.00012	0.00000
59			2PZ	(I)	0.00000	0.00000	0.00000	0.00000	0.06116
60			2S	(O)	0.09262	0.00001	-0.06790	0.00000	0.00000
61			2PX	(O)	-0.00023	0.01703	0.00013	-0.26796	0.00000
62			2PY	(O)	0.05924	-0.00001	-0.13059	-0.00010	0.00000
63			2PZ	(O)	0.00000	0.00000	0.00000	0.00000	0.04506
64	8	H	1S	(I)	0.11122	-0.00003	-0.13953	-0.00013	0.00000
65			1S	(O)	0.06535	-0.00003	-0.11838	-0.00011	0.00000
66	9	H	1S	(I)	-0.12576	0.13569	-0.06269	-0.02929	0.00000
67			1S	(O)	-0.06601	0.09919	-0.04794	-0.01664	0.00000
68	10	H	1S	(I)	0.13687	0.12551	0.08035	0.07328	0.00000
69			1S	(O)	0.08740	0.10745	0.06486	0.05117	0.00000
70	11	H	1S	(I)	-0.12571	-0.13568	-0.06267	0.02936	0.00000
71			1S	(O)	-0.06597	-0.09916	-0.04791	0.01669	0.00000
72	12	H	1S	(I)	0.13684	-0.12547	0.08042	-0.07325	0.00000
73			1S	(O)	0.08739	-0.10743	0.06491	-0.05116	0.00000
74	13	H	1S	(I)	0.06847	0.00491	-0.08823	-0.19840	0.00000
75			1S	(O)	0.06629	0.00349	-0.08166	-0.16959	0.00000
76	14	H	1S	(I)	0.06883	-0.00492	-0.08836	0.19834	0.00000
77			1S	(O)	0.06656	-0.00350	-0.08174	0.16952	0.00000
					21	22	23	24	25
					(A')	(A')	(A")	(A")	(A")
	EIGENVALUES --				-0.49834	-0.47889	-0.37762	-0.36044	0.11535
1	1	C	1S		0.00251	0.00001	0.00000	0.00000	0.00000
2			2S	(I)	-0.00038	-0.00001	0.00000	0.00000	0.00000
3			2PX	(I)	-0.00009	-0.25802	0.00000	0.00000	0.00000
4			2PY	(I)	0.18908	-0.00011	0.00000	0.00000	0.00000
5			2PZ	(I)	0.00000	0.00000	0.34244	-0.00013	-0.04236
6			2S	(O)	-0.00858	-0.00007	0.00000	0.00000	0.00000
7			2PX	(O)	-0.00016	-0.25052	0.00000	0.00000	0.00000
8			2PY	(O)	0.23363	-0.00012	0.00000	0.00000	0.00000
9			2PZ	(O)	0.00000	0.00000	0.41204	-0.00017	-0.09229
10	2	C	1S		0.00308	0.00000	0.00000	0.00000	0.00000
11			2S	(I)	-0.00341	0.00000	0.00000	0.00000	0.00000
12			2PX	(I)	0.00010	0.19006	0.00000	0.00000	0.00000
13			2PY	(I)	-0.20247	0.00006	0.00000	0.00000	0.00000

