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COMPUTED STRUCTURES OF POLYIMIDES MODEL COMPOUNDS

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Abstract -- Using a semiempirical approach, a computer study has been made of 8 model compounds of polyimides. The compounds represent subunits from which NASA-Langley Research Center has successfully synthesized polymers for aerospace high performance material application, including one of the most promising, LaRC-TPI polymer. Three dimensional graphic display as well as important molecular structure data pertaining to these eight compounds are obtained.

I. Introduction

The utilization of computational chemistry as a routine procedure in chemical research is rapidly coming of age. The greatest economic and scientific benefits of these techniques come from allowing chemists to build three-dimensional models of chemical structures whose activity

and properties can be predicted before they are synthesized and tested. Molecular computer graphics are used to simulate and visualize what various prototype compounds look like in terms of their molecular structure, shape, and topology. It is well known that the chemical and physical properties of molecules are dependent upon their equilibrium and transition electronic structures, and much of quantum chemical research is concerned with the accurate prediction of molecular structure and properties. Properties such as electronic densities, electron affinities, electrostatic potentials, chemical reactivity, dipole and quadrupole moments can all be calculated using quantum chemical computational techniques. Other physical properties, such as ionization potentials, heats of formation and activation energies, harmonic force constants, and vibrational frequencies can also be estimated. Currently, there are three types of calculations that are being applied. (1) LCAO-SCF approaches to ab initio Hartree Fock calculations historically break down into two steps: the calculation and storage of all 2-electron integrals over the operators in the Hamiltonian; and the iterating over the Fock matrix in order to achieve a self-consistent energy[1] . On the order of N^4 molecular integrals (where N is the number of basis functions) must be evaluated to determine the energy[2] . This method is capable of giving accurate results; however, as the system becomes larger, it utilizes extensive computing resources. (2) Semi-Empirical methods have evolved that describe the backbone framework of the structure on the basis of classical mechanics and add a semiempirical Hamiltonian to describe the electron system. (3) Simpler (empirical) methods use a purely

classical potential function model. The theory and detailed descriptions can be found in the literature[3]. In this report, the intermediate semiempirical approach has been adopted for the investigation of eight compounds. Langley researchers recently have successfully synthesized some promising polymers incorporating these groups, including LaRC-TPI.

II. Methods and Procedures

In this calculation, we opt to use two existing software packages which are available to us at this time. The first package, XIRIS molecular modeling system, version 1.0, a commercial package[4] allows us to set up and create the molecule by inputting the relevant information, such as different atomic species and bond types (single bond, or double bond, or ring structure etc.) Then, the XIRIS takes this two dimensional graphic input information and calculates a low energy conformation of the molecule using a classical molecular mechanics approach. Essentially, this package adopts the view that a molecule is a collection of particles held together by simple harmonic or elastic forces. These forces can be defined by a potential energy function whose terms depend on the atomic coordinates. This function can then be minimized to obtain a least strain, three dimensional model of the molecule. To implement a molecular modeling system, a potential energy function to calculate a strain for the molecule and an algorithm to minimize the strain are required. The algorithm used in this system is a descendent of the one developed

by Wipke and colleagues at Princeton during the early 1970s. The potential energy contains five major terms:

1. A bond stretching term based upon Hooke's law. The standard bond lengths and force constants are obtained from the bond data file.

2. A bond angle term based upon Hooke's law. The standard bond angles of 109.5, 120.0, and 180.0 degrees are used for sp3, sp2, and sp type atoms, respectively.

3. A non-bonded repulsion term or Van der Waal's term calculated using a modified Hooke's law.

4. A torsional term based upon Hooke's law.

5. A stereoisomer term which increases the strain of any chiral center.

Once a molecule has been modeled, the XIRIS system has several commands that allow us to determine various parameters as well as information about the geometry of the structure. It also can orient the structure into a good position for viewing and for drawing options.

One important final output from XIRIS consists of a set of atomic coordinates corresponding to the lowest energy conformation along with other information pertaining to this particular molecule. This information can then be input to the second of our modeling programs (Quantum mechanical extension of the consistent force field to PI electron systems, by A. Warshel and M. Levitt), which is based on the CHARMM program (which stands for Chemistry at HARvard Macromolecular Mechanics) . The program uses empirical energy functions to model the σ

electrons of macromolecular systems combined with a semiempirical Hartree Fock model for the π electrons and calculates equilibrium conformations and the vibrational frequencies of normal modes of the ground states of large conjugated molecules. The energy and oscillator strengths of π electron transitions are also calculated. The equilibrium geometries are calculated by minimization of the molecular energy with respect to the complete set of 3N Cartesian coordinates. The vibrational normal modes are calculated by diagonalization of the matrix of second derivatives of the potential with respect to the mass-scaled Cartesian coordinates at the calculated minimum[4]. The empirical energy function which is based on separable internal coordinates and pairwise nonbonded interactions contains similar but more elaborate terms than XIRIS. Therefore, CHARMM should be capable of predicting more reliable results than a purely empirical model such as XIRIS. Nevertheless, the results from the two programs should be similar, and this is in fact what we have obtained. These two modeling programs have been applied to eight model compounds for polymers[7] recently developed at Langley research center. The names of the compounds as well as aliases (in brackets) are listed in the following.

1. N-phenylphthalimide [ltp1]
2. N-(3-benzoylphenyl)phthalimide [ltp2]
3. 4-benzoyl-N-phenylphthalimide [ltp3]
4. N-(4-phenoxyphenyl)phthalimide [ltp4]
5. N-phenyl-4-phenoxyphthalimide [ltp5]

6. N,N'-diphenylpyromellitimide [ltp6]

7. N,N'-diphenyl-3,4,3',4'-benzophenoetetra-

carboxylicdiimide [ltp7]

8. N,N'-diphenyl-3,4,3',4'-oxydiphthalimide [ltp8]

III. Results

For brevity, the compounds are renamed ltp1....to ltp8 and each output is listed separately. As mentioned earlier, the results predicted by the two programs are similar, so we choose to present the structure results generated by CHARMM, while the graphic results are created by the XIRIS program (simply, the CHARMM program does not have the graphic capability). With the atoms labelled, one can easily identify each atom and the relevant structure data associated with specific atom or bonds. For each molecule, the graphic presentations are given first, e.g. Fig. na and Fig. nb. n being from 1 to 8. Fig. na labels the atoms, while Fig. nb uses a space filled mode which shows dihedral angles and other aspects of the geometry more clearly. After the graphic output, we list the structure results predicted by CHARMM. The main products are the equilibrium structure constants, such as bond lengths and bond angles. With the graphic display, we can easily identify those constants that would be considered the major contribution for this exercise. In addition, the coordinates of each atom and the I.R. spectrum

of the molecule are listed. Finally, a plot of the I.R. radiation intensity (in arbitrary units) versus wave number is given and denoted Fig. nc.

IV. Discussion

We have successfully applied two pieces of software to 8 LaRC-TPI compounds to obtain some molecular structure constants - thereby gaining some understanding of those molecules. Initial results, although not totally satisfactory, are quite encouraging. For example, we have compared the I.R. spectrum of ltp1 to the experimental result. Our calculation is able to predict the major peaks, but misses one or two. The implication of this is not clear at this time. Whether we can fine tune the force constants so that the I.R. spectrum is totally in agreement with the experimental work without invalidating the structure constants is not clear. We will probably look into this in the future. However, we believe the molecular constants given in this report are fairly reliable.

References

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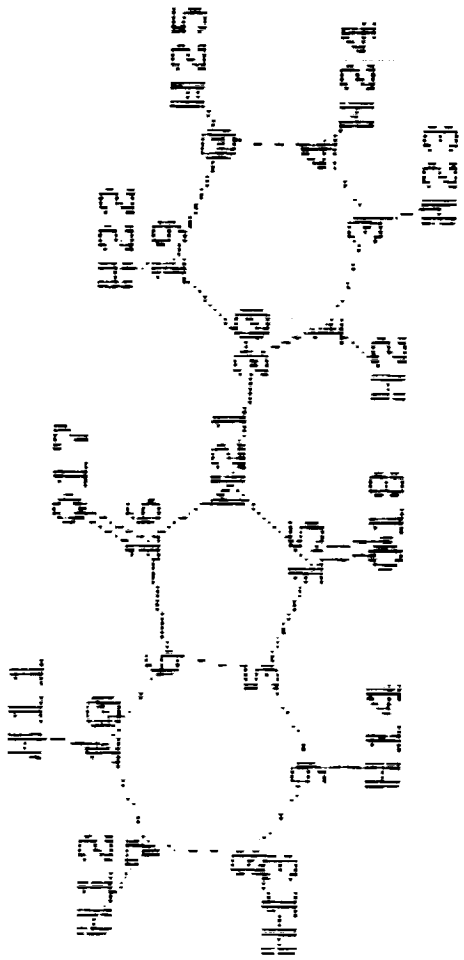

Fig. 1a

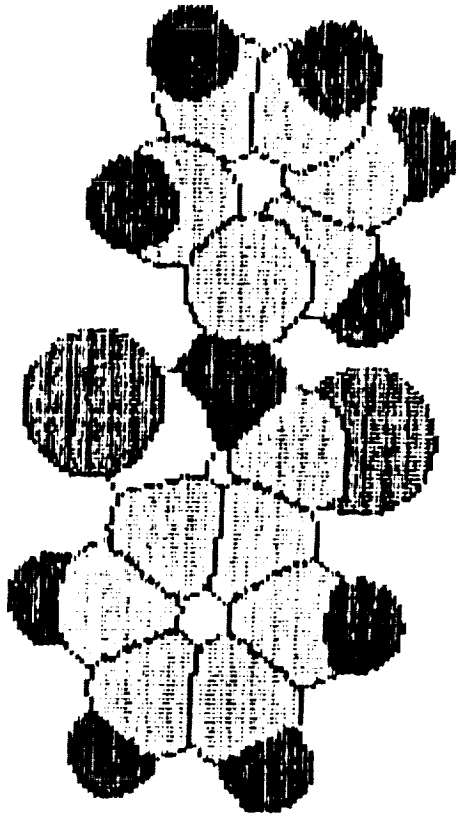

Fig. 1b

F I N A L R E S U L T S

ltp1

BOND LENGTHS (IN ANGSTROMS)	TYPE	ATOMS INVOLVED
1.5167	AA	6 16
1.4194	AA	6 5
1.2560	AO	16 17
1.4120	AN	16 21
1.4842	NA	21 20
1.4663	NA	21 15
1.4246	AA	20 19
1.4229	AA	20 1
1.0794	AH	19 22
1.4037	AA	19 0
1.0836	AH	0 25
1.4012	AA	0 4
1.0830	AH	4 24
1.4006	AA	4 3
1.0836	AH	3 23
1.4049	AA	3 1
1.0792	AH	1 2
1.2548	AO	15 18
1.4895	AA	15 5
1.4237	AA	5 9
1.0903	AH	9 14
1.3865	AA	9 8
1.0913	AH	8 13
1.4192	AA	8 7
1.0873	AH	7 12
1.3971	AA	7 10
1.0815	AH	10 11

BOND ANGLES (IN DEGREES)	TYPE	ATOMS INVOLVED
107.2721	AAA	16 6 5
121.9306	AAO	6 16 17
109.0341	AAN	6 16 21
107.6175	AAA	6 5 15
127.8592	AAA	6 5 9
128.9704	OAN	17 16 21
126.4385	ANA	16 21 20
107.4881	ANA	16 21 15
126.0041	ANA	20 21 15
121.5632	NAA	21 20 19
121.6451	NAA	21 20 1

127.3825	NAO	21 15 18
108.4881	NAA	21 15 5
116.7647	AAA	19 20 1
121.9641	AAH	20 19 22
121.5068	AAA	20 19 0
121.4800	AAA	20 1 3
122.0691	AAH	20 1 2
116.5294	HAA	22 19 0
119.5311	AAH	19 0 25
120.4133	AAA	19 0 4
120.0558	HAA	25 0 4
120.2925	AAH	0 4 24
119.3849	AAA	0 4 3
120.3228	HAA	24 4 3
120.0552	AAH	4 3 23
120.4404	AAA	4 3 1
119.5021	HAA	23 3 1
116.4433	AAH	3 1 2
124.1274	OAA	18 15 5
124.5013	AAA	15 5 9
115.5950	AAH	5 9 14
130.3099	AAA	5 9 8
114.0935	HAA	14 9 8
114.6534	AAH	9 8 13
131.3209	AAA	9 8 7
113.9673	HAA	13 8 7
115.7490	AAH	8 7 12
126.7259	AAA	8 7 10
117.3768	HAA	12 7 10
120.5397	AAH	7 10 11

DIHEDRAL ANGLES (IN DEGREES)	TYPE	ATOMS INVOLVED
177.2698	AAAO	5 6 16 17
359.9604	AAAN	5 6 16 21
1.9422	AAAA	16 6 5 15
180.2727	AAAA	16 6 5 9
175.1867	AANA	6 16 21 20
358.0881	AANA	6 16 21 15
358.1261	OANA	17 16 21 20
181.0268	OANA	17 16 21 15
11.8695	ANAA	16 21 20 19
193.8308	ANAA	16 21 20 1
188.4483	ANAA	15 21 20 19
10.4095	ANAA	15 21 20 1
183.6496	ANAO	16 21 15 18
3.1152	ANAA	16 21 15 5
6.5348	ANAO	20 21 15 18
186.0004	ANAA	20 21 15 5

2.8660	NAAH	21	20	19	22
182.8748	NAAA	21	20	19	0
180.9962	AAAH	1	20	19	22
1.0050	AAAA	1	20	19	0
177.8759	NAAA	21	20	1	3
358.9374	NAAH	21	20	1	2
359.7467	AAAA	19	20	1	3
180.8089	AAAH	19	20	1	2
178.9603	AAAH	20	19	0	25
359.1006	AAAA	20	19	0	4
358.9687	HAAH	22	19	0	25
179.1091	HAAA	22	19	0	4
179.9477	AAAH	19	0	4	24
-0.0000	AAAA	19	0	4	3
0.0862	HAAH	25	0	4	24
180.1399	HAAA	25	0	4	3
180.1519	AAAH	0	4	3	23
0.7449	AAAA	0	4	3	1
0.2075	HAAH	24	4	3	23
180.7997	HAAA	24	4	3	1
359.3839	AAAA	20	1	3	4
179.9720	AAAH	20	1	3	23
178.3797	AAAH	4	3	1	2
358.9683	HAAH	23	3	1	2
356.8451	AAAN	6	5	15	21
176.3320	AAAO	6	5	15	18
178.4453	NAAA	21	15	5	9
357.9322	OAAA	18	15	5	9
191.8158	AAAH	6	5	9	14
11.2807	AAAA	6	5	9	8
9.8840	AAAH	15	5	9	14
189.3489	AAAA	15	5	9	8
186.0443	AAAH	5	9	8	13
9.0444	AAAA	5	9	8	7
5.5157	HAAH	14	9	8	13
188.5158	HAAA	14	9	8	7
181.5847	AAAH	9	8	7	12
6.1606	AAAA	9	8	7	10
4.5687	HAAH	13	8	7	12
189.1446	HAAA	13	8	7	10
177.6306	AAAH	8	7	10	11
2.2719	HAAH	12	7	10	11
176.7257	AOAN	6	17	16	21
181.6001	AAAA	6	15	5	9
176.5788	AANA	16	20	21	15
178.1300	NAAA	21	19	20	1
180.6120	NOAA	21	18	15	5
180.0000	AHAA	20	22	19	0
178.9952	AAAH	20	3	1	2
179.8629	AHAA	19	25	0	4
179.9477	AHAA	0	24	4	3

179.4138	AHAA	4 23 3 1
180.4476	AHAA	5 14 9 8
177.5346	AHAA	9 13 8 7
175.8707	AHAA	8 12 7 10

TOTAL ENERGY = -2600.4799804688 KCAL

DIAGONAL CORE CONTRIBUTION =	-71.6000900269 KCAL
BOND CONTRIBUTION =	-2680.5073242188 KCAL
NON-BOND CONTRIBUTION =	13.6627359390 KCAL
REPULS CONTRIBUTION =	782.0302124023 KCAL
THETA CONTRIBUTION =	36.3170356750 KCAL
PHI CONTRIBUTION =	-680.3825073242 KCAL

ltp1

-1.5550	1.2108	0.6166
-0.0402	1.2858	0.6196
0.5712	2.3588	0.8486
0.4842	0.0211	0.2745
1.9151	-0.3126	0.0652
2.9534	0.5883	0.4392
2.7460	1.5271	0.9297
4.3032	0.2975	0.1866
5.0658	1.0135	0.4696
4.6660	-0.9075	-0.4295
5.7080	-1.1294	-0.6242
3.6686	-1.8215	-0.7920
3.9371	-2.7578	-1.2668
2.3150	-1.5288	-0.5557
1.5992	-2.2663	-0.8850
-0.6493	-0.8908	0.0911
-0.6058	-2.1197	-0.1585
-1.9105	-0.1173	0.2635
-3.2174	-0.6647	0.1257
-3.2670	-1.7508	0.0438
-4.4533	-0.0372	0.0876
-5.3081	-0.7156	0.0766
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-3.9339	2.4113	-0.1811
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VIBRATIONAL FREQUENCY	I.R. INTENSITY
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3091.93	0.05
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3088.58	2.32
3079.36	1.16
3075.73	1.65
3074.97	0.66
3013.29	1.21
1632.80	0.63
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1603.48	0.87
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1570.63	1.20
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1483.14	2.48
1476.27	0.72
1436.93	2.11
1410.26	0.20
1401.74	0.03
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1285.93	0.23
1255.79	0.57
1224.92	1.37
1205.33	0.63
1189.09	1.02
1171.86	0.07
1120.15	0.08
1087.00	0.35
1064.75	0.00
1059.49	0.20
1050.88	1.01
1028.91	1.94
1027.04	0.07
1015.52	0.17
989.21	0.04
966.06	0.47
943.11	0.19
906.61	0.09
874.03	1.28
863.85	0.61
854.23	0.00
815.55	0.74
771.34	3.44
746.75	0.35
720.92	0.36
682.88	0.03
664.76	1.71
627.72	0.20
620.10	0.78
604.69	0.86
564.84	2.05

554.88	0.56
501.51	0.08
478.53	1.27
471.82	1.22
407.10	0.95
391.06	2.30
369.83	0.99
349.01	0.25
320.85	0.53
297.98	1.63
274.94	1.00
232.02	0.14
193.96	0.71
145.42	1.57
134.12	1.20
112.22	1.37
60.61	1.20
32.58	0.65
14.87	0.05
8.58	1.81
8.58	0.05
7.11	1.53
7.11	0.05

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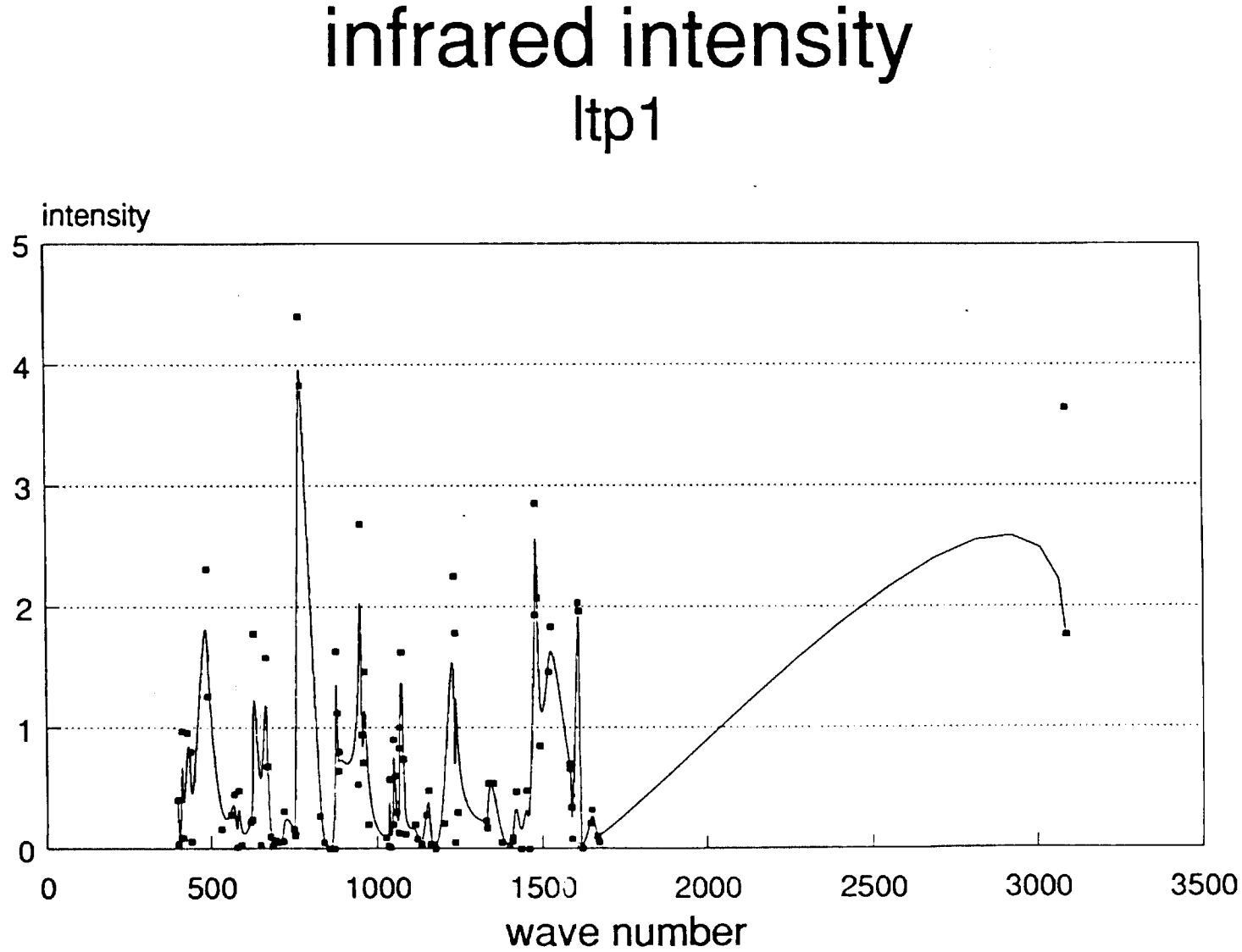
infrared intensity
ltp1
intensity
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1000
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wave number

Fig. 1c

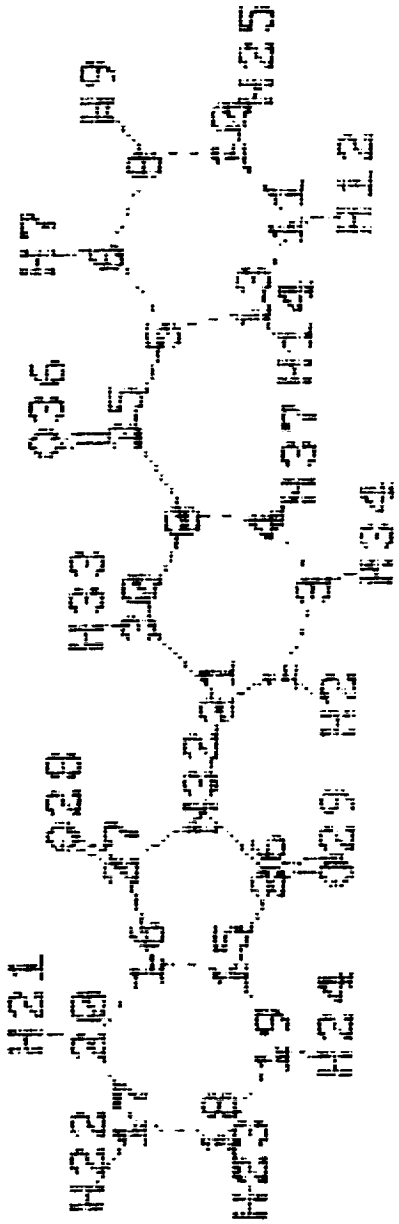


Fig. 2a

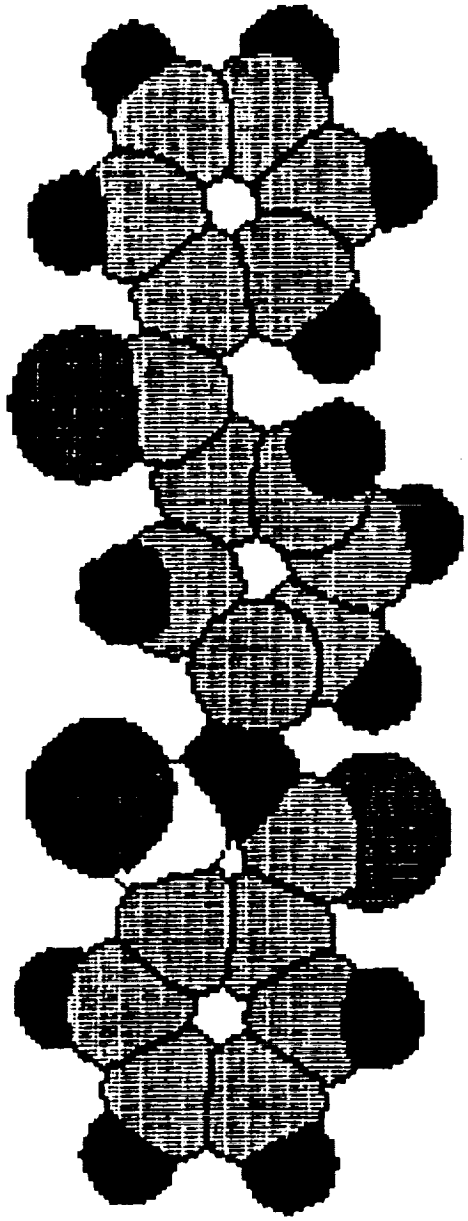


Fig. 2b

F I N A L R E S U L T S

ltp2

BOND LENGTHS (IN ANGSTROMS)	TYPE	ATOMS INVOLVED
1.0823	AH	30 33
1.4240	AA	30 0
1.4159	AA	30 31
1.5108	AA	0 35
1.4143	AA	0 4
1.2604	AO	35 36
1.4941	AA	35 5
1.4240	AA	5 6
1.4172	AA	5 13
1.0832	AH	6 7
1.4007	AA	6 8
1.0835	AH	8 9
1.4035	AA	8 10
1.0831	AH	10 25
1.4026	AA	10 11
1.0832	AH	11 12
1.4065	AA	11 13
1.0823	AH	13 14
1.0800	AH	4 37
1.4044	AA	4 3
1.0839	AH	3 34
1.3978	AA	3 1
1.0824	AH	1 2
1.4168	AA	1 31
1.4747	AN	31 32
1.4488	NA	32 26
1.4442	NA	32 27
1.2549	AO	26 29
1.4878	AA	26 15
1.4018	AA	15 19
1.4200	AA	15 16
1.0815	AH	19 24
1.4106	AA	19 18
1.0830	AH	18 23
1.4099	AA	18 17
1.0830	AH	17 22
1.4114	AA	17 20
1.0817	AH	20 21
1.3985	AA	20 16
1.4975	AA	16 27
1.2509	AO	27 28

THETA ANGLES	TYPE	ATOMS INVOLVED

(IN DEGREES)

119.2105	HAA	33	30	0
118.7510	HAA	33	30	31
122.0303	AAA	0	30	31
119.7588	AAA	30	0	35
117.6019	AAA	30	0	4
118.3099	AAA	30	31	1
121.0586	AAN	30	31	32
122.4811	AAA	35	0	4
119.3792	AAO	0	35	36
122.1502	AAA	0	35	5
122.1130	AAH	0	4	37
120.8932	AAA	0	4	3
118.2205	OAA	36	35	5
119.5562	AAA	35	5	6
122.4294	AAA	35	5	13
117.9939	AAA	6	5	13
120.2585	AAH	5	6	7
120.9478	AAA	5	6	8
120.6678	AAA	5	13	11
120.9008	AAH	5	13	14
118.7666	HAA	7	6	8
119.7783	AAH	6	8	9
120.1637	AAA	6	8	10
120.0576	HAA	9	8	10
120.0145	AAH	8	10	25
119.7884	AAA	8	10	11
120.1956	HAA	25	10	11
119.8982	AAH	10	11	12
120.3580	AAA	10	11	13
119.7441	HAA	12	11	13
118.4267	AAH	11	13	14
116.9832	HAA	37	4	3
119.5123	AAH	4	3	34
120.6663	AAA	4	3	1
119.7905	HAA	34	3	1
118.5509	AAH	3	1	2
120.3849	AAA	3	1	31
120.9844	HAA	2	1	31
120.5148	AAN	1	31	32
125.6276	ANA	31	32	26
124.8577	ANA	31	32	27
109.2029	ANA	26	32	27
127.1440	NAO	32	26	29
107.2022	NAA	32	26	15
106.9416	NAA	32	27	16
127.3734	NAO	32	27	28
125.6384	OAA	29	26	15
130.7406	AAA	26	15	19
108.3649	AAA	26	15	16

120.8679	AAA	19 15 16
121.7896	AAH	15 19 24
118.0236	AAA	15 19 18
121.1428	AAA	15 16 20
108.2676	AAA	15 16 27
120.1833	HAA	24 19 18
119.6645	AAH	19 18 23
121.0110	AAA	19 18 17
119.3236	HAA	23 18 17
119.4327	AAH	18 17 22
120.9519	AAA	18 17 20
119.6147	HAA	22 17 20
120.2020	AAH	17 20 21
118.0032	AAA	17 20 16
121.7927	HAA	21 20 16
130.5669	AAA	20 16 27
125.2135	AAO	16 27 28

PHI ANGLES (IN DEGREES)	TYPE	ATOMS INVOLVED
356.1916	HAAA	33 30 0 35
180.6540	HAAA	33 30 0 4
175.1219	AAAA	31 30 0 35
359.5846	AAAA	31 30 0 4
181.9128	HAAA	33 30 31 1
5.8266	HAAN	33 30 31 32
2.9777	AAAA	0 30 31 1
186.8916	AAAN	0 30 31 32
355.7806	AAAO	30 0 35 36
181.6340	AAAA	30 0 35 5
171.0927	AAAO	4 0 35 36
356.9457	AAAA	4 0 35 5
176.2860	AAAH	30 0 4 37
357.5227	AAAA	30 0 4 3
0.8783	AAAH	35 0 4 37
182.1148	AAAA	35 0 4 3
139.9417	AAAA	0 35 5 6
318.2512	AAAA	0 35 5 13
325.7300	OAAA	36 35 5 6
144.0394	OAAA	36 35 5 13
359.5429	AAAH	35 5 6 7
181.4709	AAAA	35 5 6 8
181.1586	AAAH	13 5 6 7
3.0867	AAAA	13 5 6 8
178.5291	AAAA	35 5 13 11
357.7021	AAAH	35 5 13 14
356.8637	AAAA	6 5 13 11
176.0365	AAAH	6 5 13 14
178.6070	AAAH	5 6 8 9

358.9165	AAAA	5	6	8	10
0.5067	HAAH	7	6	8	9
180.8161	HAAA	7	6	8	10
179.5489	AAAH	6	8	10	25
359.0575	AAAA	6	8	10	11
359.8574	HAAH	9	8	10	25
179.3679	HAAA	9	8	10	11
180.9820	AAAH	8	10	11	12
0.8856	AAAA	8	10	11	13
0.4902	HAAH	25	10	11	12
180.3937	HAAA	25	10	11	13
1.2035	AAAA	5	13	11	10
181.1078	AAAH	5	13	11	12
182.0101	AAAH	10	11	13	14
1.9145	HAAH	12	11	13	14
180.7301	AAAH	0	4	3	34
2.7695	AAAA	0	4	3	1
1.9058	HAAH	37	4	3	34
183.9448	HAAA	37	4	3	1
176.6876	AAAH	4	3	1	2
359.9094	AAAA	4	3	1	31
358.7324	HAAH	34	3	1	2
181.9538	HAAA	34	3	1	31
357.2904	AAAA	30	31	1	3
180.5908	AAAH	30	31	1	2
173.3985	AAAN	3	1	31	32
356.6995	HAAN	2	1	31	32
209.9622	AANA	30	31	32	26
37.0784	AANA	30	31	32	27
33.9621	AANA	1	31	32	26
221.0783	AANA	1	31	32	27
8.9640	ANAO	31	32	26	29
187.5748	ANAA	31	32	26	15
182.7845	ANAO	27	32	26	29
1.3953	ANAA	27	32	26	15
172.3962	ANAA	31	32	27	16
-0.0000	ANAO	31	32	27	28
358.5171	ANAA	26	32	27	16
186.1346	ANAO	26	32	27	28
177.3259	NAAA	32	26	15	19
359.2488	NAAA	32	26	15	16
355.9635	OAAA	29	26	15	19
177.8867	OAAA	29	26	15	16
1.5390	AAAH	26	15	19	24
182.2483	AAAA	26	15	19	18
179.4128	AAAH	16	15	19	24
0.1187	AAAA	16	15	19	18
178.2742	AAAA	26	15	16	20
359.8430	AAAA	26	15	16	27
359.9720	AAAA	19	15	16	20
181.5423	AAAA	19	15	16	27

179.4872	AAAH	15	19	18	23
359.8847	AAAA	15	19	18	17
0.1856	HAAH	24	19	18	23
180.5825	HAAA	24	19	18	17
179.6368	AAAH	19	18	17	22
-0.0000	AAAA	19	18	17	20
0.0280	HAAH	23	18	17	22
180.4117	HAAA	23	18	17	20
179.5224	AAAH	18	17	20	21
0.0791	AAAA	18	17	20	16
359.9011	HAAH	22	17	20	21
180.4593	HAAA	22	17	20	16
359.9234	AAAA	15	16	20	17
180.4934	AAAH	15	16	20	21
177.9632	AAAA	17	20	16	27
358.5305	HAAA	21	20	16	27
1.0056	NAAA	32	27	16	15
182.7747	NAAA	32	27	16	20
173.5970	AAAO	15	16	27	28
355.3663	AAAO	20	16	27	28
178.9306	HAAA	33	0	30	31
175.3119	AAAA	30	35	0	4
176.1083	AAAN	30	1	31	32
174.3766	AOAA	0	36	35	5
178.8091	AHAA	0	37	4	3
181.6159	AAAA	35	6	5	13
178.1136	AHAA	5	7	6	8
180.8067	AAAH	5	11	13	14
179.6904	AHAA	6	9	8	10
180.4926	AHAA	8	25	10	11
180.0969	AHAA	10	12	11	13
177.9789	AHAA	4	34	3	1
176.7584	AHAA	3	2	1	31
173.8205	AANA	31	26	32	27
181.6330	NOAA	32	29	26	15
172.5916	NAAO	32	16	27	28
177.8732	AAAA	26	19	15	16
179.2756	AHAA	15	24	19	18
178.0368	AAAA	15	20	16	27
179.6093	AHAA	19	23	18	17
179.6278	AHAA	18	22	17	20
179.4199	AHAA	17	21	20	16

TOTAL ENERGY = -4304.0869140625 KCAL

DIAGONAL CORE CONTRIBUTION = -159.2570343018 KCAL
BOND CONTRIBUTION = -4064.2814941406 KCAL
NON-BOND CONTRIBUTION = 23.6613464355 KCAL

REPULS CONTRIBUTION = 1013.5626220703 KCAL
THETA CONTRIBUTION = 40.9228553772 KCAL
PHI CONTRIBUTION = -1158.6954345703 KCAL

ltp2

0.2170	0.1039	0.4734
-0.0367	0.9842	1.0498
1.5858	-0.1748	0.1965
2.6531	0.8013	0.6333
2.3131	1.8909	1.1678
4.1011	0.5801	0.3394
4.9161	1.6825	-0.0459
4.4880	2.6737	-0.1326
6.2698	1.5032	-0.3577
6.8668	2.3515	-0.6705
6.8504	0.2283	-0.2720
7.8956	0.0912	-0.5208
6.0757	-0.8635	0.1462
6.5260	-1.8452	0.2283
4.7160	-0.6908	0.4622
4.1558	-1.5478	0.8133
1.8778	-1.3261	-0.5713
2.8844	-1.5743	-0.8738
0.8538	-2.1879	-0.9967
1.1041	-3.0704	-1.5741
-0.4848	-1.8961	-0.7192
-1.2496	-2.5551	-1.1097
-0.8289	-0.7242	-0.0011
-2.2418	-0.3376	0.1682
-3.3557	-1.2526	0.3131
-3.2990	-2.4957	0.4748
-4.6012	-0.4400	0.2691
-5.9479	-0.8268	0.3137
-6.2400	-1.8629	0.4174
-6.9304	0.1794	0.2035
-7.9790	-0.0905	0.2263
-6.5692	1.5342	0.0554
-7.3446	2.2851	-0.0329
-5.2133	1.9235	0.0127
-4.9499	2.9656	-0.1090
-4.2398	0.9251	0.1200
-2.7457	1.0123	0.0693
-2.0915	2.0514	-0.1695

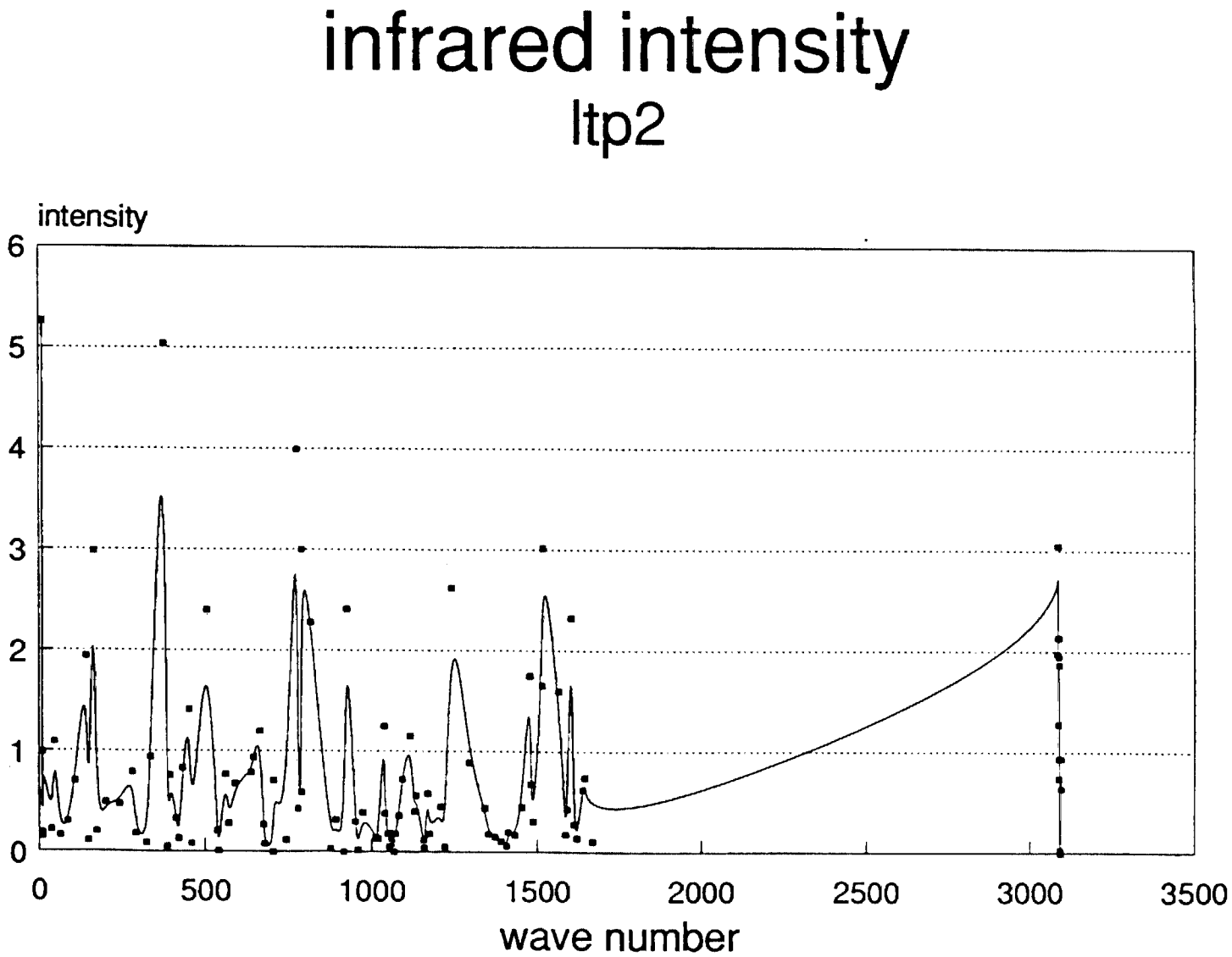
VIBRATIONAL FREQUENCY	I.R. INTENSITY
3094.10	0.51
3093.55	0.94
3092.86	0.01

3092.60	0.00
3090.27	0.06
3090.02	2.03
3089.39	1.04
3089.20	0.72
3088.54	1.95
3087.97	1.83
3087.95	1.48
3086.28	2.86
3085.34	2.15
1668.63	0.11
1644.13	0.72
1638.14	0.66
1620.67	0.15
1612.12	0.28
1603.67	2.35
1590.51	0.40
1586.53	0.15
1565.14	1.58
1514.59	3.05
1511.81	1.61
1486.81	0.32
1480.30	0.74
1476.45	1.75
1452.92	0.44
1431.84	0.16
1412.02	0.22
1407.20	0.07
1390.28	0.11
1372.15	0.15
1351.03	0.16
1341.98	0.45
1295.58	0.83
1242.06	2.63
1222.37	0.05
1206.99	0.40
1175.59	0.29
1169.63	0.50
1159.11	0.04
1157.20	0.11
1137.27	0.60
1128.47	0.39
1116.27	1.10
1091.26	0.75
1079.95	0.45
1069.85	0.14
1067.17	0.00
1060.17	0.11
1054.96	0.18
1052.10	0.07
1048.46	0.19

1039.83	0.44
1037.47	1.19
1020.07	0.13
1011.70	0.15
971.55	0.39
959.95	0.01
953.89	0.34
926.28	2.39
917.93	0.00
890.96	0.31
875.59	0.02
815.70	2.32
788.87	3.45
786.92	0.09
776.94	0.44
772.28	3.97
739.81	0.11
703.19	0.73
699.69	0.00
675.60	0.30
674.31	0.07
661.42	1.19
642.39	1.00
635.08	0.82
588.02	0.43
570.22	0.26
559.57	0.75
538.88	0.01
536.72	0.26
504.25	2.54
459.89	0.11
452.33	1.51
434.97	0.68
421.27	0.16
413.35	0.39
392.67	0.60
388.22	0.07
377.98	5.22
340.84	0.92
325.02	0.08
290.82	0.26
282.95	0.71
245.84	0.42
203.73	0.47
176.27	0.30
164.75	3.01
150.36	0.55
146.55	1.29
109.81	0.72
88.73	0.25
62.13	0.14

46.01	1.25
38.35	0.11
17.00	1.07
9.81	1.64
9.81	1.07
9.81	1.64
9.78	1.06
9.78	1.64

VIBRATIONAL ENTHALPY AT ROOM TEMPERATURE = 187.41
ZERO POINT ENERGY = 177.39
ATOMIZATION ENERGY = -4126.70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ltp2
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Fig. 2c