14			2PZ	(I)	0.00000	0.00000	-0.15519	0.00007	-0.21254
15			2S	(O)	-0.01106	-0.00002	0.00000	0.00000	0.00000
16			2PX	(O)	0.00005	0.13094	0.00000	0.00000	0.00000
17			2PY	(O)	-0.23080	0.00004	0.00000	0.00000	0.00000
18			2PZ	(O)	0.00000	0.00000	-0.15374	0.00007	-0.43407
19	3	C	1S		-0.00606	0.01092	0.00000	0.00000	0.00000
20			2S	(I)	0.00725	-0.01217	0.00000	0.00000	0.00000
21			2PX	(I)	0.00892	0.20079	0.00000	0.00000	0.00000
22			2PY	(I)	-0.20700	-0.03794	0.00000	0.00000	0.00000
23			2PZ	(I)	0.00000	0.00000	0.04634	-0.14230	0.17117
24			2S	(O)	0.02525	-0.01800	0.00000	0.00000	0.00000
25			2PX	(O)	-0.03538	0.19065	0.00000	0.00000	0.00000
26			2PY	(O)	-0.16935	0.03846	0.00000	0.00000	0.00000
27			2PZ	(O)	0.00000	0.00000	0.04371	-0.14664	0.32342
28	4	C	1S		0.00027	-0.00675	0.00000	0.00000	0.00000
29			2S	(I)	0.00163	0.00763	0.00000	0.00000	0.00000
30			2PX	(I)	0.02182	-0.18003	0.00000	0.00000	0.00000
31			2PY	(I)	0.22430	-0.00250	0.00000	0.00000	0.00000
32			2PZ	(I)	0.00000	0.00000	-0.18834	-0.31208	0.01633
33			2S	(O)	-0.01072	0.03746	0.00000	0.00000	0.00000
34			2PX	(O)	-0.02838	-0.19559	0.00000	0.00000	0.00000
35			2PY	(O)	0.17269	0.04808	0.00000	0.00000	0.00000
36			2PZ	(O)	0.00000	0.00000	-0.22941	-0.38565	0.05914
37	5	C	1S		-0.00604	-0.01093	0.00000	0.00000	0.00000
38			2S	(I)	0.00724	0.01218	0.00000	0.00000	0.00000
39			2PX	(I)	-0.00873	0.20080	0.00000	0.00000	0.00000
40			2PY	(I)	-0.20708	0.03810	0.00000	0.00000	0.00000
41			2PZ	(I)	0.00000	0.00000	0.04646	0.14225	0.17113
42			2S	(O)	0.02503	0.01796	0.00000	0.00000	0.00000
43			2PX	(O)	0.03552	0.19062	0.00000	0.00000	0.00000
44			2PY	(O)	-0.16945	-0.03827	0.00000	0.00000	0.00000
45			2PZ	(O)	0.00000	0.00000	0.04383	0.14659	0.32333
46	6	C	1S		0.00025	0.00674	0.00000	0.00000	0.00000
47			2S	(I)	0.00164	-0.00763	0.00000	0.00000	0.00000
48			2PX	(I)	-0.02198	-0.18002	0.00000	0.00000	0.00000
49			2PY	(I)	0.22439	0.00236	0.00000	0.00000	0.00000
50			2PZ	(I)	0.00000	0.00000	-0.18812	0.31219	0.01638
51			2S	(O)	-0.01065	-0.03736	0.00000	0.00000	0.00000
52			2PX	(O)	0.02825	-0.19556	0.00000	0.00000	0.00000
53			2PY	(O)	0.17276	-0.04815	0.00000	0.00000	0.00000
54			2PZ	(O)	0.00000	0.00000	-0.22915	0.38578	0.05925
55	7	C	1S		-0.02414	0.00001	0.00000	0.00000	0.00000
56			2S	(I)	0.03111	-0.00001	0.00000	0.00000	0.00000
57			2PX	(I)	-0.00005	0.09069	0.00000	0.00000	0.00000
58			2PY	(I)	-0.16955	0.00010	0.00000	0.00000	0.00000
59			2PZ	(I)	0.00000	0.00000	0.11388	-0.00004	-0.24623
60			2S	(O)	0.00670	0.00000	0.00000	0.00000	0.00000
61			2PX	(O)	-0.00003	0.11283	0.00000	0.00000	0.00000
62			2PY	(O)	-0.07725	0.00007	0.00000	0.00000	0.00000
63			2PZ	(O)	0.00000	0.00000	0.11092	-0.00004	-0.48687
64	8	H	1S	(I)	0.16807	-0.00006	0.00000	0.00000	0.00000
65			1S	(O)	0.14267	-0.00006	0.00000	0.00000	0.00000
66	9	H	1S	(I)	-0.07267	-0.11682	0.00000	0.00000	0.00000
67			1S	(O)	-0.05462	-0.09102	0.00000	0.00000	0.00000
68	10	H	1S	(I)	-0.07440	0.12628	0.00000	0.00000	0.00000
69			1S	(O)	-0.06434	0.11591	0.00000	0.00000	0.00000
70	11	H	1S	(I)	-0.07259	0.11687	0.00000	0.00000	0.00000
71			1S	(O)	-0.05453	0.09107	0.00000	0.00000	0.00000
72	12	H	1S	(I)	-0.07457	-0.12623	0.00000	0.00000	0.00000
73			1S	(O)	-0.06450	-0.11587	0.00000	0.00000	0.00000