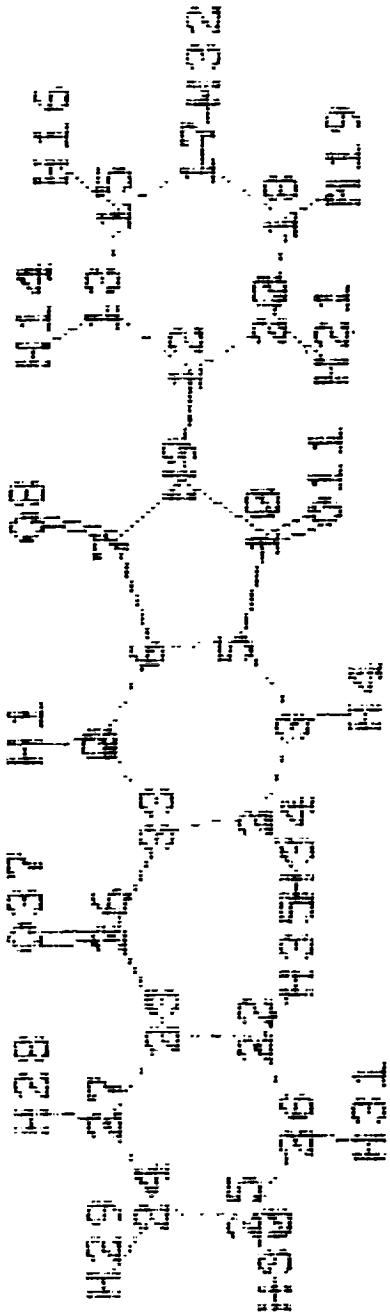


Fig. 3a

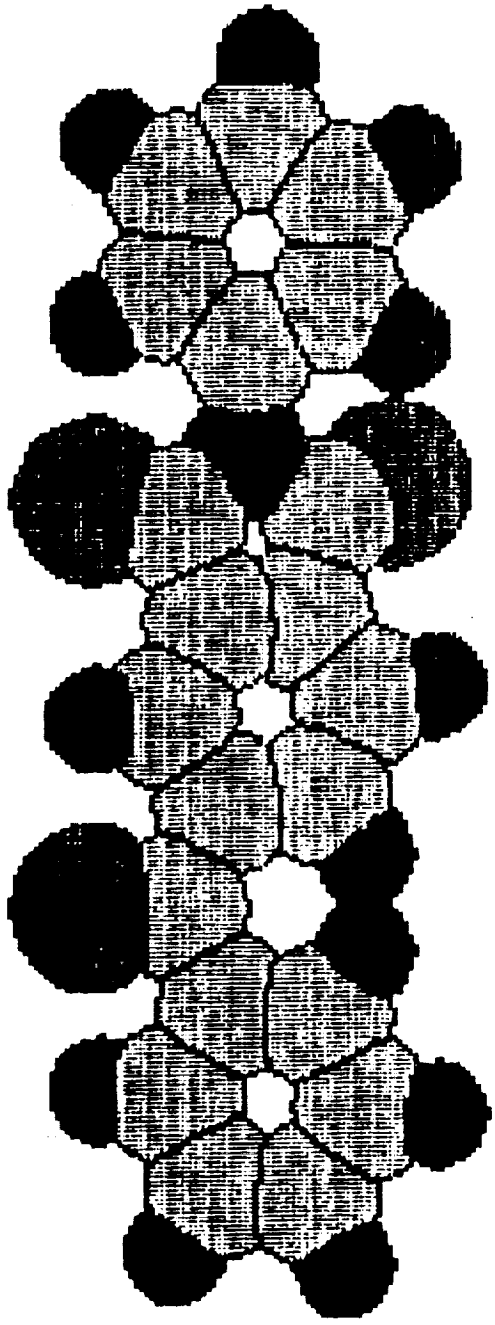


Fig. 3b

F I N A L R E S U L T S

ltp3

BOND LENGTHS (IN ANGSTROMS)	TYPE	ATOMS INVOLVED
1.3943	AA	5 3
1.4199	AA	5 6
1.4919	AA	5 10
1.0821	AH	3 4
1.4124	AA	3 2
1.0819	AH	2 34
1.4215	AA	2 33
1.5012	AA	33 36
1.4320	AA	33 0
1.2626	AO	36 37
1.4905	AA	36 23
1.4211	AA	23 22
1.4241	AA	23 27
1.0823	AH	22 35
1.4044	AA	22 26
1.0833	AH	26 31
1.4034	AA	26 25
1.0831	AH	25 30
1.4029	AA	25 24
1.0835	AH	24 29
1.4010	AA	24 27
1.0831	AH	27 28
1.0817	AH	0 1
1.3936	AA	0 6
1.4946	AA	6 7
1.2540	AO	7 8
1.4406	AN	7 9
1.4694	NA	9 12
1.4421	NA	9 10
1.4196	AA	12 13
1.4216	AA	12 20
1.0822	AH	13 14
1.4050	AA	13 15
1.0834	AH	15 16
1.4019	AA	15 17
1.0831	AH	17 32
1.4036	AA	17 18
1.0833	AH	18 19
1.4038	AA	18 20
1.0822	AH	20 21
1.2549	AO	10 11

THETA ANGLES (IN DEGREES)	TYPE	ATOMS INVOLVED		
120.7790	AAA	3	5	6
130.8622	AAA	3	5	10
121.8648	AAH	5	3	4
118.3215	AAA	5	3	2
108.3174	AAA	6	5	10
121.2527	AAA	5	6	0
108.0324	AAA	5	6	7
107.1123	AAN	5	10	9
125.2038	AAO	5	10	11
119.7957	HAA	4	3	2
117.4590	AAH	3	2	34
121.9050	AAA	3	2	33
120.6060	HAA	34	2	33
121.3308	AAA	2	33	36
118.7021	AAA	2	33	0
119.8198	AAA	36	33	0
118.9818	AAO	33	36	37
121.8371	AAA	33	36	23
120.5574	AAH	33	0	1
119.0280	AAA	33	0	6
119.1260	OAA	37	36	23
121.8722	AAA	36	23	22
120.1684	AAA	36	23	27
117.9235	AAA	22	23	27
120.8353	AAH	23	22	35
120.7183	AAA	23	22	26
120.9188	AAA	23	27	24
120.4000	AAH	23	27	28
118.4385	HAA	35	22	26
119.7539	AAH	22	26	31
120.3470	AAA	22	26	25
119.8989	HAA	31	26	25
120.1314	AAH	26	25	30
119.8114	AAA	26	25	24
120.0561	HAA	30	25	24
119.9936	AAH	25	24	29
120.2423	AAA	25	24	27
119.7644	HAA	29	24	27
118.6660	AAH	24	27	28
120.4090	HAA	1	0	6
130.6774	AAA	0	6	7
125.4018	AAO	6	7	8
107.2046	AAN	6	7	9
127.3321	OAN	8	7	9
125.3900	ANA	7	9	12
109.3093	ANA	7	9	10
125.2500	ANA	12	9	10
120.8231	NAA	9	12	13

121.1291	NAA	9 12 20
127.4238	NAO	9 10 11
118.0370	AAA	13 12 20
120.7964	AAH	12 13 14
120.8390	AAA	12 13 15
120.7707	AAA	12 20 18
120.7304	AAH	12 20 21
118.3395	HAA	14 13 15
119.6970	AAH	13 15 16
120.2589	AAA	13 15 17
120.0432	HAA	16 15 17
120.0964	AAH	15 17 32
119.7990	AAA	15 17 18
120.1049	HAA	32 17 18
119.9302	AAH	17 18 19
120.2952	AAA	17 18 20
119.7749	HAA	19 18 20
118.4888	AAH	18 20 21

PHI ANGLES (IN DEGREES)	TYPE	ATOMS INVOLVED
178.9025	AAAH	6 5 3 4
0.4656	AAAA	6 5 3 2
1.5451	AAAH	10 5 3 4
183.1086	AAAA	10 5 3 2
0.4059	AAAA	3 5 6 0
182.4191	AAAA	3 5 6 7
178.3011	AAAA	10 5 6 0
0.3140	AAAA	10 5 6 7
176.4273	AAAN	3 5 10 9
1.9325	AAAO	3 5 10 11
358.8193	AAAN	6 5 10 9
184.3242	AAAO	6 5 10 11
176.7658	AAAH	5 3 2 34
358.7543	AAAA	5 3 2 33
358.2958	HAAH	4 3 2 34
180.2832	HAAA	4 3 2 33
176.7148	AAAA	3 2 33 36
1.1404	AAAA	3 2 33 0
358.7652	HAAA	34 2 33 36
183.1908	HAAA	34 2 33 0
206.2329	AAAO	2 33 36 37
23.5013	AAAA	2 33 36 23
21.7584	AAAO	0 33 36 37
199.0268	AAAA	0 33 36 23
178.8754	AAAH	2 33 0 1
359.7545	AAAA	2 33 0 6
3.2328	AAAH	36 33 0 1
184.1127	AAAA	36 33 0 6

31.4041	AAAA	33	36	23	22
209.1697	AAAA	33	36	23	27
208.6686	OAAA	37	36	23	22
26.4342	OAAA	37	36	23	27
1.0025	AAAH	36	23	22	35
179.9407	AAAA	36	23	22	26
183.1890	AAAH	27	23	22	35
2.1334	AAAA	27	23	22	26
179.9184	AAAA	36	23	27	24
1.3601	AAAH	36	23	27	28
357.7659	AAAA	22	23	27	24
179.2127	AAAH	22	23	27	28
179.5106	AAAH	23	22	26	31
359.2506	AAAA	23	22	26	25
358.4792	HAAH	35	22	26	31
178.2197	HAAA	35	22	26	25
179.8165	AAAH	22	26	25	30
359.3938	AAAA	22	26	25	24
359.5559	HAAH	31	26	25	30
179.1339	HAAA	31	26	25	24
180.4343	AAAH	26	25	24	29
0.5090	AAAA	26	25	24	27
-0.0000	HAAH	30	25	24	29
180.0885	HAAA	30	25	24	27
0.9429	AAAA	23	27	24	25
181.0176	AAAH	23	27	24	29
179.5203	AAAH	25	24	27	28
359.5960	HAAH	29	24	27	28
359.4891	AAAA	5	6	0	33
180.3690	AAAH	5	6	0	1
176.9653	AAAA	33	0	6	7
357.8440	HAAA	1	0	6	7
183.3572	AAAO	5	6	7	8
0.6688	AAAN	5	6	7	9
5.6264	AAAO	0	6	7	8
182.9381	AAAN	0	6	7	9
176.0854	AANA	6	7	9	12
358.5749	AANA	6	7	9	10
353.3296	OANA	8	7	9	12
175.8192	OANA	8	7	9	10
326.1286	ANAA	7	9	12	13
147.3591	ANAA	7	9	12	20
143.2513	ANAA	10	9	12	13
324.4818	ANAA	10	9	12	20
1.6121	AANA	5	10	9	7
184.0975	AANA	5	10	9	12
175.9475	ANAO	7	9	10	11
358.4328	ANAO	12	9	10	11
359.5922	NAAH	9	12	13	14
181.4543	NAAA	9	12	13	15
178.3989	AAAH	20	12	13	14

0.2602	AAAA	20	12	13	15
178.7339	NAAA	9	12	20	18
357.5400	NAAH	9	12	20	21
359.9315	AAAA	13	12	20	18
178.7370	AAAH	13	12	20	21
179.3919	AAAH	12	13	15	16
359.7898	AAAA	12	13	15	17
1.2085	HAAH	14	13	15	16
181.6066	HAAA	14	13	15	17
179.8847	AAAH	13	15	17	32
359.9658	AAAA	13	15	17	18
0.2811	HAAH	16	15	17	32
180.3621	HAAA	16	15	17	18
180.2046	AAAH	15	17	18	19
0.2290	AAAA	15	17	18	20
0.2860	HAAH	32	17	18	19
180.3096	HAAA	32	17	18	20
359.8253	AAAA	12	20	18	17
179.8493	AAAH	12	20	18	19
180.9927	AAAH	17	18	20	21
1.0170	HAAH	19	18	20	21
177.8947	AAAA	3	6	5	10
178.4142	AHAA	5	4	3	2
177.4760	AAAA	5	0	6	7
174.3353	ANAO	5	9	10	11
178.0387	AHAA	3	34	2	33
175.5256	AAAA	2	36	33	0
182.6567	AOAA	33	37	36	23
179.1078	AHAA	33	1	0	6
182.1864	AAAA	36	22	23	27
181.0319	AHAA	23	35	22	26
178.5774	AAAH	23	24	27	28
180.2579	AHAA	22	31	26	25
180.4224	AHAA	26	30	25	24
179.9234	AHAA	25	29	24	27
183.2302	AOAN	6	8	7	9
177.1228	AANA	7	12	9	10
178.8068	NAAA	9	13	12	20
178.1834	AHAA	12	14	13	15
181.1674	AAAH	12	18	20	21
179.6034	AHAA	13	16	15	17
179.9209	AHAA	15	32	17	18
179.9802	AHAA	17	19	18	20

TOTAL ENERGY = -4304.8632812500 KCAL

DIAGONAL CORE CONTRIBUTION = -148.0831909180 KCAL
BOND CONTRIBUTION = -4061.7929687500 KCAL

NON-BOND CONTRIBUTION = 23.1864223480 KCAL
REPULS CONTRIBUTION = 1008.2837524414 KCAL
THETA CONTRIBUTION = 40.6211509705 KCAL
PHI CONTRIBUTION = -1167.0787353516 KCAL

ltp3

0.6498	-0.7426	-0.3782
-0.5364	-1.3805	-0.7388
-0.5408	-2.3545	-1.2102
-1.7565	-0.7085	-0.5048
-2.6647	-1.1927	-0.8385
-1.8026	0.5744	0.1056
-3.0999	1.3087	0.2823
-3.0856	2.5697	0.3446
-4.4077	0.5950	0.3259
-4.5271	-0.7214	0.8479
-3.6651	-1.2403	1.2467
-5.7719	-1.3709	0.8783
-5.8436	-2.3774	1.2724
-6.9226	-0.7208	0.4062
-7.8803	-1.2261	0.4285
-6.8307	0.5894	-0.0869
-7.7184	1.0966	-0.4457
-5.5935	1.2460	-0.1193
-5.5506	2.2543	-0.5125
-0.5707	1.2077	0.4691
-0.5699	2.1915	0.9187
0.6297	0.5457	0.2182
2.0442	0.9795	0.4303
2.4017	2.0424	0.9914
2.8920	-0.0733	-0.0681
4.3593	-0.0264	-0.1308
5.0378	1.1939	-0.3867
4.4865	2.1114	-0.5469
6.4393	1.2336	-0.4768
6.9375	2.1733	-0.6826
7.1914	0.0622	-0.3098
8.2716	0.0955	-0.3817
6.5401	-1.1539	-0.0510
7.1193	-2.0596	0.0817
5.1399	-1.2027	0.0366
4.6691	-2.1526	0.2534
2.0725	-1.1575	-0.5505
2.4558	-2.2093	-1.1175

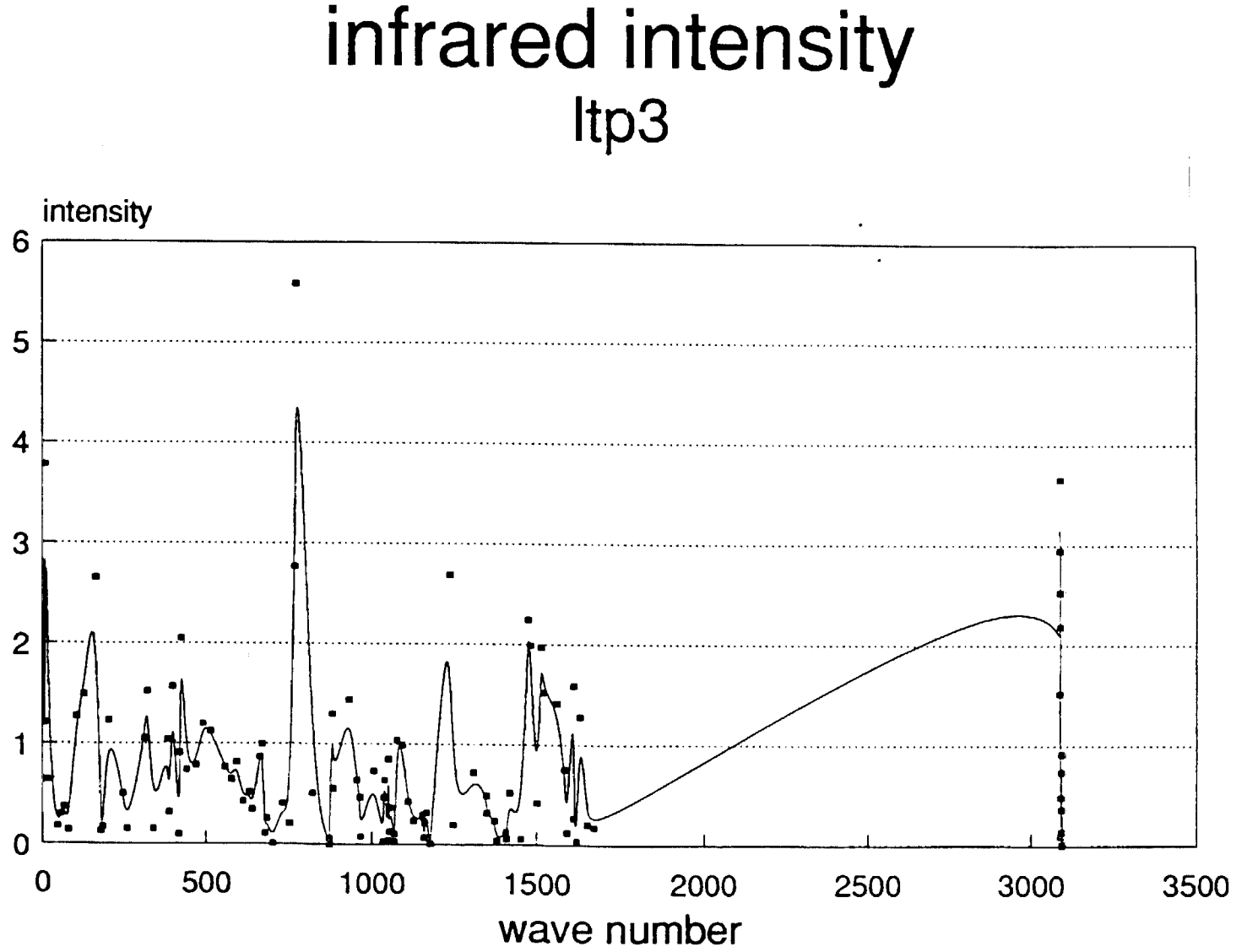
VIBRATIONAL FREQUENCY	I.R. INTENSITY
3092.84	0.01
3092.62	0.02

3092.43	0.92
3090.77	0.74
3090.59	0.15
3090.28	0.37
3089.43	0.10
3089.22	0.49
3088.63	2.19
3088.17	2.53
3087.30	3.66
3086.94	1.52
3086.36	2.95
1669.66	0.18
1650.84	0.21
1628.57	1.28
1618.27	0.04
1610.24	0.27
1609.45	1.59
1588.96	0.13
1583.21	0.76
1557.74	1.41
1518.90	1.52
1512.67	1.97
1500.82	0.42
1479.64	1.99
1474.15	2.25
1452.46	0.06
1418.90	0.52
1409.22	0.06
1407.11	0.13
1379.46	0.04
1374.22	0.24
1349.64	0.32
1348.16	0.49
1308.65	0.72
1246.20	0.20
1235.55	2.69
1178.90	0.01
1176.72	0.01
1164.78	0.32
1161.16	0.22
1159.33	0.07
1154.92	0.29
1127.77	0.24
1110.89	0.43
1092.10	0.99
1077.12	1.04
1069.29	0.03
1067.93	0.11
1055.76	0.37
1053.91	0.13
1050.56	0.85

1050.09	0.04
1039.66	0.64
1037.40	0.47
1034.50	0.03
1005.99	0.73
965.30	0.08
963.37	0.47
954.03	0.64
930.69	1.44
882.89	0.56
881.03	1.30
871.29	0.06
871.18	0.00
822.07	0.51
771.21	5.59
768.76	2.77
752.45	0.21
732.44	0.41
702.30	0.01
683.64	0.26
678.26	0.11
669.52	1.00
664.07	0.87
639.80	0.35
631.11	0.52
612.47	0.43
592.80	0.82
577.84	0.65
558.56	0.77
514.63	1.13
491.97	1.20
469.50	0.79
440.48	0.74
424.40	2.05
419.17	0.91
415.81	0.10
397.83	1.57
386.52	0.32
381.24	1.04
337.30	0.15
318.92	1.52
311.79	1.05
257.35	0.15
244.47	0.50
200.21	1.23
181.36	0.17
174.89	0.13
159.77	2.65
123.81	1.49
102.40	1.27
76.70	0.14

64.77	0.37
55.36	0.30
45.44	0.18
21.75	0.64
8.22	3.78
8.22	0.64
8.22	3.78
6.18	1.21
6.18	3.78
6.18	1.21

VIBRATIONAL ENTHALPY AT ROOM TEMPERATURE = 187.41
ZERO POINT ENERGY = 177.38
ATOMIZATION ENERGY = -4127.48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ltp3
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wave number

Fig. 3c

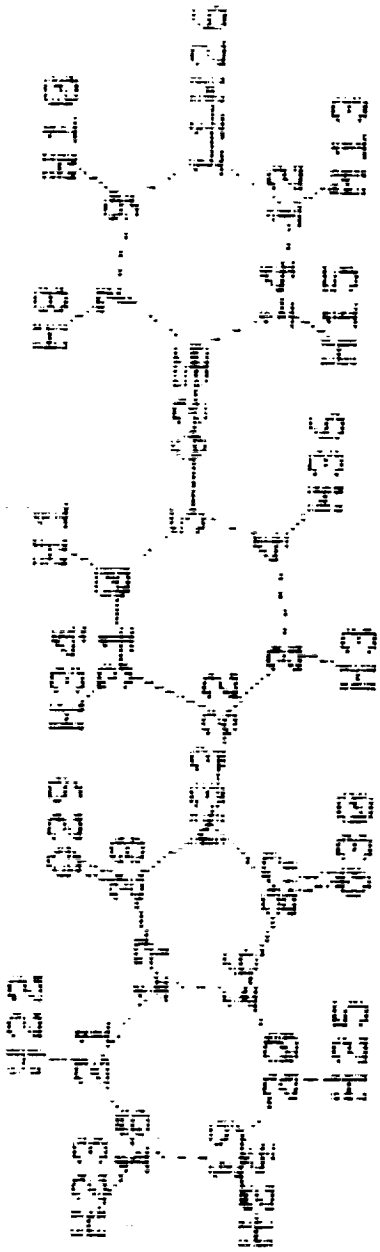

Fig. 4a

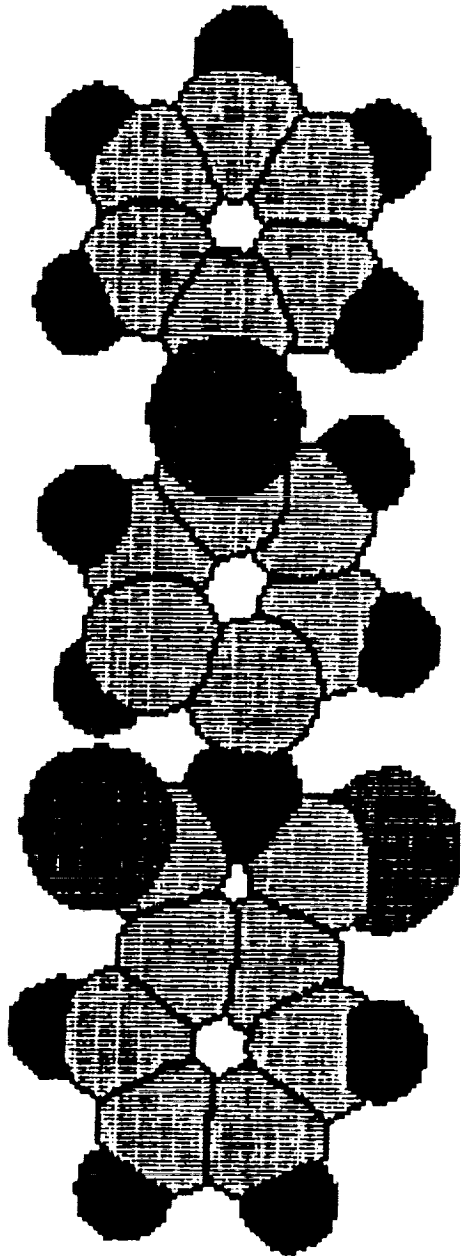

Fig. 4b

F I N A L R E S U L T S

LTP4

BOND LENGTHS (IN ANGSTROMS)	TYPE	ATOMS INVOLVED
1.0797	AH	31 34
1.4039	AA	31 0
1.4230	AA	31 32
1.0839	AH	0 1
1.4047	AA	0 5
1.4830	AQ	5 35
1.4061	AA	5 4
1.4751	QA	35 6
1.4110	AA	6 7
1.4108	AA	6 14
1.0833	AH	7 8
1.4046	AA	7 9
1.0830	AH	9 10
1.4054	AA	9 11
1.0829	AH	11 26
1.4054	AA	11 12
1.0830	AH	12 13
1.4055	AA	12 14
1.0832	AH	14 15
1.0837	AH	4 36
1.4035	AA	4 2
1.0792	AH	2 3
1.4235	AA	2 32
1.4828	AN	32 33
1.4430	NA	33 27
1.4637	NA	33 28
1.2563	AO	27 30
1.4935	AA	27 16
1.3989	AA	16 20
1.4177	AA	16 17
1.0816	AH	20 25
1.4126	AA	20 19
1.0830	AH	19 24
1.4093	AA	19 18
1.0830	AH	18 23
1.4110	AA	18 21
1.0817	AH	21 22
1.4003	AA	21 17
1.4870	AA	17 28
1.2529	AO	28 29

THETA ANGLES	TYPE	ATOMS INVOLVED

(IN DEGREES)

116.6820	HAA	34	31	0
121.8511	HAA	34	31	32
121.3604	AAA	0	31	32
119.0313	AAH	31	0	1
120.5406	AAA	31	0	5
116.6754	AAA	31	32	2
121.5097	AAN	31	32	33
120.3295	HAA	1	0	5
120.1440	AAQ	0	5	35
118.8716	AAA	0	5	4
120.3558	QAA	35	5	4
124.7328	AQA	5	35	6
120.3938	AAH	5	4	36
120.4828	AAA	5	4	2
119.7758	QAA	35	6	7
120.3572	QAA	35	6	14
119.5097	AAA	7	6	14
120.1442	AAH	6	7	8
120.2150	AAA	6	7	9
120.1297	AAA	6	14	12
120.2966	AAH	6	14	15
119.6292	HAA	8	7	9
119.9074	AAH	7	9	10
120.0514	AAA	7	9	11
120.0320	HAA	10	9	11
119.9770	AAH	9	11	26
119.9915	AAA	9	11	12
120.0297	HAA	26	11	12
119.9532	AAH	11	12	13
120.1012	AAA	11	12	14
119.9364	HAA	13	12	14
119.5589	AAH	12	14	15
118.9990	HAA	36	4	2
116.3596	AAH	4	2	3
121.4058	AAA	4	2	32
122.0761	HAA	3	2	32
121.3968	AAN	2	32	33
125.8652	ANA	32	33	27
125.0059	ANA	32	33	28
108.0456	ANA	27	33	28
128.3107	NAO	33	27	30
107.7310	NAA	33	27	16
107.4522	NAA	33	28	17
128.4439	NAO	33	28	29
123.9486	OAA	30	27	16
130.6379	AAA	27	16	20
108.2704	AAA	27	16	17
120.9674	AAA	20	16	17
121.8730	AAH	16	20	25

118.0418	AAA	16 20 19
121.1036	AAA	16 17 21
108.2777	AAA	16 17 28
120.0665	HAA	25 20 19
119.6557	AAH	20 19 24
120.9653	AAA	20 19 18
119.3748	HAA	24 19 18
119.4580	AAH	19 18 23
120.9087	AAA	19 18 21
119.6269	HAA	23 18 21
120.1764	AAH	18 21 22
118.0078	AAA	18 21 17
121.8007	HAA	22 21 17
130.5106	AAA	21 17 28
123.8841	AAO	17 28 29

PHI ANGLES (IN DEGREES)	TYPE	ATOMS INVOLVED
2.0200	HAAH	34 31 0 1
178.4158	HAAA	34 31 0 5
185.7101	AAAH	32 31 0 1
2.1057	AAAA	32 31 0 5
175.9019	HAAA	34 31 32 2
348.5753	HAAN	34 31 32 33
352.0200	AAAA	0 31 32 2
164.6933	AAAN	0 31 32 33
193.8766	AAAQ	31 0 5 35
4.8195	AAAA	31 0 5 4
10.2254	HAAQ	1 0 5 35
181.1684	HAAA	1 0 5 4
263.7473	AAQA	0 5 35 6
92.9399	AAQA	4 5 35 6
178.5302	AAAH	0 5 4 36
354.4300	AAAA	0 5 4 2
349.4536	QAAH	35 5 4 36
165.3531	QAAA	35 5 4 2
97.1509	AQAA	5 35 6 7
270.2521	AQAA	5 35 6 14
354.4191	QAAH	35 6 7 8
173.1606	QAAA	35 6 7 9
181.2588	AAAH	14 6 7 8
-0.0000	AAAA	14 6 7 9
186.9317	QAAA	35 6 14 12
5.5093	QAAH	35 6 14 15
0.0523	AAAA	7 6 14 12
178.6291	AAAH	7 6 14 15
180.8067	AAAH	6 7 9 10
359.6923	AAAA	6 7 9 11
359.5546	HAAH	8 7 9 10

178.4395	HAAA	8	7	9	11
181.0965	AAAH	7	9	11	26
0.5640	AAAA	7	9	11	12
360.0000	HAAH	10	9	11	26
179.4486	HAAA	10	9	11	12
180.6094	AAAH	9	11	12	13
359.4872	AAAA	9	11	12	14
0.0766	HAAH	26	11	12	13
178.9545	HAAA	26	11	12	14
0.2056	AAAA	6	14	12	11
179.0827	AAAH	6	14	12	13
181.6167	AAAH	11	12	14	15
0.4938	HAAH	13	12	14	15
183.9095	AAAH	5	4	2	3
359.4206	AAAA	5	4	2	32
359.8659	HAAH	36	4	2	3
175.3764	HAAA	36	4	2	32
7.2230	AAAA	31	32	2	4
182.4749	AAAH	31	32	2	3
194.5407	AAAN	4	2	32	33
9.7927	HAAN	3	2	32	33
180.0560	AANA	31	32	33	27
346.7085	AANA	31	32	33	28
352.3823	AANA	2	32	33	27
159.0367	AANA	2	32	33	28
344.8653	ANAO	32	33	27	30
163.7326	ANAA	32	33	27	16
176.3348	ANAO	28	33	27	30
355.2022	ANAA	28	33	27	16
195.8076	ANAA	32	33	28	17
10.5157	ANAO	32	33	28	29
4.4614	ANAA	27	33	28	17
179.1696	ANAO	27	33	28	29
187.4671	NAAA	33	27	16	20
3.3450	NAAA	33	27	16	17
6.3957	OAAA	30	27	16	20
182.2737	OAAA	30	27	16	17
357.2002	AAAH	27	16	20	25
175.6134	AAAA	27	16	20	19
181.7658	AAAH	17	16	20	25
0.1791	AAAA	17	16	20	19
182.8461	AAAA	27	16	17	21
359.4395	AAAA	27	16	17	28
359.1989	AAAA	20	16	17	21
175.7912	AAAA	20	16	17	28
181.1817	AAAH	16	20	19	24
0.4064	AAAA	16	20	19	18
359.6257	HAAH	25	20	19	24
178.8499	HAAA	25	20	19	18
180.5529	AAAH	20	19	18	23
359.6064	AAAA	20	19	18	21

359.7833	HAAH	24 19 18 23
178.8337	HAAA	24 19 18 21
181.1889	AAAH	19 18 21 22
359.7833	AAAA	19 18 21 17
0.2390	HAAH	23 18 21 22
178.8362	HAAA	23 18 21 17
0.8021	AAAA	16 17 21 18
179.3744	AAAH	16 17 21 22
185.0595	AAAA	18 21 17 28
3.6318	HAAA	22 21 17 28
357.6201	NAAA	33 28 17 16
173.7814	NAAA	33 28 17 21
182.6117	AAAO	16 17 28 29
358.7732	AAAO	21 17 28 29
183.6902	HAAA	34 0 31 32
183.5965	AHAA	31 1 0 5
187.3177	AAAN	31 2 32 33
189.1926	AQAA	0 35 5 4
184.0402	AHAA	5 36 4 2
186.8399	QAAA	35 7 6 14
181.2512	AHAA	6 8 7 9
181.4117	AAAH	6 12 14 15
181.1152	AHAA	7 10 9 11
180.5319	AHAA	9 26 11 12
181.1207	AHAA	11 13 12 14
184.5221	AHAA	4 3 2 32
191.4696	AANA	32 27 33 28
181.3009	NOAA	33 30 27 16
184.9918	NAAO	33 17 28 29
184.5658	AAAA	27 20 16 17
181.6181	AHAA	16 25 20 19
184.2576	AAAA	16 21 17 28
180.7621	AHAA	20 24 19 18
180.9350	AHAA	19 23 18 21
181.4581	AHAA	18 22 21 17

TOTAL ENERGY = -3961.2145996094 KCAL

DIAGONAL CORE CONTRIBUTION = -77.6206130981 KCAL
BOND CONTRIBUTION = -3706.6564941406 KCAL
NON-BOND CONTRIBUTION = 20.3816623688 KCAL
REPULS CONTRIBUTION = 893.4633789063 KCAL
THETA CONTRIBUTION = 39.5680885315 KCAL
PHI CONTRIBUTION = -1130.3505859375 KCAL

LTP4

-0.1061	1.2608	-0.2844
-0.5715	2.2188	-0.4618
1.2367	1.2786	0.1249
1.7283	2.2328	0.2748
1.9119	0.0802	0.4101
3.2097	0.1091	1.1272
4.5318	0.0700	0.4741
5.2337	1.2715	0.2402
4.7668	2.2250	0.4557
6.5502	1.2375	-0.2480
7.0888	2.1624	-0.4134
7.1760	0.0045	-0.4995
8.1971	-0.0207	-0.8590
6.4801	-1.1955	-0.2736
6.9662	-2.1455	-0.4581
5.1622	-1.1650	0.2139
4.6433	-2.0954	0.4098
1.2537	-1.1410	0.1809
1.7598	-2.0805	0.3698
-0.0932	-1.1609	-0.2130
-0.5505	-2.1338	-0.3073
-0.8350	0.0425	-0.3803
-2.3143	0.0304	-0.4813
-3.1453	-1.1451	-0.5813
-2.8011	-2.3208	-0.8597
-4.5468	-0.7399	-0.2618
-5.6999	-1.5115	-0.0822
-5.6940	-2.5854	-0.2102
-6.8859	-0.8519	0.3097
-7.7890	-1.4263	0.4748
-6.9088	0.5436	0.5054
-7.8294	1.0231	0.8146
-5.7449	1.3203	0.3232
-5.7712	2.3878	0.4952
-4.5675	0.6622	-0.0529
-3.1832	1.1790	-0.2201
-2.8603	2.3780	-0.0526

VIBRATIONAL FREQUENCY	I.R. INTENSITY
3096.29	0.68
3093.51	0.91
3093.41	0.09
3093.08	1.28
3092.83	0.01
3091.41	0.57
3090.99	0.01
3090.30	0.08
3088.88	2.47
3088.84	2.67
3088.56	1.98

3088.03	1.76
3087.96	3.28
1668.26	0.09
1638.71	0.54
1619.87	0.00
1607.86	2.03
1604.22	0.00
1587.51	0.05
1586.05	0.05
1575.71	1.08
1530.19	1.45
1502.27	2.13
1485.18	0.74
1477.12	1.86
1472.67	1.61
1453.81	1.44
1432.36	0.15
1407.33	0.05
1403.45	0.01
1371.88	0.00
1356.58	0.00
1341.57	0.43
1326.58	0.23
1241.19	2.45
1224.56	0.10
1209.39	0.38
1171.82	0.07
1158.20	0.03
1157.28	0.01
1156.14	0.01
1143.96	0.18
1132.55	0.40
1115.55	0.97
1105.22	0.08
1079.26	1.02
1066.89	0.01
1066.80	0.00
1063.26	0.40
1060.35	0.84
1049.79	0.29
1043.88	0.00
1038.17	1.36
1037.26	0.77
1028.55	0.08
1019.61	0.13
997.16	0.24
963.34	0.29
929.46	2.38
917.72	0.02
881.77	0.20
871.38	0.00

865.40	2.15
854.01	0.86
804.80	0.20
788.74	3.45
778.93	1.17
775.90	0.25
760.21	1.06
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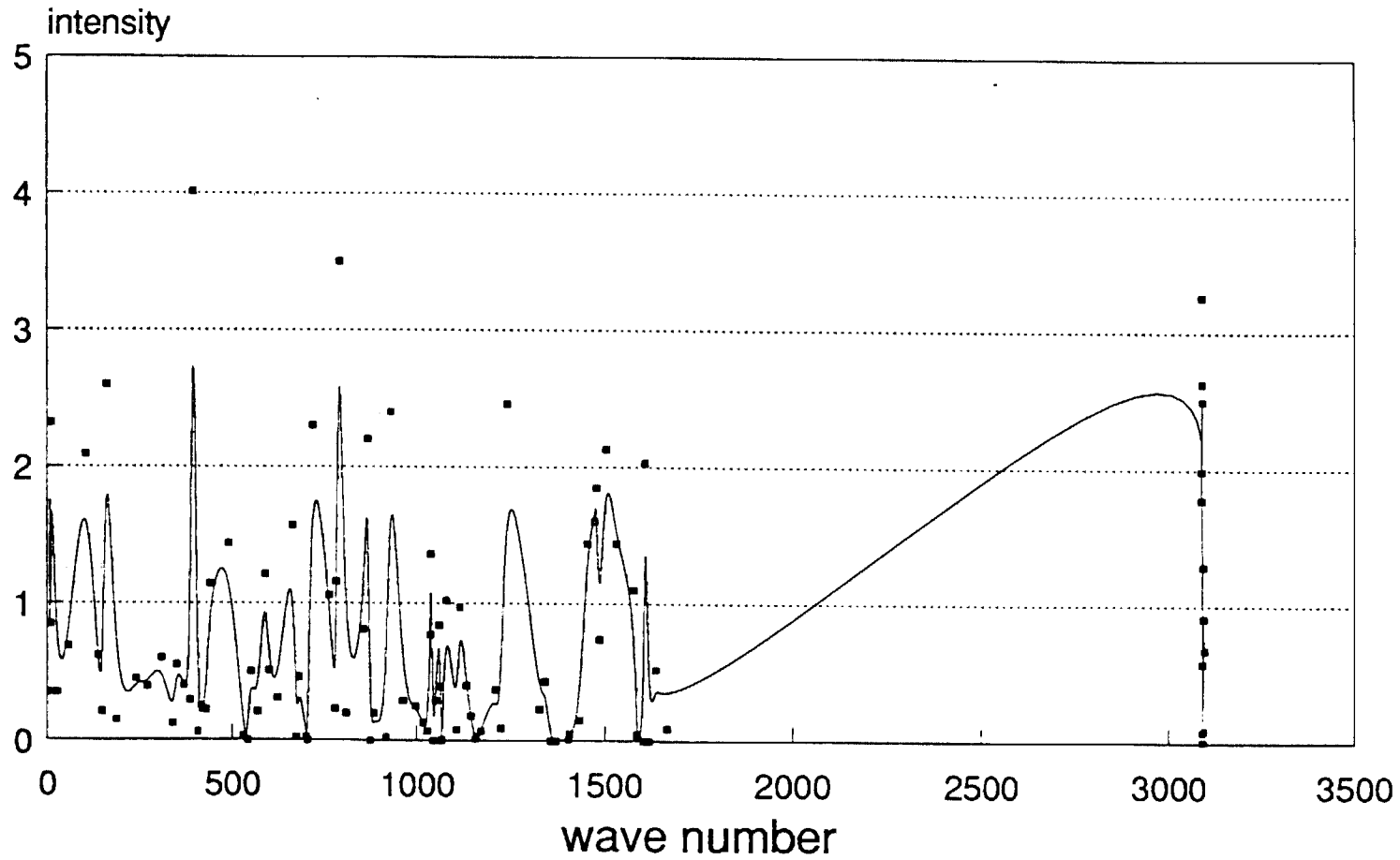
699.66	0.00
697.79	0.02
677.32	0.46
670.88	0.02
660.53	1.56
620.02	0.32
598.44	0.48
587.85	1.23
567.39	0.21
549.57	0.50
539.51	0.00
530.38	0.03
490.72	1.50
440.79	1.16
427.79	0.23
415.48	0.25
407.15	0.06
394.33	3.97
386.51	0.33
370.01	0.40
349.64	0.56
339.44	0.12
309.40	0.60
269.64	0.39
241.88	0.45
186.84	0.15
161.87	2.55
149.11	0.20
136.51	0.59
103.65	2.05
57.41	0.73
27.19	0.40
10.28	0.16
10.28	0.34
10.28	0.16
9.00	1.60
9.00	0.16

VIBRATIONAL ENTHALPY AT ROOM TEMPERATURE = 184.45
ZERO POINT ENERGY = 173.03
ATOMIZATION ENERGY = -3788.19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wave number

Fig. 4c

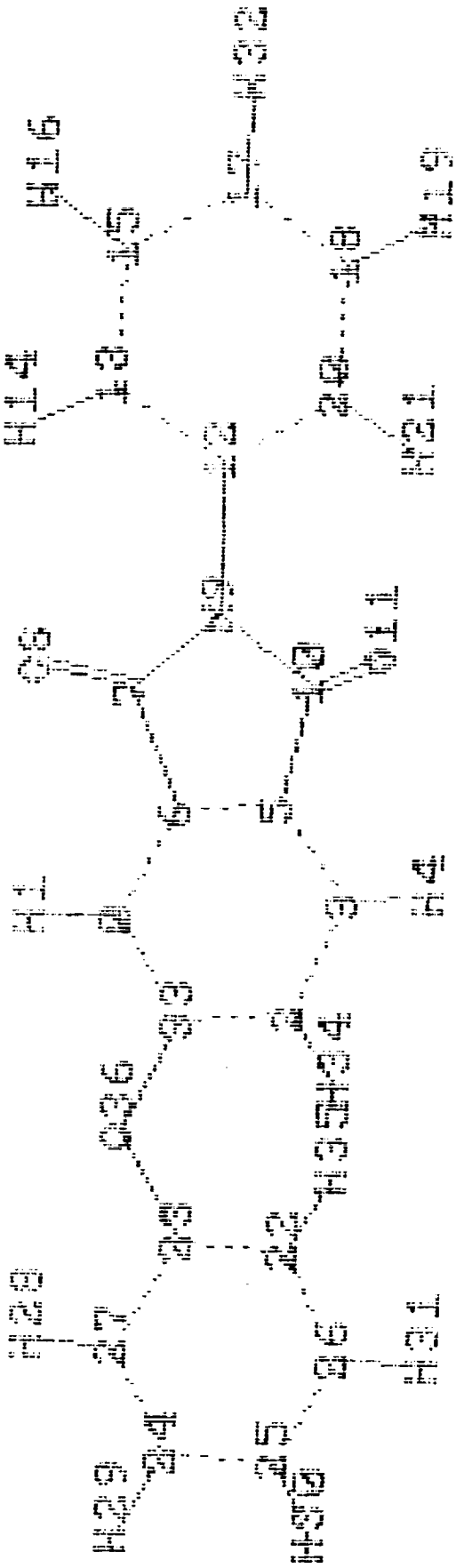


Fig. 5a

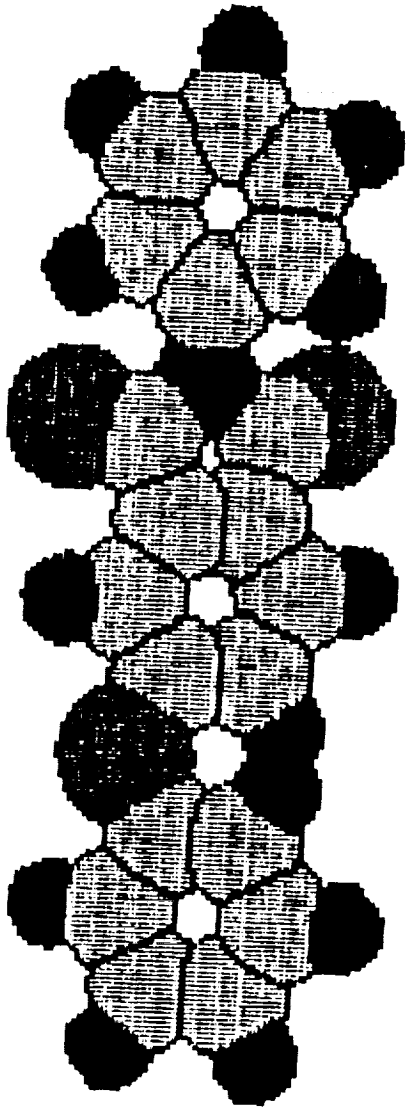


Fig. 5b

F I N A L R E S U L T S

ltp5

BOND LENGTHS (IN ANGSTROMS)	TYPE	ATOMS INVOLVED	
1.5098	AA	6	7
1.4958	AA	6	5
1.3725	AA	6	0
1.2581	AO	7	8
1.4293	AN	7	9
1.4819	NA	9	12
1.4228	NA	9	10
1.4159	AA	12	13
1.4198	AA	12	20
1.0824	AH	13	14
1.4069	AA	13	15
1.0832	AH	15	16
1.4018	AA	15	17
1.0831	AH	17	32
1.4035	AA	17	18
1.0834	AH	18	19
1.4038	AA	18	20
1.0825	AH	20	21
1.2626	AO	10	11
1.4945	AA	10	5
1.3977	AA	5	3
1.0846	AH	3	4
1.4074	AA	3	2
1.0786	AH	2	34
1.4363	AA	2	33
1.4349	AQ	33	36
1.4804	QA	36	23
1.5077	QA	36	0
1.4102	AA	23	22
1.4124	AA	23	27
1.0829	AH	22	35
1.4079	AA	22	26
1.0830	AH	26	31
1.4020	AA	26	25
1.0831	AH	25	30
1.4050	AA	25	24
1.0830	AH	24	29
1.4062	AA	24	27
1.0830	AH	27	28
1.0824	AH	0	1