74	13	H	1S	(I)	-0.04508	0.07590	0.00000	0.00000	0.00000
75			1S	(O)	-0.06076	0.07631	0.00000	0.00000	0.00000
76	14	H	1S	(I)	-0.04498	-0.07585	0.00000	0.00000	0.00000
77			1S	(O)	-0.06064	-0.07624	0.00000	0.00000	0.00000
					26	27	28	29	30
					(A")	(A")	(A')	(A')	(A')
	EIGENVALUES --				0.18177	0.22950	0.26658	0.31228	0.31290
1	1	C	1S		0.00000	0.00000	0.01968	-0.00009	-0.00433
2			2S	(I)	0.00000	0.00000	-0.00287	0.00051	0.04161
3			2PX	(I)	0.00000	0.00000	-0.00002	0.05666	-0.00067
4			2PY	(I)	0.00000	0.00000	-0.00115	0.00002	0.00295
5			2PZ	(I)	-0.00005	-0.21226	0.00000	0.00000	0.00000
6			2S	(O)	0.00000	0.00000	-0.35584	-0.00654	-0.58562
7			2PX	(O)	0.00000	0.00000	-0.00009	-0.06232	0.00092
8			2PY	(O)	0.00000	0.00000	-0.00079	0.00333	0.29468
9			2PZ	(O)	-0.00016	-0.49619	0.00000	0.00000	0.00000
10	2	C	1S		0.00000	0.00000	0.04420	-0.00008	-0.00554
11			2S	(I)	0.00000	0.00000	-0.02233	-0.00021	-0.01774
12			2PX	(I)	0.00000	0.00000	0.00001	0.03291	-0.00041
13			2PY	(I)	0.00000	0.00000	0.10711	-0.00109	-0.09053
14			2PZ	(I)	-0.00009	-0.23908	0.00000	0.00000	0.00000
15			2S	(O)	0.00000	0.00000	-0.51650	0.00556	0.44071
16			2PX	(O)	0.00000	0.00000	-0.00004	-0.02504	0.00030
17			2PY	(O)	0.00000	0.00000	0.43081	-0.00172	-0.13782
18			2PZ	(O)	-0.00020	-0.62095	0.00000	0.00000	0.00000
19	3	C	1S		0.00000	0.00000	0.04666	-0.00884	0.02946
20			2S	(I)	0.00000	0.00000	-0.02816	-0.01379	-0.02363
21			2PX	(I)	0.00000	0.00000	-0.07022	0.15583	-0.04938
22			2PY	(I)	0.00000	0.00000	-0.04265	0.03833	-0.04028
23			2PZ	(I)	-0.25677	0.02886	0.00000	0.00000	0.00000
24			2S	(O)	0.00000	0.00000	-0.48378	0.40206	-0.22614
25			2PX	(O)	0.00000	0.00000	-0.33984	0.46055	-0.56761
26			2PY	(O)	0.00000	0.00000	-0.20563	0.29443	-0.04136
27			2PZ	(O)	-0.60791	0.11153	0.00000	0.00000	0.00000
28	4	C	1S		0.00000	0.00000	0.04536	-0.04017	-0.04097
29			2S	(I)	0.00000	0.00000	-0.01472	0.00742	0.02811
30			2PX	(I)	0.00000	0.00000	-0.08500	0.12489	0.05076
31			2PY	(I)	0.00000	0.00000	0.06756	-0.04401	-0.00248
32			2PZ	(I)	0.17420	0.13666	0.00000	0.00000	0.00000
33			2S	(O)	0.00000	0.00000	-0.66909	0.72518	0.45669
34			2PX	(O)	0.00000	0.00000	-0.27130	0.44049	0.44810
35			2PY	(O)	0.00000	0.00000	0.19034	-0.18682	-0.08013
36			2PZ	(O)	0.41358	0.30366	0.00000	0.00000	0.00000
37	5	C	1S		0.00000	0.00000	0.04668	0.00959	0.02921
38			2S	(I)	0.00000	0.00000	-0.02815	0.01321	-0.02394
39			2PX	(I)	0.00000	0.00000	0.07024	0.15696	0.04562
40			2PY	(I)	0.00000	0.00000	-0.04265	-0.03933	-0.03933
41			2PZ	(I)	0.25679	0.02872	0.00000	0.00000	0.00000
42			2S	(O)	0.00000	0.00000	-0.48405	-0.40818	-0.21584
43			2PX	(O)	0.00000	0.00000	0.33993	0.47388	0.55640
44			2PY	(O)	0.00000	0.00000	-0.20564	-0.29540	-0.03408
45			2PZ	(O)	0.60799	0.11122	0.00000	0.00000	0.00000
46	6	C	1S		0.00000	0.00000	0.04535	0.03918	-0.04191
47			2S	(I)	0.00000	0.00000	-0.01471	-0.00675	0.02827
48			2PX	(I)	0.00000	0.00000	0.08498	0.12360	-0.05373
49			2PY	(I)	0.00000	0.00000	0.06755	0.04390	-0.00354
50			2PZ	(I)	-0.17410	0.13676	0.00000	0.00000	0.00000
51			2S	(O)	0.00000	0.00000	-0.66916	-0.71396	0.47390
52			2PX	(O)	0.00000	0.00000	0.27126	0.42947	-0.45851
53			2PY	(O)	0.00000	0.00000	0.19044	0.18502	-0.08467