THETA ANGLES (IN DEGREES)	TYPE	ATOMS INVOLVED

105.7075	AAA	7	6	5
123.5796	AAA	7	6	0
125.0078	AAO	6	7	8
108.7614	AAN	6	7	9
130.6021	AAA	5	6	0
106.6733	AAA	6	5	10
128.9440	AAA	6	5	3
124.0200	AAQ	6	0	36
120.0767	AAH	6	0	1
126.1572	OAN	8	7	9
125.3444	ANA	7	9	12
109.8048	ANA	7	9	10
124.8508	ANA	12	9	10
120.8687	NAA	9	12	13
120.8431	NAA	9	12	20
126.2791	NAO	9	10	11
109.0456	NAA	9	10	5
118.2805	AAA	13	12	20
120.6969	AAH	12	13	14
120.6866	AAA	12	13	15
120.7446	AAA	12	20	18
120.6520	AAH	12	20	21
118.6001	HAA	14	13	15
119.7213	AAH	13	15	16
120.2615	AAA	13	15	17
120.0162	HAA	16	15	17
120.1408	AAH	15	17	32
119.8116	AAA	15	17	18
120.0479	HAA	32	17	18
120.0001	AAH	17	18	19
120.2133	AAA	17	18	20
119.7869	HAA	19	18	20
118.5993	AAH	18	20	21
124.5704	OAA	11	10	5
123.3058	AAA	10	5	3
118.6028	AAH	5	3	4
120.8106	AAA	5	3	2
119.4653	HAA	4	3	2
119.5973	AAH	3	2	34
114.9421	AAA	3	2	33
123.5604	HAA	34	2	33
116.4710	AAQ	2	33	36
123.9206	AQA	33	36	23
112.1596	AQA	33	36	0
123.5554	AQA	23	36	0
119.9012	QAA	36	23	22
120.7988	QAA	36	23	27
115.7955	QAH	36	0	1
119.2977	AAA	22	23	27
120.3318	AAH	23	22	35

120.3437	AAA	23 22 26
120.1447	AAA	23 27 24
120.3490	AAH	23 27 28
119.3192	HAA	35 22 26
119.7521	AAH	22 26 31
120.0430	AAA	22 26 25
120.2051	HAA	31 26 25
119.9736	AAH	26 25 30
119.9717	AAA	26 25 24
120.0550	HAA	30 25 24
119.8643	AAH	25 24 29
120.1926	AAA	25 24 27
119.9434	HAA	29 24 27
119.4953	AAH	24 27 28

PHI ANGLES (IN DEGREES)	TYPE	ATOMS INVOLVED
183.6353	AAAO	5 6 7 8
0.6673	AAAN	5 6 7 9
0.1643	AAAO	0 6 7 8
177.1966	AAAN	0 6 7 9
359.8220	AAAA	7 6 5 10
168.0716	AAAA	7 6 5 3
183.6311	AAAA	0 6 5 10
351.8801	AAAA	0 6 5 3
173.6111	AAAQ	7 6 0 36
357.5544	AAAH	7 6 0 1
349.2094	AAAQ	5 6 0 36
173.1527	AAAH	5 6 0 1
178.8978	AANA	6 7 9 12
359.0730	AANA	6 7 9 10
355.8869	OANA	8 7 9 12
176.0621	OANA	8 7 9 10
320.5450	ANAA	7 9 12 13
141.5936	ANAA	7 9 12 20
140.3441	ANAA	10 9 12 13
321.3928	ANAA	10 9 12 20
177.2063	ANAO	7 9 10 11
0.8132	ANAA	7 9 10 5
357.3804	ANAO	12 9 10 11
180.9875	ANAA	12 9 10 5
-0.0000	NAAH	9 12 13 14
181.5257	NAAA	9 12 13 15
178.9964	AAAH	20 12 13 14
0.5036	AAAA	20 12 13 15
178.4669	NAAA	9 12 20 18
357.6912	NAAH	9 12 20 21
359.4887	AAAA	13 12 20 18
178.7132	AAAH	13 12 20 21

179.4751	AAAH	12	13	15	16
359.8797	AAAA	12	13	15	17
0.9506	HAAH	14	13	15	16
181.3545	HAAA	14	13	15	17
179.7066	AAAH	13	15	17	32
359.7346	AAAA	13	15	17	18
0.1119	HAAH	16	15	17	32
180.1371	HAAA	16	15	17	18
180.1958	AAAH	15	17	18	19
0.2579	AAAA	15	17	18	20
0.2255	HAAH	32	17	18	19
180.2860	HAAA	32	17	18	20
0.1342	AAAA	12	20	18	17
180.1988	AAAH	12	20	18	19
180.8953	AAAH	17	18	20	21
0.9561	HAAH	19	18	20	21
359.6263	AAAN	6	5	10	9
183.1580	AAAO	6	5	10	11
190.5524	NAAA	9	10	5	3
14.0833	OAAA	11	10	5	3
204.5963	AAAH	6	5	3	4
12.4262	AAAA	6	5	3	2
11.0967	AAAH	10	5	3	4
178.9268	AAAA	10	5	3	2
227.1399	AAAH	5	3	2	34
32.0096	AAAA	5	3	2	33
34.8660	HAAH	4	3	2	34
199.7359	HAAA	4	3	2	33
269.2703	AAAQ	3	2	33	36
73.4657	HAAQ	34	2	33	36
262.5284	AAQA	2	33	36	23
75.7996	AAQA	2	33	36	0
61.0307	AQAA	33	36	23	22
241.6288	AQAA	33	36	23	27
248.5127	AQAA	0	36	23	22
69.1108	AQAA	0	36	23	27
344.1784	AAQA	6	0	36	33
157.4784	AAQA	6	0	36	23
160.3886	AQAH	33	36	0	1
333.6887	AQAH	23	36	0	1
1.2966	QAAH	36	23	22	35
180.4312	QAAA	36	23	22	26
180.7075	AAAH	27	23	22	35
359.8430	AAAA	27	23	22	26
178.7876	QAAA	36	23	27	24
0.0280	QAAH	36	23	27	28
359.3813	AAAA	22	23	27	24
180.6139	AAAH	22	23	27	28
180.5974	AAAH	23	22	26	31
0.7228	AAAA	23	22	26	25
359.7436	HAAH	35	22	26	31

179.8688	HAAA	35 22 26 25
179.4696	AAAH	22 26 25 30
359.4880	AAAA	22 26 25 24
359.5960	HAAH	31 26 25 30
179.6149	HAAA	31 26 25 24
179.6029	AAAH	26 25 24 29
359.7346	AAAA	26 25 24 27
359.6216	HAAH	30 25 24 29
179.7553	HAAA	30 25 24 27
0.8320	AAAA	23 27 24 25
180.9655	AAAH	23 27 24 29
179.6108	AAAH	25 24 27 28
359.7444	HAAH	29 24 27 28
183.8085	AAAA	7 5 6 0
183.4814	AOAN	6 8 7 9
190.9252	AAAA	6 10 5 3
176.2102	AQAH	6 36 0 1
179.7983	AANA	7 12 9 10
178.9776	NAAA	9 13 12 20
175.8588	NOAA	9 11 10 5
178.5238	AHAA	12 14 13 15
180.7600	AAAH	12 18 20 21
179.5975	AHAA	13 16 15 17
179.9720	AHAA	15 32 17 18
179.9375	AHAA	17 19 18 20
192.0029	AHAA	5 4 3 2
196.4999	AHAA	3 34 2 33
179.4112	QAAA	36 22 23 27
180.8557	AHAA	23 35 22 26
178.7791	AAAH	23 24 27 28
179.8749	AHAA	22 31 26 25
179.9802	AHAA	26 30 25 24
179.8673	AHAA	25 29 24 27

TOTAL ENERGY = -3757.5158691406 KCAL

DIAGONAL CORE CONTRIBUTION = -80.1948013306 KCAL
BOND CONTRIBUTION = -3615.6689453125 KCAL
NON-BOND CONTRIBUTION = 17.6576061249 KCAL
REPULS CONTRIBUTION = 897.3578491211 KCAL
THETA CONTRIBUTION = 38.6332626343 KCAL
PHI CONTRIBUTION = -1015.3007812500 KCAL

ltp5

0.0269 0.0848 -0.3206
1.3231 0.7385 0.0940

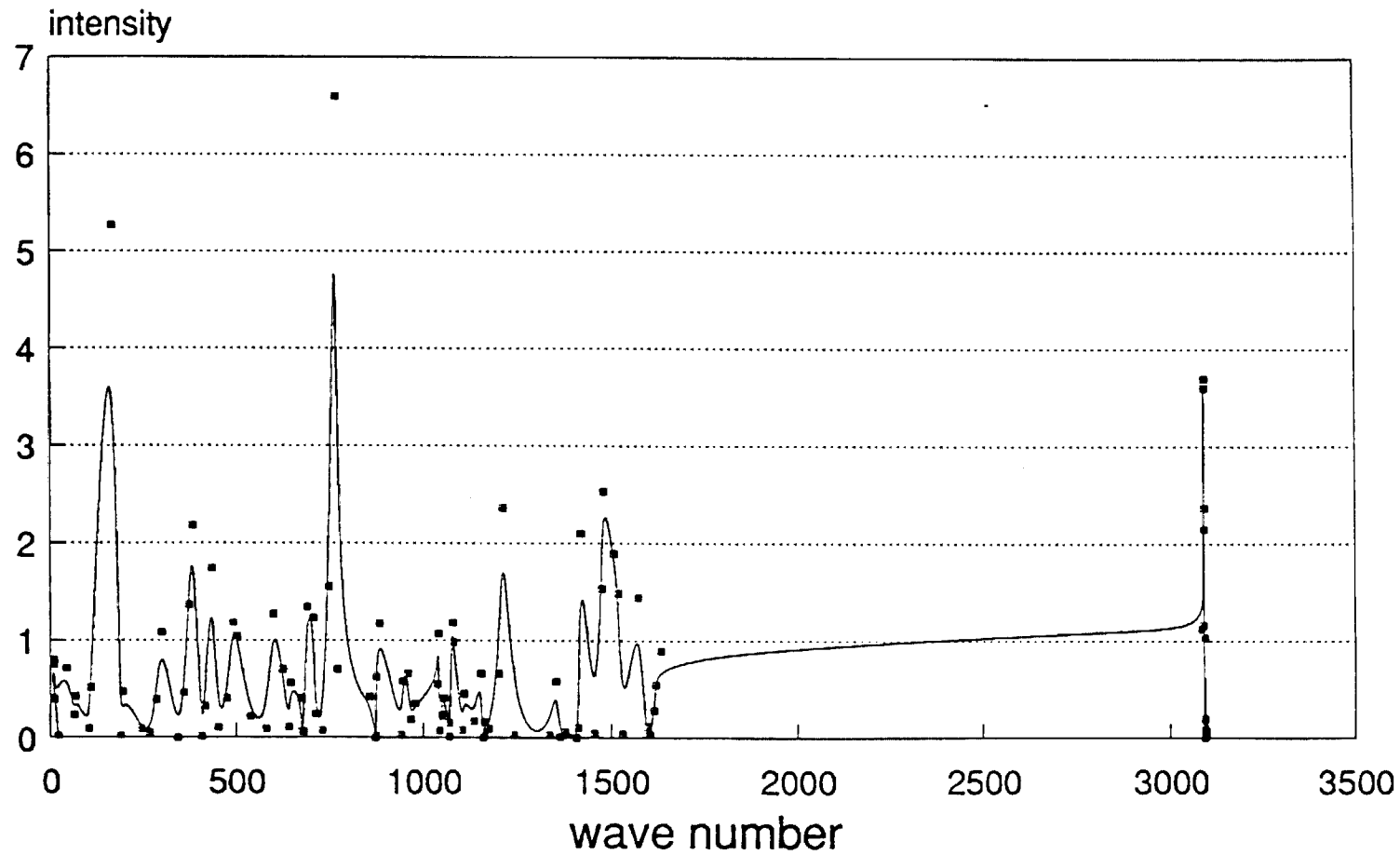
1.4152	1.8284	0.7156
2.4075	-0.1167	-0.2741
3.8436	0.1791	-0.0592
4.3531	1.4858	-0.2536
3.7012	2.2928	-0.5628
5.7228	1.7556	-0.0795
6.0972	2.7592	-0.2406
6.6031	0.7300	0.2926
7.6581	0.9389	0.4214
6.1139	-0.5694	0.4974
6.7910	-1.3636	0.7881
4.7483	-0.8453	0.3255
4.3967	-1.8534	0.5046
1.9034	-1.2990	-0.8842
2.5905	-2.2402	-1.3703
0.4121	-1.2198	-0.9429
-0.4011	-2.3034	-1.2866
0.0457	-3.2899	-1.3449
-1.8026	-2.1760	-1.3035
-2.4117	-2.9285	-0.8279
-2.2881	-0.8736	-1.6654
-2.5028	0.0507	-0.5891
-3.8212	0.2972	0.0375
-4.5046	-0.7584	0.6758
-4.0605	-1.7447	0.7284
-5.7630	-0.5366	1.2668
-6.2750	-1.3519	1.7629
-6.3508	0.7350	1.2101
-7.3227	0.9023	1.6577
-5.6785	1.7911	0.5723
-6.1370	2.7711	0.5238
-4.4142	1.5784	-0.0053
-3.9089	2.3989	-0.4996
-1.2101	0.6204	-0.0622
-1.2958	1.5412	0.5001

VIBRATIONAL FREQUENCY	I.R. INTENSITY
3093.56	0.07
3092.85	0.01
3091.89	1.03
3091.00	0.00
3090.55	0.19
3090.37	0.09
3089.46	0.15
3088.97	2.37
3088.58	2.15
3087.97	3.70
3087.19	3.60
3086.57	1.16
3082.38	1.11

1634.67	0.88
1619.61	0.51
1614.42	0.31
1603.69	0.02
1597.87	0.12
1592.95	0.04
1571.82	1.46
1529.57	0.04
1517.72	1.48
1505.85	1.89
1478.63	2.53
1473.95	1.53
1453.81	0.05
1417.45	2.10
1410.36	0.10
1406.08	0.00
1376.36	0.06
1362.42	0.01
1350.91	0.58
1334.31	0.03
1239.27	0.03
1212.09	2.35
1199.15	0.66
1172.18	0.09
1162.05	0.16
1160.22	0.02
1156.89	0.01
1152.26	0.66
1132.67	0.17
1109.13	0.45
1103.02	0.07
1081.06	0.97
1078.32	1.19
1068.37	0.00
1068.08	0.14
1054.84	0.41
1051.78	0.40
1049.52	0.24
1043.45	0.09
1040.63	1.05
1038.70	0.54
978.44	0.35
966.07	0.16
959.64	0.68
946.17	0.60
940.02	0.03
883.84	1.17
873.82	0.63
872.70	0.01
871.18	0.00
857.10	0.42

770.02	0.72
768.98	6.57
747.78	1.54
728.09	0.08
710.58	0.22
705.76	1.25
689.07	1.34
678.44	0.06
672.43	0.06
670.67	0.40
644.19	0.56
639.62	0.11
622.01	0.69
598.78	1.26
578.03	0.09
535.46	0.22
502.61	1.06
491.74	1.18
474.52	0.39
451.16	0.09
437.31	1.74
416.32	0.32
408.30	0.01
386.53	2.15
374.98	1.41
361.00	0.45
343.53	0.00
302.07	1.08
286.18	0.39
268.12	0.05
245.30	0.10
195.00	0.47
189.12	0.03
167.24	5.25
108.26	0.50
102.94	0.09
68.96	0.41
62.91	0.24
43.44	0.71
11.22	0.63
11.22	0.86
11.22	0.63
6.44	0.73
6.44	0.63

VIBRATIONAL ENTHALPY AT ROOM TEMPERATURE = 183.06
ZERO POINT ENERGY = 171.55
ATOMIZATION ENERGY = -3585.97


infrared intensity
ltp5
intensity
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6
5
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3
2
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0
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500
1000
1500
2000
2500
3000
3500
wave number

Fig. 5c

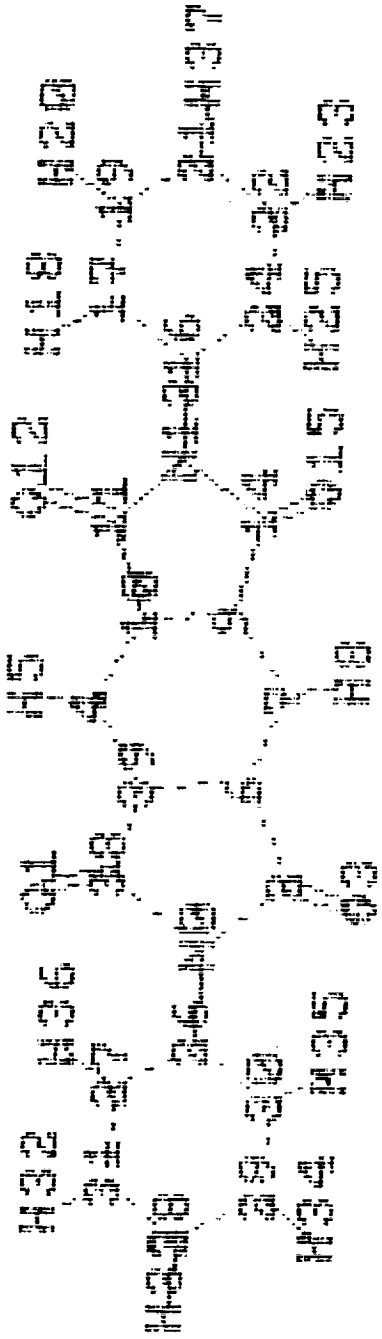


Fig. 6a

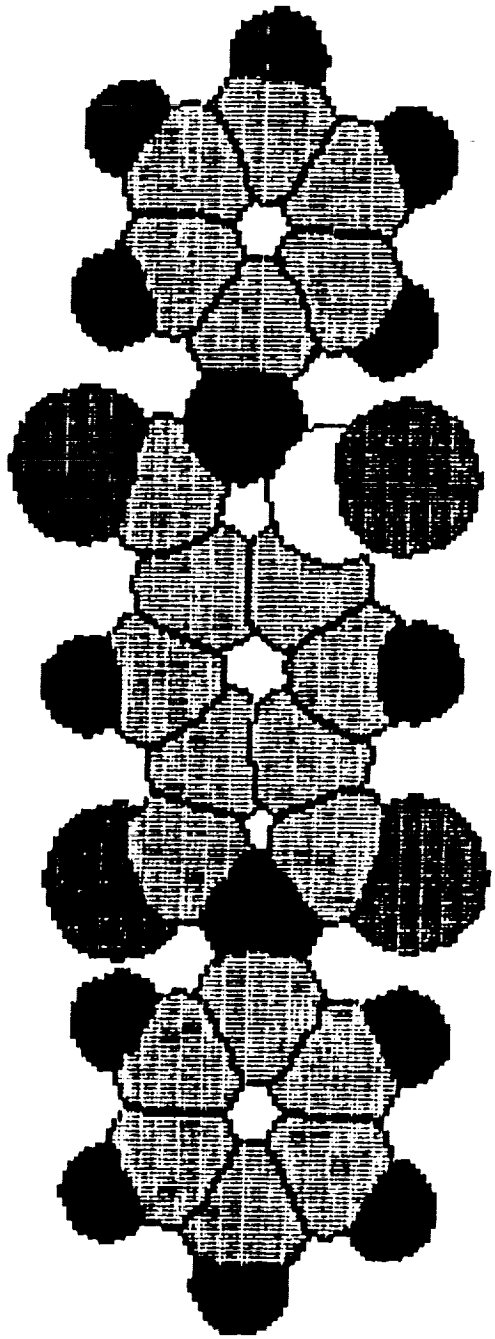


Fig. 6b

F I N A L R E S U L T S

LTP6

BOND LENGTHS (IN ANGSTROMS)	TYPE	ATOMS INVOLVED
1.4975	AA	10 11
1.4230	AA	10 9
1.4050	AA	10 4
1.2535	AO	11 12
1.4372	AN	11 13
1.4730	NA	13 16
1.4446	NA	13 14
1.4209	AA	16 17
1.4220	AA	16 24
1.0817	AH	17 18
1.4049	AA	17 19
1.0834	AH	19 20
1.4018	AA	19 21
1.0831	AH	21 37
1.4023	AA	21 22
1.0834	AH	22 23
1.4043	AA	22 24
1.0817	AH	24 25
1.2518	AO	14 15
1.4962	AA	14 9
1.4057	AA	9 7
1.0805	AH	7 8
1.4043	AA	7 6
1.4969	AA	6 2
1.4258	AA	6 39
1.2537	AO	2 3
1.4342	AN	2 0
1.4707	NA	0 26
1.4419	NA	0 38
1.4190	AA	26 30
1.4199	AA	26 27
1.0825	AH	30 35
1.4048	AA	30 29
1.0833	AH	29 34
1.4026	AA	29 28
1.0831	AH	28 33
1.4031	AA	28 31
1.0833	AH	31 32
1.4044	AA	31 27
1.0825	AH	27 36
1.2527	AO	38 1
1.4937	AA	38 39
1.4053	AA	39 4

1.0805 AH 4 5

THETA ANGLES (IN DEGREES)	TYPE	ATOMS INVOLVED
108.0051	AAA	11 10 9
130.0802	AAA	11 10 4
124.7437	AAO	10 11 12
107.5153	AAN	10 11 13
121.9150	AAA	9 10 4
107.9751	AAA	10 9 14
121.9142	AAA	10 9 7
116.2192	AAA	10 4 39
121.8980	AAH	10 4 5
127.5810	OAN	12 11 13
125.5118	ANA	11 13 16
109.1144	ANA	11 13 14
125.3728	ANA	16 13 14
121.1755	NAA	13 16 17
121.0811	NAA	13 16 24
127.5811	NAO	13 14 15
107.3851	NAA	13 14 9
117.7435	AAA	17 16 24
121.0150	AAH	16 17 18
120.9522	AAA	16 17 19
120.9549	AAA	16 24 22
120.9961	AAH	16 24 25
118.0229	HAA	18 17 19
119.6742	AAH	17 19 20
120.3210	AAA	17 19 21
120.0048	HAA	20 19 21
120.1506	AAH	19 21 37
119.7209	AAA	19 21 22
120.1288	HAA	37 21 22
120.0033	AAH	21 22 23
120.3071	AAA	21 22 24
119.6894	HAA	23 22 24
118.0372	AAH	22 24 25
124.8898	OAA	15 14 9
130.1085	AAA	14 9 7
121.8801	AAH	9 7 8
116.2131	AAA	9 7 6
121.9063	HAA	8 7 6
130.1414	AAA	7 6 2
121.8760	AAA	7 6 39
107.9825	AAA	2 6 39
125.3692	AAO	6 2 3
107.2752	AAN	6 2 0
107.9875	AAA	6 39 38
121.8478	AAA	6 39 4

127.2674	OAN	3	2	0	
125.3147	ANA	2	0	26	
109.5416	ANA	2	0	38	
125.1428	ANA	26	0	38	
120.8510	NAA	0	26	30	
120.8665	NAA	0	26	27	
127.2260	NAO	0	38	1	
107.2031	NAA	0	38	39	
118.2826	AAA	30	26	27	
120.6148	AAH	26	30	35	
120.6838	AAA	26	30	29	
120.6676	AAA	26	27	31	
120.5968	AAH	26	27	36	
118.6819	HAA	35	30	29	
119.7511	AAH	30	29	34	
120.2513	AAA	30	29	28	
119.9977	HAA	34	29	28	
120.0722	AAH	29	28	33	
119.8615	AAA	29	28	31	
120.0666	HAA	33	28	31	
119.9754	AAH	28	31	32	
120.2512	AAA	28	31	27	
119.7736	HAA	32	31	27	
118.7183	AAH	31	27	36	
125.4473	OAA	1	38	39	
130.1633	AAA	38	39	4	
121.8830	AAH	39	4	5	

PHI ANGLES (IN DEGREES)	TYPE	ATOMS INVOLVED			
184.7502	AAAO	9	10	11	12
0.4406	AAAN	9	10	11	13
4.6525	AAAO	4	10	11	12
180.3427	AAAN	4	10	11	13
359.2840	AAAA	11	10	9	14
178.7643	AAAA	11	10	9	7
179.3722	AAAA	4	10	9	14
358.8523	AAAA	4	10	9	7
180.7391	AAAA	11	10	4	39
0.6104	AAAH	11	10	4	5
0.6299	AAAA	9	10	4	39
180.5013	AAAH	9	10	4	5
180.4187	AANA	10	11	13	16
0.0280	AANA	10	11	13	14
355.9505	OANA	12	11	13	16
175.5572	OANA	12	11	13	14
330.2682	ANAA	11	13	16	17
150.0677	ANAA	11	13	16	24
150.7238	ANAA	14	13	16	17

330.5233	ANAA	14	13	16	24
175.3073	ANAO	11	13	14	15
359.5420	ANAA	11	13	14	9
354.9149	ANAO	16	13	14	15
179.1496	ANAA	16	13	14	9
358.4428	NAAH	13	16	17	18
179.6310	NAAA	13	16	17	19
178.6369	AAAH	24	16	17	18
359.8253	AAAA	24	16	17	19
180.0523	NAAA	13	16	24	22
358.7643	NAAH	13	16	24	25
359.8630	AAAA	17	16	24	22
178.5704	AAAH	17	16	24	25
180.1119	AAAH	16	17	19	20
0.3147	AAAA	16	17	19	21
1.2647	HAAH	18	17	19	20
181.4684	HAAA	18	17	19	21
179.8781	AAAH	17	19	21	37
359.8644	AAAA	17	19	21	22
0.0839	HAAH	20	19	21	37
180.0656	HAAA	20	19	21	22
180.1028	AAAH	19	21	22	23
359.8264	AAAA	19	21	22	24
0.0839	HAAH	37	21	22	23
179.8103	HAAA	37	21	22	24
0.3140	AAAA	16	24	22	21
180.0485	AAAH	16	24	22	23
181.5685	AAAH	21	22	24	25
1.2957	HAAH	23	22	24	25
0.7351	AAAN	10	9	14	13
184.8260	AAAO	10	9	14	15
181.3121	NAAA	13	14	9	7
5.4027	OAAA	15	14	9	7
180.7605	AAAH	10	9	7	8
0.4352	AAAA	10	9	7	6
0.1136	AAAH	14	9	7	8
179.7906	AAAA	14	9	7	6
180.9903	AAAA	9	7	6	2
0.7171	AAAA	9	7	6	39
0.6644	HAAA	8	7	6	2
180.3922	HAAA	8	7	6	39
357.2678	AAAO	7	6	2	3
180.4862	AAAN	7	6	2	0
177.5116	AAAO	39	6	2	3
0.7303	AAAN	39	6	2	0
179.1815	AAAA	7	6	39	38
358.7613	AAAA	7	6	39	4
358.9620	AAAA	2	6	39	38
178.5416	AAAA	2	6	39	4
180.2805	AANA	6	2	0	26
359.8864	AANA	6	2	0	38

3.5795	OANA	3	2	0	26
183.1826	OANA	3	2	0	38
39.0549	ANAA	2	0	26	30
218.8816	ANAA	2	0	26	27
219.5124	ANAA	38	0	26	30
39.3390	ANAA	38	0	26	27
183.3871	ANAO	2	0	38	1
359.4887	ANAA	2	0	38	39
2.9910	ANAO	26	0	38	1
179.0919	ANAA	26	0	38	39
1.2061	NAAH	0	26	30	35
179.5652	NAAA	0	26	30	29
181.3747	AAAH	27	26	30	35
359.7346	AAAA	27	26	30	29
179.9558	NAAA	0	26	27	31
1.5008	NAAH	0	26	27	36
359.7898	AAAA	30	26	27	31
181.3316	AAAH	30	26	27	36
180.6567	AAAH	26	30	29	34
0.4829	AAAA	26	30	29	28
359.0474	HAAH	35	30	29	34
178.8739	HAAA	35	30	29	28
179.7944	AAAH	30	29	28	33
359.7824	AAAA	30	29	28	31
359.6205	HAAH	34	29	28	33
179.6083	HAAA	34	29	28	31
179.6294	AAAH	29	28	31	32
359.7413	AAAA	29	28	31	27
359.6164	HAAH	33	28	31	32
179.7288	HAAA	33	28	31	27
0.4764	AAAA	26	27	31	28
180.5885	AAAH	26	27	31	32
178.9611	AAAH	28	31	27	36
359.0730	HAAH	32	31	27	36
0.9705	AAAN	6	39	38	0
177.1599	AAAO	6	39	38	1
181.4380	NAAA	0	38	39	4
357.6274	OAAA	1	38	39	4
0.5230	AAAA	10	4	39	6
180.0000	AAAA	10	4	39	38
180.6510	AAAH	6	39	4	5
0.1297	AAAH	38	39	4	5
180.0885	AAAA	11	9	10	4
185.1880	AOAN	10	12	11	13
180.5761	AAAA	10	14	9	7
180.1282	AAAH	10	39	4	5
180.4546	AANA	11	16	13	14
180.1958	NAAA	13	17	16	24
175.0724	NOAA	13	15	14	9
178.8453	AHAA	16	18	17	19
181.2545	AAAH	16	22	24	25

179.7983	AHAA	17	20	19	21
180.0000	AHAA	19	37	21	22
180.2727	AHAA	21	23	22	24
180.3432	AHAA	9	8	7	6
180.2423	AAAA	7	2	6	39
176.1367	AOAN	6	3	2	0
180.4673	AAAA	6	38	39	4
180.4580	AANA	2	26	0	38
180.1679	NAAA	0	30	26	27
184.5730	NOAA	0	1	38	39
181.6089	AHAA	26	35	30	29
178.4852	AAAH	26	31	27	36
180.1713	AHAA	30	34	29	28
180.0000	AHAA	29	33	28	31
179.8881	AHAA	28	32	31	27

TOTAL ENERGY =	-4246.6811523438 KCAL
DIAGONAL CORE CONTRIBUTION =	-105.1765365601 KCAL
BOND CONTRIBUTION =	-4406.6074218750 KCAL
NON-BOND CONTRIBUTION =	19.6340141296 KCAL
REPULS CONTRIBUTION =	1424.4631347656 KCAL
THETA CONTRIBUTION =	66.4076690674 KCAL
PHI CONTRIBUTION =	-1245.4017333984 KCAL

LTP6

1.1921	0.6803	0.1821
2.6200	1.1120	0.3137
2.9963	2.1839	0.8435
3.4428	0.0405	-0.1765
4.9151	0.0437	-0.2207
5.6437	1.2536	-0.3759
5.1336	2.2006	-0.4906
7.0482	1.2521	-0.4098
7.5829	2.1870	-0.5272
7.7575	0.0483	-0.2968
8.8402	0.0501	-0.3252
7.0593	-1.1585	-0.1464
7.6029	-2.0914	-0.0571
5.6556	-1.1648	-0.1051
5.1554	-2.1131	0.0379
2.5955	-1.0457	-0.6112
2.9450	-2.1104	-1.1693
1.1783	-0.6318	-0.3686
-0.0204	-1.3311	-0.5927
-0.0297	-2.3320	-0.9997

-1.2045	-0.6578	-0.2511
-2.6297	-1.1071	-0.3385
-3.0171	-2.2060	-0.8012
-3.4469	-0.0251	0.1290
-4.9149	-0.0446	0.2166
-5.6033	-1.2119	0.6375
-5.0566	-2.1026	0.9200
-7.0050	-1.2239	0.7286
-7.5145	-2.1200	1.0619
-7.7447	-0.0802	0.3936
-8.8256	-0.0937	0.4617
-7.0814	1.0815	-0.0298
-7.6512	1.9639	-0.2948
-5.6797	1.1050	-0.1141
-5.1946	2.0088	-0.4600
-2.6074	1.0838	0.5095
-2.9707	2.1707	1.0155
-1.1920	0.6661	0.2781
0.0074	1.3603	0.5110
0.0180	2.3596	0.9217

VIBRATIONAL FREQUENCY	I.R. INTENSITY
3094.96	0.00
3094.61	2.26
3092.96	0.01
3092.85	0.02
3090.79	0.08
3090.54	0.16
3089.51	0.02
3089.49	0.11
3088.83	2.25
3088.60	2.17
3087.61	3.74
3087.27	3.64
1679.18	0.00
1653.52	0.00
1645.21	0.29
1619.63	4.25
1618.45	0.01
1616.84	0.02
1609.75	0.02
1587.78	0.63
1583.56	0.00
1571.71	0.00
1519.83	1.64
1518.26	1.24
1507.64	0.04
1479.72	1.33
1478.76	3.32
1468.19	0.11

1453.77	1.63
1410.08	0.04
1409.44	0.09
1384.00	0.05
1375.86	0.05
1352.86	0.26
1345.77	1.01
1290.11	0.00
1266.59	0.01
1265.46	0.26
1207.76	4.00
1182.08	0.24
1171.79	0.13
1167.76	0.01
1162.66	0.08
1157.14	0.00
1137.68	0.00
1116.64	0.55
1107.14	0.60
1098.98	0.08
1074.85	2.12
1069.34	0.09
1067.62	0.65
1055.05	0.50
1053.57	0.31
1052.36	0.41
1048.47	0.31
1038.55	0.55
1035.89	0.37
1026.46	0.01
973.11	1.28
963.99	0.28
960.29	0.08
959.64	0.04
901.54	3.52
900.81	1.05
872.21	0.00
870.56	0.00
869.43	0.00
846.90	0.01
770.44	5.88
768.21	3.16
760.05	0.00
718.21	0.03
708.88	0.00
679.74	0.05
677.87	0.17
672.02	0.73
669.32	1.27
658.14	0.00
629.98	0.01

627.25	0.00
622.10	0.27
610.92	0.00
600.31	2.13
563.74	0.41
543.62	0.00
496.59	0.01
489.82	2.43
450.55	0.00
440.15	1.65
428.16	5.58
423.13	0.01
414.82	0.01
413.08	0.25
388.72	0.05
369.35	1.27
345.64	0.02
322.83	0.04
319.29	0.03
304.30	3.31
297.06	1.21
232.66	0.01
220.63	2.26
206.41	0.00
188.36	0.00
172.89	0.17
161.42	3.69
126.62	4.61
109.43	0.10
90.52	0.06
69.82	0.01
65.25	0.67
54.09	0.02
51.84	0.03
20.88	0.01
8.09	2.53
8.09	0.01
8.09	2.53
5.88	0.61
5.88	2.53
5.88	0.61

VIBRATIONAL ENTHALPY AT ROOM TEMPERATURE = 191.12
ZERO POINT ENERGY = 179.88
ATOMIZATION ENERGY = -4066.81

infrared intensity

ltp6

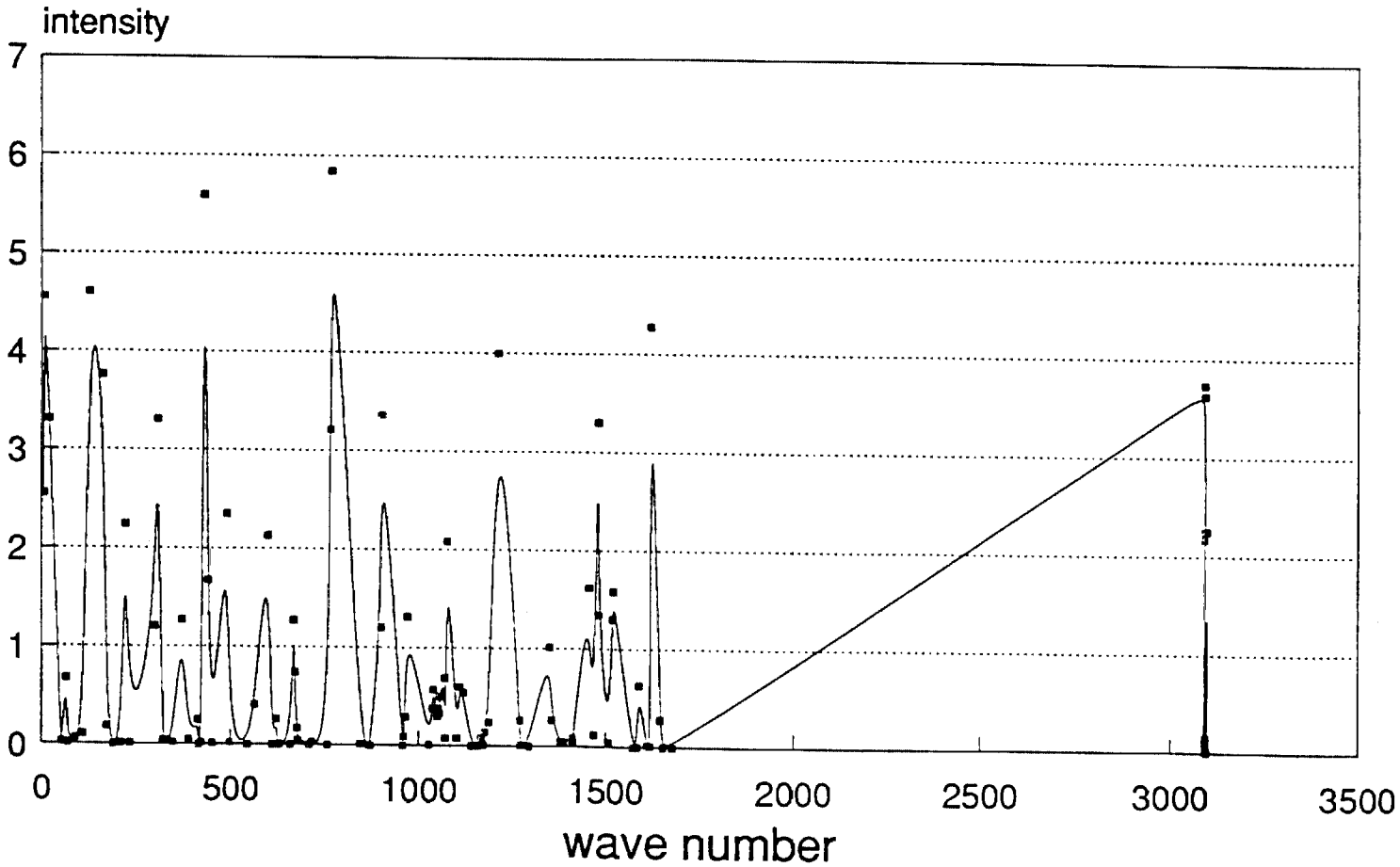


Fig. 6c

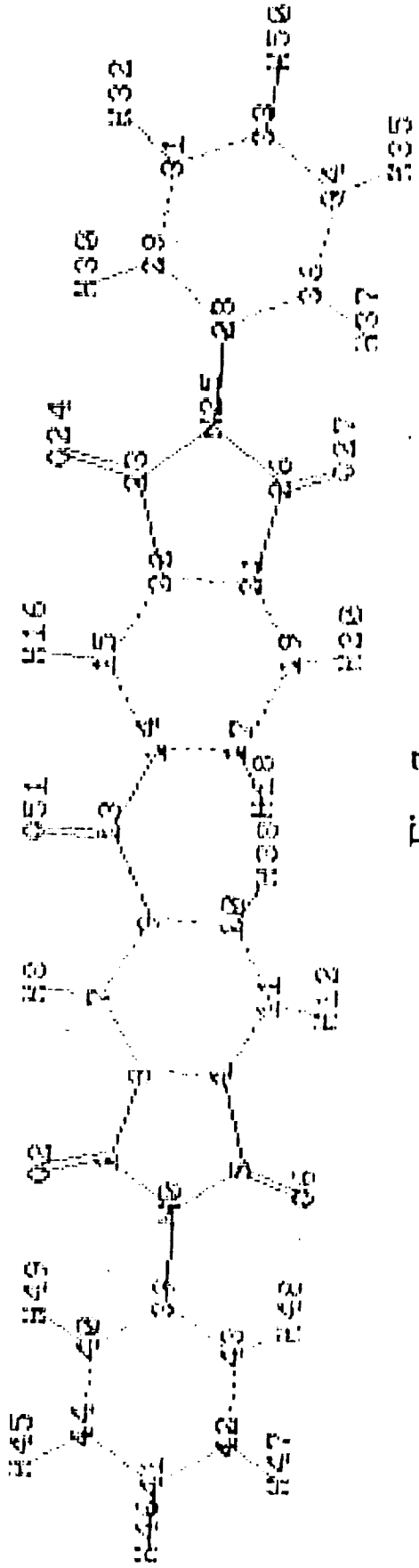


Fig. 7a

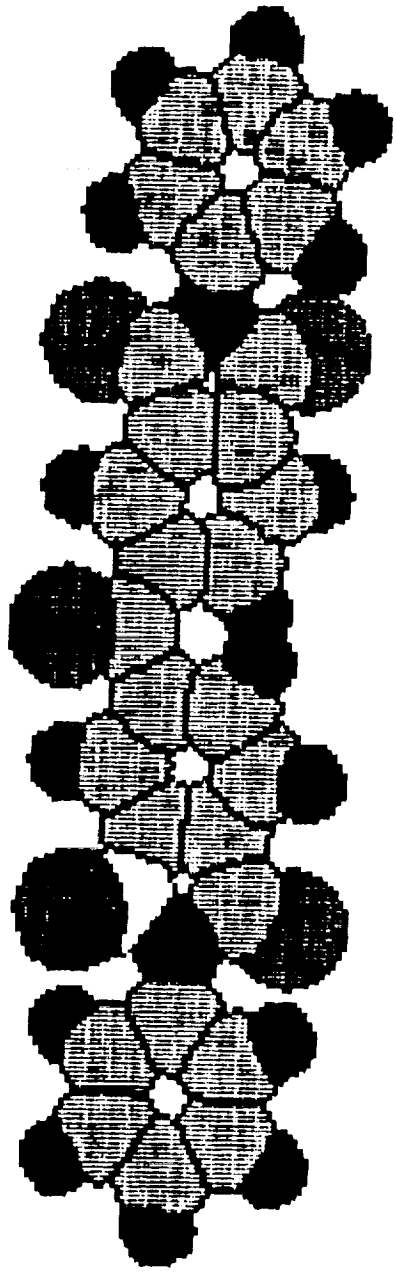


Fig. 7b

F I N A L R E S U L T S

LTP7

BOND LENGTHS (IN ANGSTROMS)	TYPE	ATOMS INVOLVED
1.2581	AO	13 51
1.4964	AA	13 14
1.5027	AA	13 9
1.4307	AA	14 15
1.4259	AA	14 17
1.0818	AH	15 16
1.3944	AA	15 22
1.4940	AA	22 23
1.4179	AA	22 21
1.2530	AO	23 24
1.4427	AN	23 25
1.4658	NA	25 28
1.4422	NA	25 26
1.4201	AA	28 29
1.4225	AA	28 36
1.0823	AH	29 30
1.4048	AA	29 31
1.0834	AH	31 32
1.4021	AA	31 33
1.0831	AH	33 5
1.4035	AA	33 34
1.0833	AH	34 35
1.4036	AA	34 36
1.0821	AH	36 37
1.2546	AO	26 27
1.4918	AA	26 21
1.3972	AA	21 19
1.0821	AH	19 20
1.4103	AA	19 17
1.0820	AH	17 18
1.4260	AA	9 10
1.4270	AA	9 7
1.0820	AH	10 38
1.4102	AA	10 11
1.0821	AH	11 12
1.3973	AA	11 4
1.4971	AA	4 5
1.4118	AA	4 3
1.2540	AO	5 6
1.4421	AN	5 0
1.4792	NA	0 39
1.4534	NA	0 1
1.4249	AA	39 43