54			2PZ	(O)	-0.41340	0.30393	0.00000	0.00000	0.00000
55	7	C	1S		0.00000	0.00000	0.00947	0.00139	0.11616
56			2S	(I)	0.00000	0.00000	0.00100	-0.00057	-0.04677
57			2PX	(I)	0.00000	0.00000	0.00002	0.14103	-0.00170
58			2PY	(I)	0.00000	0.00000	-0.08303	-0.00148	-0.12810
59			2PZ	(I)	0.00002	0.22941	0.00000	0.00000	0.00000
60			2S	(O)	0.00000	0.00000	-0.20154	-0.01879	-1.57251
61			2PX	(O)	0.00000	0.00000	0.00014	0.68810	-0.00822
62			2PY	(O)	0.00000	0.00000	-0.35629	-0.00777	-0.66350
63			2PZ	(O)	0.00009	0.63328	0.00000	0.00000	0.00000
64	8	H	1S	(I)	0.00000	0.00000	0.03983	0.00007	0.00642
65			1S	(O)	0.00000	0.00000	0.85423	-0.00477	-0.38277
66	9	H	1S	(I)	0.00000	0.00000	0.04212	-0.02695	-0.01748
67			1S	(O)	0.00000	0.00000	0.82791	-0.94920	-0.65518
68	10	H	1S	(I)	0.00000	0.00000	0.02604	-0.01284	-0.02858
69			1S	(O)	0.00000	0.00000	0.74484	-0.84990	0.57001
70	11	H	1S	(I)	0.00000	0.00000	0.04211	0.02649	-0.01811
71			1S	(O)	0.00000	0.00000	0.82793	0.93309	-0.67774
72	12	H	1S	(I)	0.00000	0.00000	0.02604	0.01216	-0.02887
73			1S	(O)	0.00000	0.00000	0.74499	0.86367	0.54906
74	13	H	1S	(I)	0.00000	0.00000	-0.00226	-0.00700	0.01452
75			1S	(O)	0.00000	0.00000	0.27474	-0.68048	1.11103
76	14	H	1S	(I)	0.00000	0.00000	-0.00226	0.00734	0.01437
77			1S	(O)	0.00000	0.00000	0.27485	0.70681	1.09435

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VITA

Henry Ntiri Berko

Candidate for the Degree of

Doctor of Philosophy

Thesis: MERCURY PHOTOSENSITIZATION OF TOLUENE VAPOR AND AEROSOL FORMATION

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