1.4247	AA	39 40
1.0790	AH	43 48
1.4053	AA	43 42
1.0836	AH	42 47
1.4002	AA	42 41
1.0832	AH	41 46
1.3998	AA	41 44
1.0837	AH	44 45
1.4053	AA	44 40
1.0789	AH	40 49
1.2519	AO	1 2
1.4925	AA	1 3
1.3972	AA	3 7
1.0818	AH	7 8

THETA ANGLES (IN DEGREES)	TYPE	ATOMS INVOLVED
118.9631	OAA	51 13 14
118.6702	OAA	51 13 9
122.3637	AAA	14 13 9
119.6263	AAA	13 14 15
121.6628	AAA	13 14 17
121.5796	AAA	13 9 10
119.5991	AAA	13 9 7
118.6333	AAA	15 14 17
120.5975	AAH	14 15 16
119.1168	AAA	14 15 22
121.8065	AAA	14 17 19
120.3631	AAH	14 17 18
120.2848	HAA	16 15 22
130.5495	AAA	15 22 23
121.2721	AAA	15 22 21
108.1761	AAA	23 22 21
125.3360	AAO	22 23 24
107.1371	AAN	22 23 25
108.2736	AAA	22 21 26
120.7260	AAA	22 21 19
127.3865	OAN	24 23 25
125.2331	ANA	23 25 28
109.2150	ANA	23 25 26
125.5512	ANA	28 25 26
120.9316	NAA	25 28 29
121.0488	NAA	25 28 36
127.4073	NAO	25 26 27
107.1940	NAA	25 26 21
118.0199	AAA	29 28 36
120.7662	AAH	28 29 30
120.8295	AAA	28 29 31
120.7680	AAA	28 36 34

120.7135	AAH	28 36 37
118.3846	HAA	30 29 31
119.7111	AAH	29 31 32
120.2702	AAA	29 31 33
120.0189	HAA	32 31 33
120.0947	AAH	31 33 5
119.8127	AAA	31 33 34
120.0929	HAA	5 33 34
119.9296	AAH	33 34 35
120.2990	AAA	33 34 36
119.7714	HAA	35 34 36
118.4971	AAH	34 36 37
125.2575	OAA	27 26 21
130.9941	AAA	26 21 19
121.7331	AAH	21 19 20
118.4181	AAA	21 19 17
119.8452	HAA	20 19 17
117.8174	AAH	19 17 18
118.7077	AAA	10 9 7
120.3806	AAH	9 10 38
121.7169	AAA	9 10 11
119.0821	AAA	9 7 3
120.5771	AAH	9 7 8
117.8783	HAA	38 10 11
119.8599	AAH	10 11 12
118.3785	AAA	10 11 4
121.7537	HAA	12 11 4
130.9509	AAA	11 4 5
120.8320	AAA	11 4 3
108.2014	AAA	5 4 3
123.6071	AAO	4 5 6
107.7952	AAN	4 5 0
108.1523	AAA	4 3 1
121.2760	AAA	4 3 7
128.5512	OAN	6 5 0
126.1327	ANA	5 0 39
108.1255	ANA	5 0 1
125.7334	ANA	39 0 1
121.7692	NAA	0 39 43
121.6527	NAA	0 39 40
128.4503	NAO	0 1 2
107.7125	NAA	0 1 3
116.5755	AAA	43 39 40
122.0834	AAH	39 43 48
121.5431	AAA	39 43 42
121.5860	AAA	39 40 44
122.1431	AAH	39 40 49
116.3729	HAA	48 43 42
119.4965	AAH	43 42 47
120.4817	AAA	43 42 41
120.0220	HAA	47 42 41

120.3351	AAH	42 41 46
119.3613	AAA	42 41 44
120.3039	HAA	46 41 44
120.0830	AAH	41 44 45
120.4477	AAA	41 44 40
119.4688	HAA	45 44 40
116.2678	AAH	44 40 49
123.8012	OAA	2 1 3
130.5591	AAA	1 3 7
120.3405	AAH	3 7 8

PHI ANGLES (IN DEGREES)	TYPE	ATOMS INVOLVED
22.0489	OAAA	51 13 14 15
205.3046	OAAA	51 13 14 17
202.7262	AAAA	9 13 14 15
25.9819	AAAA	9 13 14 17
209.2630	OAAA	51 13 9 10
25.3323	OAAA	51 13 9 7
28.5876	AAAA	14 13 9 10
204.6570	AAAA	14 13 9 7
2.1321	AAAH	13 14 15 16
181.7337	AAAA	13 14 15 22
178.9749	AAAH	17 14 15 16
358.5766	AAAA	17 14 15 22
178.7297	AAAA	13 14 17 19
0.0839	AAAH	13 14 17 18
1.9541	AAAA	15 14 17 19
183.3116	AAAH	15 14 17 18
179.3713	AAAA	14 15 22 23
0.0396	AAAA	14 15 22 21
358.9742	HAAA	16 15 22 23
179.6331	HAAA	16 15 22 21
4.3418	AAAO	15 22 23 24
180.2880	AAAN	15 22 23 25
183.7483	AAAO	21 22 23 24
359.6948	AAAN	21 22 23 25
180.0862	AAAA	15 22 21 26
0.9239	AAAA	15 22 21 19
0.6161	AAAA	23 22 21 26
181.4516	AAAA	23 22 21 19
179.5314	AANA	22 23 25 28
359.8601	AANA	22 23 25 26
355.3697	OANA	24 23 25 28
175.6969	OANA	24 23 25 26
325.2000	ANAA	23 25 28 29
145.1639	ANAA	23 25 28 36
144.8204	ANAA	26 25 28 29
324.7843	ANAA	26 25 28 36

176.3349	ANAO	23 25 26 27
0.5120	ANAA	23 25 26 21
356.6633	ANAO	28 25 26 27
180.8405	ANAA	28 25 26 21
358.4061	NAAH	25 28 29 30
180.0593	NAAA	25 28 29 31
178.4413	AAAH	36 28 29 30
0.0969	AAAA	36 28 29 31
180.2907	NAAA	25 28 36 34
358.5688	NAAH	25 28 36 37
0.2549	AAAA	29 28 36 34
178.5337	AAAH	29 28 36 37
179.5122	AAAH	28 29 31 32
359.6732	AAAA	28 29 31 33
1.1297	HAAH	30 29 31 32
181.2903	HAAA	30 29 31 33
180.1958	AAAH	29 31 33 5
0.2017	AAAA	29 31 33 34
0.3593	HAAH	32 31 33 5
180.3632	HAAA	32 31 33 34
180.3461	AAAH	31 33 34 35
0.1506	AAAA	31 33 34 36
0.3511	HAAH	5 33 34 35
180.1545	HAAA	5 33 34 36
359.6175	AAAA	28 36 34 33
179.4219	AAAH	28 36 34 35
181.3024	AAAH	33 34 36 37
1.1068	HAAH	35 34 36 37
359.2956	AAAN	22 21 26 25
183.3594	AAAO	22 21 26 27
178.3448	NAAA	25 26 21 19
2.4082	OAAA	27 26 21 19
178.8497	AAAH	22 21 19 20
359.5785	AAAA	22 21 19 17
359.8954	AAAH	26 21 19 20
180.6290	AAAA	26 21 19 17
358.9736	AAAA	14 17 19 21
179.6872	AAAH	14 17 19 20
177.6493	AAAH	21 19 17 18
358.3638	HAAH	20 19 17 18
358.7545	AAAH	13 9 10 38
176.9135	AAAA	13 9 10 11
182.6511	AAAH	7 9 10 38
0.8101	AAAA	7 9 10 11
183.2248	AAAA	13 9 7 3
2.9402	AAAH	13 9 7 8
359.4072	AAAA	10 9 7 3
179.1229	AAAH	10 9 7 8
180.1494	AAAH	9 10 11 12
359.1216	AAAA	9 10 11 4
358.3488	HAAH	38 10 11 12

177.3252	HAAA	38	10	11	4
182.3783	AAAA	10	11	4	5
0.7399	AAAA	10	11	4	3
1.3343	HAAA	12	11	4	5
179.6974	HAAA	12	11	4	3
0.8009	AAAO	11	4	5	6
178.5034	AAAN	11	4	5	0
182.2811	AAAO	3	4	5	6
360.0000	AAAN	3	4	5	0
180.6120	AAAA	11	4	3	1
359.4395	AAAA	11	4	3	7
359.3102	AAAA	5	4	3	1
178.1369	AAAA	5	4	3	7
181.7588	AANA	4	5	0	39
0.7343	AANA	4	5	0	1
359.3125	OANA	6	5	0	39
178.2874	OANA	6	5	0	1
350.0325	ANAA	5	0	39	43
169.3929	ANAA	5	0	39	40
171.2325	ANAA	1	0	39	43
350.5930	ANAA	1	0	39	40
176.6969	ANAO	5	0	1	2
358.8513	ANAA	5	0	1	3
355.6771	ANAO	39	0	1	2
177.8313	ANAA	39	0	1	3
358.6280	NAAH	0	39	43	48
178.9948	NAAA	0	39	43	42
179.2369	AAAH	40	39	43	48
359.6044	AAAA	40	39	43	42
180.3251	NAAA	0	39	40	44
359.6347	NAAH	0	39	40	49
359.7175	AAAA	43	39	40	44
179.0274	AAAH	43	39	40	49
180.5808	AAAH	39	43	42	47
0.6853	AAAA	39	43	42	41
0.9279	HAAH	48	43	42	47
181.0327	HAAA	48	43	42	41
179.7626	AAAH	43	42	41	46
359.7217	AAAA	43	42	41	44
359.8688	HAAH	47	42	41	46
179.8264	HAAA	47	42	41	44
179.9260	AAAH	42	41	44	45
359.6044	AAAA	42	41	44	40
359.8749	HAAH	46	41	44	45
179.5630	HAAA	46	41	44	40
0.6858	AAAA	39	40	44	41
180.3743	AAAH	39	40	44	45
181.3365	AAAH	41	44	40	49
1.0247	HAAH	45	44	40	49
1.1465	AAAN	4	3	1	0
183.1768	AAAO	4	3	1	2

182.4663	NAAA	0	1	3	7
4.4965	OAAA	2	1	3	7
0.4793	AAAA	9	7	3	4
179.0115	AAAA	9	7	3	1
180.7631	AAAH	4	3	7	8
359.2956	AAAH	1	3	7	8
180.6770	OAAA	51	14	13	9
176.8430	AAAA	13	15	14	17
183.8967	AAAA	13	10	9	7
180.4040	AHAA	14	16	15	22
178.6757	AAAH	14	19	17	18
179.4065	AAAA	15	23	22	21
184.8759	AOAN	22	24	23	25
179.0488	AAAA	22	26	21	19
179.6205	AANA	23	28	25	26
180.0343	NAAA	25	29	28	36
175.1117	NOAA	25	27	26	21
178.3839	AHAA	28	30	29	31
181.6854	AAAH	28	34	36	37
179.8393	AHAA	29	32	31	33
180.0000	AHAA	31	5	33	34
180.1948	AHAA	33	35	34	36
179.2622	AHAA	21	20	19	17
181.7711	AHAA	9	38	10	11
180.2839	AAAH	9	3	7	8
181.0591	AHAA	10	12	11	4
181.4807	AAAA	11	5	4	3
182.7973	AOAN	4	6	5	0
181.3200	AAAA	4	1	3	7
181.2001	AANA	5	39	0	1
180.6091	NAAA	0	43	39	40
177.5303	NOAA	0	2	1	3
179.6511	AHAA	39	48	43	42
180.6507	AAAH	39	44	40	49
179.8953	AHAA	43	47	42	41
180.0485	AHAA	42	46	41	44
180.3103	AHAA	41	45	44	40

TOTAL ENERGY = -5737.8618164063 KCAL

DIAGONAL CORE CONTRIBUTION = -181.3540496826 KCAL
BOND CONTRIBUTION = -5698.6513671875 KCAL
NON-BOND CONTRIBUTION = 32.6758804321 KCAL
REPULS CONTRIBUTION = 1655.5834960938 KCAL
THETA CONTRIBUTION = 73.2184753418 KCAL
PHI CONTRIBUTION = -1619.3342285156 KCAL

LTP7

0.0712	1.2999	0.1285
0.1218	2.5435	0.3114
1.3438	0.5505	-0.1127
2.5871	1.1098	0.3215
2.6114	2.0521	0.8522
3.7700	0.4198	0.0590
5.1878	0.7660	0.3786
5.5588	1.7631	1.0405
6.0116	-0.3033	-0.1305
7.4734	-0.3615	-0.0392
8.2578	0.8190	-0.1274
7.7921	1.7824	-0.2896
9.6588	0.7607	-0.0409
10.2400	1.6717	-0.1185
10.3050	-0.4702	0.1416
11.3851	-0.5115	0.2111
9.5482	-1.6486	0.2338
10.0452	-2.6000	0.3805
8.1486	-1.6005	0.1411
7.5927	-2.5239	0.2375
5.1698	-1.2982	-0.7481
5.5337	-2.3351	-1.3534
3.7617	-0.8204	-0.6282
2.5630	-1.3782	-1.0800
2.5396	-2.3145	-1.6221
1.3622	-0.6827	-0.8282
0.4440	-1.1038	-1.2160
-1.2671	0.6182	0.1752
-1.3993	-0.7402	0.5882
-0.5250	-1.3171	0.8597
-2.6597	-1.3635	0.6945
-2.7253	-2.3955	1.0132
-3.7997	-0.6107	0.4011
-5.2528	-0.9651	0.4649
-5.6786	-2.0843	0.8372
-6.0085	0.2031	0.0854
-7.4831	0.3129	0.0452
-8.3246	-0.8277	0.1904
-7.9253	-1.8224	0.3140
-9.7252	-0.7151	0.1723
-10.3335	-1.6033	0.2951
-10.3351	0.5327	-0.0050
-11.4149	0.6163	-0.0224
-9.5360	1.6716	-0.1588
-9.9958	2.6430	-0.2980
-8.1349	1.5680	-0.1275
-7.5854	2.4908	-0.2304
-5.0692	1.2667	-0.2290
-5.3118	2.4194	-0.6531

-3.6919	0.7365	-0.0071
-2.4481	1.3629	-0.1197
-2.3838	2.3996	-0.4220

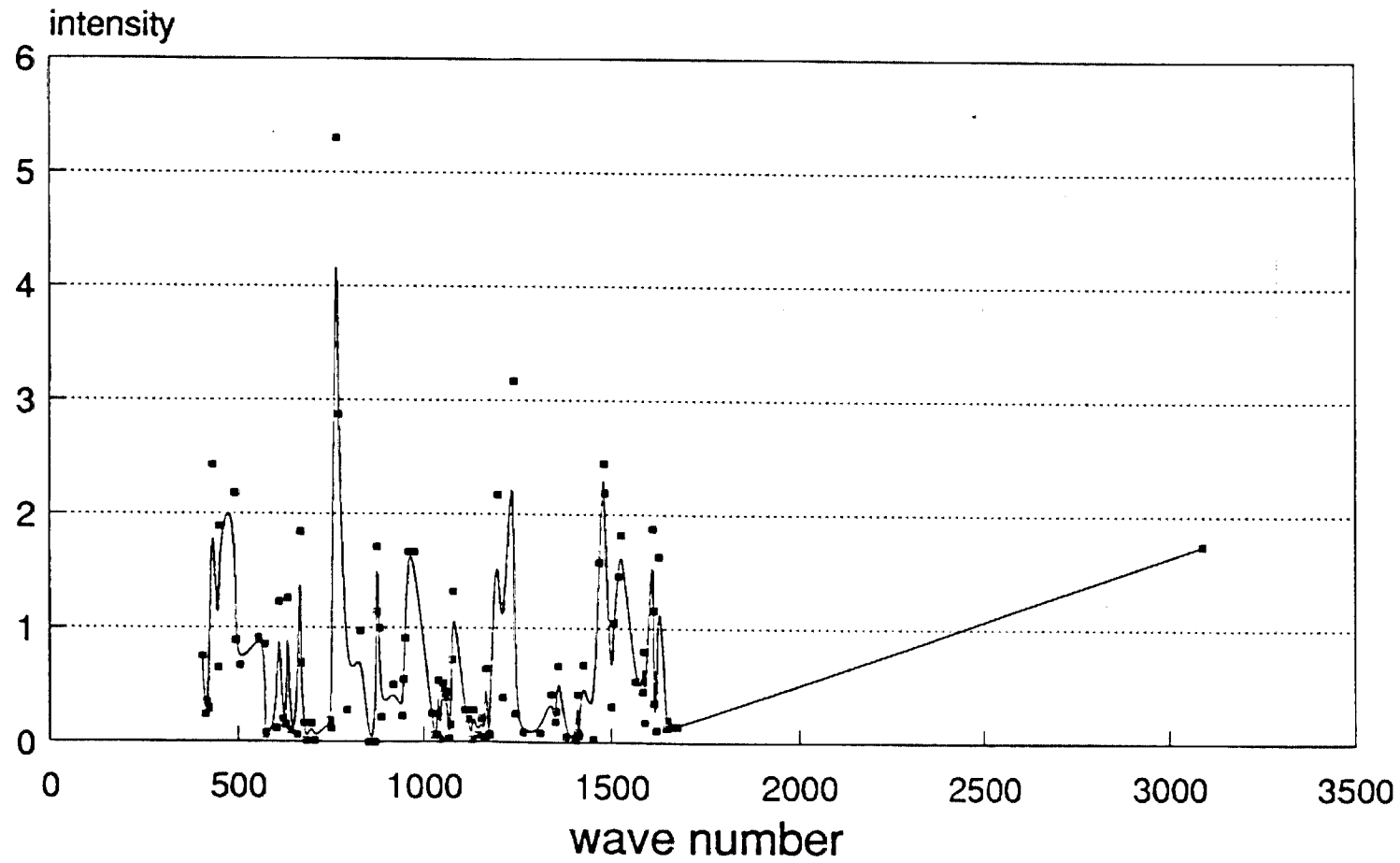
VIBRATIONAL FREQUENCY	I.R. INTENSITY
3097.00	0.21
3094.08	1.55
3092.83	0.01
3092.34	0.60
3092.31	1.24
3091.97	0.06
3090.73	0.49
3090.59	0.18
3090.55	1.14
3089.66	2.05
3089.41	0.10
3088.61	2.18
3088.52	2.25
3087.29	3.65
3087.06	1.94
3086.22	1.64
1676.36	0.13
1669.43	0.13
1649.62	0.19
1647.64	0.16
1625.65	1.57
1618.63	0.13
1613.93	0.39
1612.97	1.13
1610.30	1.79
1589.41	0.22
1585.99	0.76
1583.13	0.48
1563.78	0.56
1527.09	1.85
1519.11	1.49
1507.24	0.96
1499.55	0.34
1480.56	2.08
1479.58	2.61
1466.80	1.66
1451.30	0.04
1422.83	0.68
1412.09	0.11
1409.33	0.10
1407.84	0.38
1403.17	0.01
1379.23	0.05
1352.01	0.65
1348.57	0.27

1345.76	0.19
1335.30	0.40
1308.32	0.06
1262.06	0.09
1240.54	0.65
1238.47	2.78
1209.18	0.30
1196.37	2.22
1176.71	0.12
1173.35	0.03
1162.62	0.14
1160.68	0.56
1153.74	0.22
1142.57	0.08
1129.84	0.26
1125.95	0.05
1118.42	0.17
1109.41	0.25
1076.71	1.18
1074.35	0.86
1068.23	0.15
1065.68	0.02
1058.97	0.42
1054.36	0.47
1050.18	0.01
1049.73	1.02
1039.45	0.01
1037.46	0.45
1035.92	0.07
1026.20	0.04
1021.36	0.30
972.29	1.72
958.79	1.48
952.46	1.13
951.36	0.43
941.34	0.14
920.03	0.71
885.01	0.03
882.12	1.20
878.71	2.34
876.70	0.48
871.06	0.00
852.18	0.00
831.87	0.99
795.45	0.23
771.39	2.71
768.24	5.23
752.09	0.09
748.96	0.19
706.04	0.00
698.44	0.17

683.66	0.01
677.99	0.13
670.12	0.86
666.29	1.83
658.18	0.04
640.74	0.12
633.68	1.23
628.08	0.15
619.71	0.19
609.52	1.22
603.88	0.14
573.90	0.13
572.47	0.08
569.95	0.79
549.25	0.85
505.12	0.64
492.24	1.10
489.66	2.29
449.09	2.19
445.14	0.26
430.41	2.32
420.78	0.27
416.64	0.58
412.81	0.24
403.84	0.89
393.71	2.64
385.82	0.52
372.96	1.82
361.58	0.93
353.70	0.25
340.68	0.78
330.26	0.26
315.23	0.76
296.82	0.03
274.48	0.81
257.58	0.55
224.62	1.80
213.06	0.16
185.44	0.32
175.28	0.41
165.56	1.01
152.06	2.49
141.51	1.23
134.14	1.09
102.58	0.48
99.56	3.02
89.75	0.92
72.79	0.32
49.45	0.32
46.37	0.01
38.27	0.05

22.23	0.16
14.91	0.31
8.61	1.22
8.61	0.31
8.61	1.22
7.18	6.93
7.18	1.22
7.18	6.93

VIBRATIONAL ENTHALPY AT ROOM TEMPERATURE = 251.43
ZERO POINT ENERGY = 236.17
ATOMIZATION ENERGY = -5501.69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ltp7
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4
3
2
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0
0
500
1000
1500
2000
2500
3000
3500
wave number

Fig. 7c

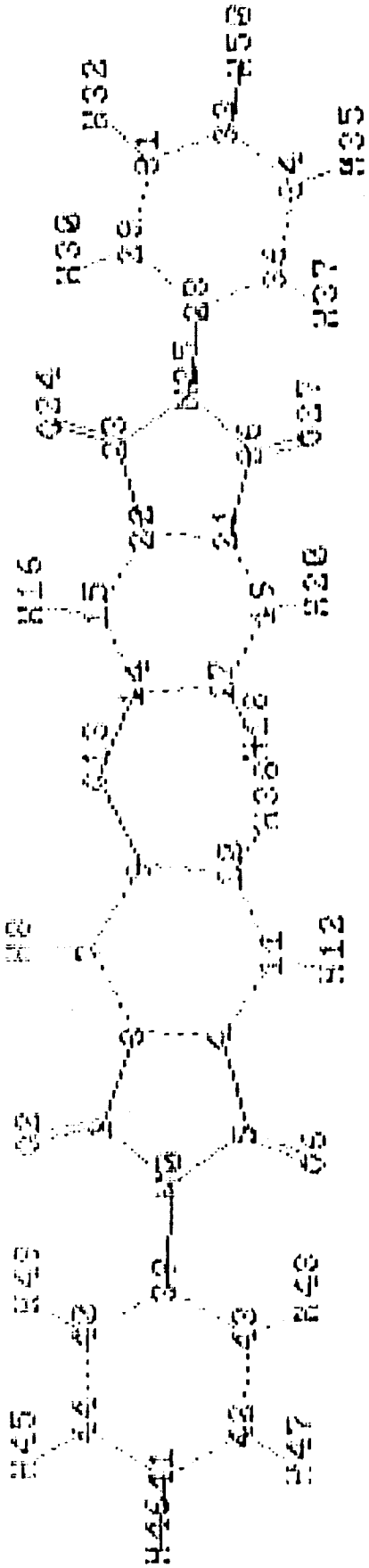

Fig. 8a

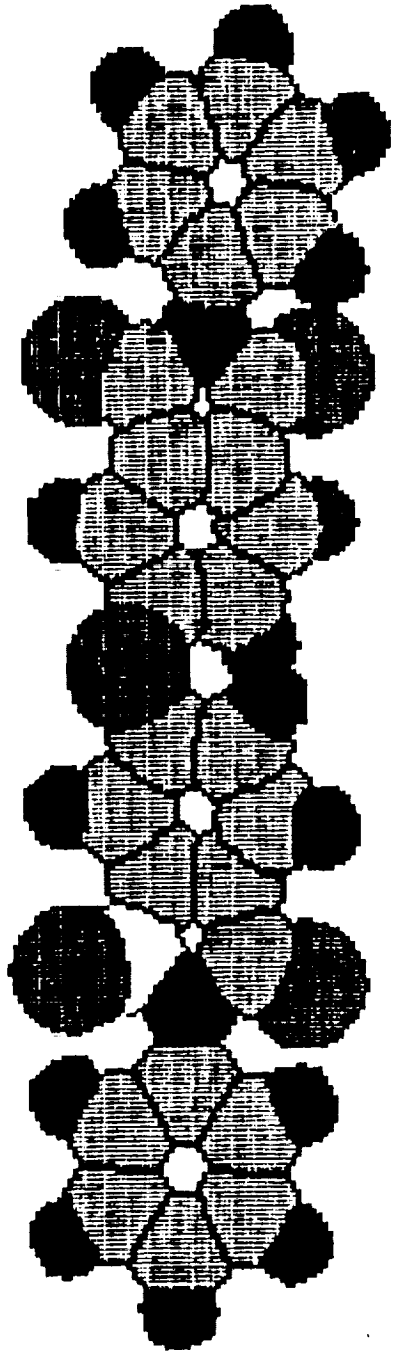

Fig. 8b

F I N A L R E S U L T S

LTP8

BOND LENGTHS (IN ANGSTROMS)	TYPE	ATOMS INVOLVED
1.5208	QA	13 14
1.5215	QA	13 9
1.4279	AA	14 15
1.4095	AA	14 17
1.0816	AH	15 16
1.4054	AA	15 22
1.4875	AA	22 23
1.4320	AA	22 21
1.2445	AO	23 24
1.5068	AN	23 25
1.3188	NA	25 28
1.4978	NA	25 26
1.5027	AA	28 29
1.5117	AA	28 36
1.0780	AH	29 30
1.3689	AA	29 31
1.0847	AH	31 32
1.4292	AA	31 33
1.0795	AH	33 50
1.4264	AA	33 34
1.0853	AH	34 35
1.3656	AA	34 36
1.0777	AH	36 37
1.2486	AO	26 27
1.4717	AA	26 21
1.3985	AA	21 19
1.0818	AH	19 20
1.4097	AA	19 17
1.0818	AH	17 18
1.4114	AA	9 10
1.4245	AA	9 7
1.0815	AH	10 38
1.4094	AA	10 11
1.0819	AH	11 12
1.3976	AA	11 4
1.4772	AA	4 5
1.4291	AA	4 3
1.2476	AO	5 6
1.4929	AN	5 0
1.3209	NA	0 39
1.5073	NA	0 1
1.5103	AA	39 43
1.5031	AA	39 40

1.0777	AH	43 48
1.3664	AA	43 42
1.0853	AH	42 47
1.4253	AA	42 41
1.0796	AH	41 46
1.4298	AA	41 44
1.0846	AH	44 45
1.3687	AA	44 40
1.0779	AH	40 49
1.2454	AO	1 2
1.4850	AA	1 3
1.4092	AA	3 7
1.0815	AH	7 8

THETA ANGLES (IN DEGREES)	TYPE	ATOMS INVOLVED
125.5694	AQA	14 13 9
119.6233	QAA	13 14 15
121.1829	QAA	13 14 17
121.1828	QAA	13 9 10
119.6481	QAA	13 9 7
119.1941	AAA	15 14 17
119.9234	AAH	14 15 16
118.9887	AAA	14 15 22
121.8858	AAA	14 17 19
120.8193	AAH	14 17 18
121.0814	HAA	16 15 22
131.4975	AAA	15 22 23
120.3433	AAA	15 22 21
108.1462	AAA	23 22 21
124.9333	AAO	22 23 24
108.1952	AAN	22 23 25
109.6284	AAA	22 21 26
120.5412	AAA	22 21 19
126.5949	OAN	24 23 25
128.0091	ANA	23 25 28
105.5495	ANA	23 25 26
126.4402	ANA	28 25 26
123.8993	NAA	25 28 29
123.1031	NAA	25 28 36
127.0634	NAO	25 26 27
108.2902	NAA	25 26 21
112.9968	AAA	29 28 36
120.0763	AAH	28 29 30
122.2084	AAA	28 29 31
122.5061	AAA	28 36 34
120.1006	AAH	28 36 37
117.5592	HAA	30 29 31
119.7945	AAH	29 31 32

121.7812	AAA	29	31	33
118.4237	HAA	32	31	33
120.6321	AAH	31	33	50
118.9607	AAA	31	33	34
120.4051	HAA	50	33	34
118.8514	AAH	33	34	35
121.4797	AAA	33	34	36
119.6669	HAA	35	34	36
117.2535	AAH	34	36	37
124.2929	OAA	27	26	21
129.8207	AAA	26	21	19
121.8553	AAH	21	19	20
118.4247	AAA	21	19	17
119.7192	HAA	20	19	17
117.2711	AAH	19	17	18
119.1691	AAA	10	9	7
120.8486	AAH	9	10	38
121.8907	AAA	9	10	11
118.9924	AAA	9	7	3
120.0193	AAH	9	7	8
117.2416	HAA	38	10	11
119.7147	AAH	10	11	12
118.4346	AAA	10	11	4
121.8506	HAA	12	11	4
129.8225	AAA	11	4	5
120.5979	AAA	11	4	3
109.5678	AAA	5	4	3
124.2289	AAO	4	5	6
108.2057	AAN	4	5	0
108.1870	AAA	4	3	1
120.3309	AAA	4	3	7
127.2153	OAN	6	5	0
126.4575	ANA	5	0	39
105.6016	ANA	5	0	1
127.9386	ANA	39	0	1
123.1444	NAA	0	39	43
123.8492	NAA	0	39	40
126.5328	NAO	0	1	2
108.2606	NAA	0	1	3
113.0046	AAA	43	39	40
120.1230	AAH	39	43	48
122.5023	AAA	39	43	42
122.2149	AAA	39	40	44
120.0923	AAH	39	40	49
117.2428	HAA	48	43	42
119.6298	AAH	43	42	47
121.5005	AAA	43	42	41
118.8681	HAA	47	42	41
120.4235	AAH	42	41	46
118.9617	AAA	42	41	44
120.6132	HAA	46	41	44

118.4280	AAH	41 44 45
121.7515	AAA	41 44 40
119.8197	HAA	45 44 40
117.5396	AAH	44 40 49
124.9479	OAA	2 1 3
131.4724	AAA	1 3 7
120.9831	AAH	3 7 8

PHI ANGLES (IN DEGREES)	TYPE	ATOMS INVOLVED
199.7395	AQAA	9 13 14 15
19.8160	AQAA	9 13 14 17
18.3313	AQAA	14 13 9 10
198.1118	AQAA	14 13 9 7
356.1975	QAAH	13 14 15 16
175.2540	QAAA	13 14 15 22
176.1225	AAAH	17 14 15 16
355.1791	AAAA	17 14 15 22
187.9586	QAAA	13 14 17 19
6.1239	QAAH	13 14 17 18
8.0347	AAAA	15 14 17 19
186.2001	AAAH	15 14 17 18
179.1087	AAAA	14 15 22 23
357.6098	AAAA	14 15 22 21
358.1535	HAAA	16 15 22 23
176.6548	HAAA	16 15 22 21
0.5082	AAAO	15 22 23 24
174.7915	AAAN	15 22 23 25
181.8689	AAAO	21 22 23 24
356.1527	AAAN	21 22 23 25
185.7499	AAAA	15 22 21 26
6.7876	AAAA	15 22 21 19
4.5688	AAAA	23 22 21 26
185.6065	AAAA	23 22 21 19
181.2265	AANA	22 23 25 28
1.6495	AANA	22 23 25 26
355.3890	OANA	24 23 25 28
175.8122	OANA	24 23 25 26
347.8182	ANAA	23 25 28 29
168.2262	ANAA	23 25 28 36
167.3114	ANAA	26 25 28 29
347.7195	ANAA	26 25 28 36
174.4277	ANAO	23 25 26 27
1.0739	ANAA	23 25 26 21
354.8422	ANAO	28 25 26 27
181.4883	ANAA	28 25 26 21
358.4423	NAAH	25 28 29 30
183.1010	NAAA	25 28 29 31
178.0708	AAAH	36 28 29 30

2.7296	AAAA	36	28	29	31
178.7108	NAAA	25	28	36	34
354.2869	NAAH	25	28	36	37
359.0785	AAAA	29	28	36	34
174.6547	AAAH	29	28	36	37
177.2005	AAAH	28	29	31	32
357.5591	AAAA	28	29	31	33
1.7475	HAAH	30	29	31	32
182.1061	HAAA	30	29	31	33
180.7141	AAAH	29	31	33	50
0.1558	AAAA	29	31	33	34
1.0681	HAAH	32	31	33	50
180.5094	HAAA	32	31	33	34
182.2386	AAAH	31	33	34	35
1.6817	AAAA	31	33	34	36
1.6809	HAAH	50	33	34	35
181.1238	HAAA	50	33	34	36
358.8000	AAAA	28	36	34	33
178.2381	AAAH	28	36	34	35
183.1046	AAAH	33	34	36	37
2.5430	HAAH	35	34	36	37
356.4565	AAAN	22	21	26	25
182.8751	AAAO	22	21	26	27
175.2929	NAAA	25	26	21	19
1.7110	OAAA	27	26	21	19
176.6857	AAAH	22	21	19	20
356.2886	AAAA	22	21	19	17
357.9584	AAAH	26	21	19	20
177.5613	AAAA	26	21	19	17
356.2907	AAAA	14	17	19	21
175.9023	AAAH	14	17	19	20
178.0633	AAAH	21	19	17	18
357.6749	HAAH	20	19	17	18
5.9476	QAAH	13	9	10	38
187.5923	QAAA	13	9	10	11
186.1662	AAAH	7	9	10	38
7.8107	AAAA	7	9	10	11
175.6685	QAAA	13	9	7	3
356.5217	QAAH	13	9	7	8
355.4535	AAAA	10	9	7	3
176.3067	AAAH	10	9	7	8
176.0547	AAAH	9	10	11	12
356.2434	AAAA	9	10	11	4
357.6428	HAAH	38	10	11	12
177.8316	HAAA	38	10	11	4
177.9527	AAAA	10	11	4	5
356.5459	AAAA	10	11	4	3
358.1459	HAAA	12	11	4	5
176.7391	HAAA	12	11	4	3
1.4988	AAAO	11	4	5	6
175.1224	AAAN	11	4	5	0

182.7843	AAAO	3	4	5	6
356.4073	AAAN	3	4	5	0
185.5619	AAAA	11	4	3	1
6.5824	AAAA	11	4	3	7
4.4153	AAAA	5	4	3	1
185.4359	AAAA	5	4	3	7
181.8534	AANA	4	5	0	39
1.2971	AANA	4	5	0	1
355.2320	OANA	6	5	0	39
174.6757	OANA	6	5	0	1
347.7853	ANAA	5	0	39	43
167.2122	ANAA	5	0	39	40
168.4647	ANAA	1	0	39	43
347.8916	ANAA	1	0	39	40
175.6876	ANAO	5	0	1	2
1.3321	ANAA	5	0	1	3
355.1202	ANAO	39	0	1	2
180.7652	ANAA	39	0	1	3
354.2586	NAAH	0	39	43	48
178.5559	NAAA	0	39	43	42
174.7757	AAAH	40	39	43	48
359.0730	AAAA	40	39	43	42
183.2107	NAAA	0	39	40	44
358.5956	NAAH	0	39	40	49
2.6893	AAAA	43	39	40	44
178.0744	AAAH	43	39	40	49
178.3321	AAAH	39	43	42	47
358.8458	AAAA	39	43	42	41
2.5122	HAAH	48	43	42	47
183.0262	HAAA	48	43	42	41
181.1363	AAAH	43	42	41	46
1.6389	AAAA	43	42	41	44
1.6461	HAAH	47	42	41	46
182.1491	HAAA	47	42	41	44
180.5293	AAAH	42	41	44	45
0.1532	AAAA	42	41	44	40
1.0334	HAAH	46	41	44	45
180.6552	HAAA	46	41	44	40
357.6058	AAAA	39	40	44	41
177.2221	AAAH	39	40	44	45
182.1086	AAAH	41	44	40	49
1.7253	HAAH	45	44	40	49
356.4401	AAAN	4	3	1	0
181.9733	AAAO	4	3	1	2
175.2644	NAAA	0	1	3	7
0.7977	OAAA	2	1	3	7
357.5479	AAAA	9	7	3	4
178.8414	AAAA	9	7	3	1
176.6862	AAAH	4	3	7	8
357.9800	AAAH	1	3	7	8
179.9260	QAAA	13	15	14	17

180.2194	QAAA	13 10 9 7
180.9639	AHAA	14 16 15 22
181.7728	AAAH	14 19 17 18
181.3610	AAAA	15 23 22 21
186.7683	AOAN	22 24 23 25
178.8367	AAAA	22 26 21 19
179.4941	AANA	23 28 25 26
179.6289	NAAA	25 29 28 36
172.3562	NOAA	25 27 26 21
175.5541	AHAA	28 30 29 31
184.3049	AAAH	28 34 36 37
179.6540	AHAA	29 32 31 33
180.5661	AHAA	31 50 33 34
180.5468	AHAA	33 35 34 36
180.4015	AHAA	21 20 19 17
178.4293	AHAA	9 38 10 11
179.1379	AAAH	9 3 7 8
179.8062	AHAA	10 12 11 4
181.2848	AAAA	11 5 4 3
187.6133	AOAN	4 6 5 0
178.8243	AAAA	4 1 3 7
180.6793	AANA	5 39 0 1
180.5174	NAAA	0 43 39 40
173.4565	NOAA	0 2 1 3
175.9241	AHAA	39 48 43 42
184.5031	AAAH	39 44 40 49
179.4999	AHAA	43 47 42 41
179.4887	AHAA	42 46 41 44
180.3701	AHAA	41 45 44 40

TOTAL ENERGY =	-4175.2290039063 KCAL
DIAGONAL CORE CONTRIBUTION =	1242.9887695313 KCAL
BOND CONTRIBUTION =	-5343.2250976563 KCAL
NON-BOND CONTRIBUTION =	31.5420131683 KCAL
REPULS CONTRIBUTION =	1392.4078369141 KCAL
THETA CONTRIBUTION =	69.2726745605 KCAL
PHI CONTRIBUTION =	-1568.2152099609 KCAL

LTP8

0.0679	1.4340	-0.0393
1.3696	0.6805	-0.2644
2.6155	1.3414	-0.0412
2.6300	2.3893	0.2263
3.8071	0.6051	-0.1553
5.2315	1.0057	-0.0030

5.6228	2.1522	0.2819
6.0827	-0.2329	-0.1118
7.3943	-0.3282	-0.0118
8.3238	0.8524	-0.0237
7.9301	1.8488	-0.1433
9.6845	0.7102	0.0200
10.3202	1.5873	-0.0364
10.3041	-0.5730	0.1314
11.3789	-0.6628	0.1758
9.4792	-1.7350	0.1953
9.9500	-2.7053	0.3168
8.1185	-1.6487	0.1183
7.5592	-2.5636	0.2254
5.1263	-1.3558	-0.3716
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-7.7094	2.5840	0.2362
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8.56	0.81
8.56	0.43

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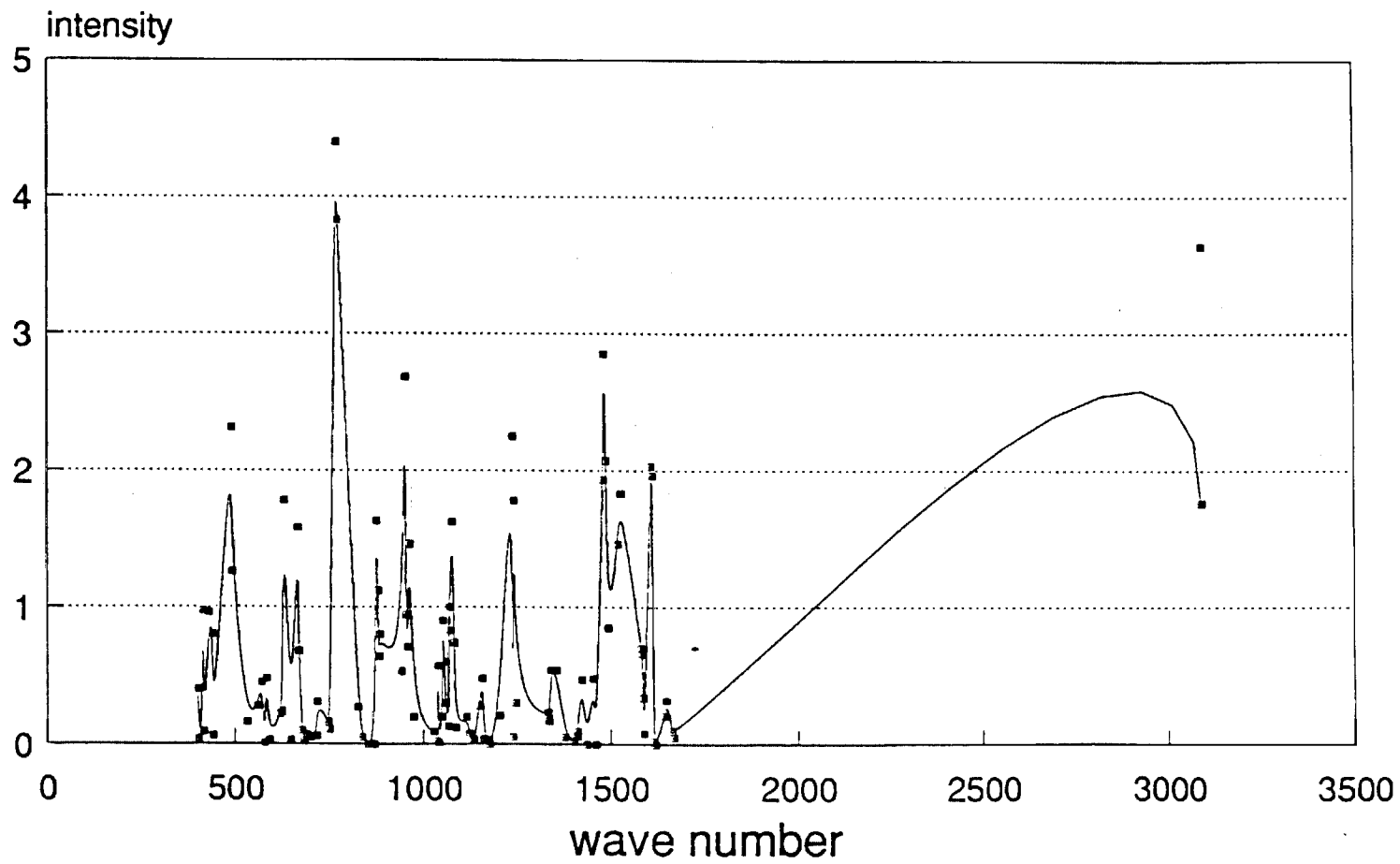
ZERO POINT ENERGY = 231.36
ATOMIZATION ENERGY = -3943.87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intensity
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4
3
2
1
0
0
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1000
1500
2000
2500
3000
3500
wave number

Fig. 8c

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16. Abstract

Using a semi-empirical approach, a computer study has been made of 8 model compounds of polyimides. The compounds represent subunits from which NASA Langley Research Center has successfully synthesized polymers for aerospace high performance material application, including one of the most promising, LARC-TPI polymer. Three-dimensional graphic display as well as important molecular structure data pertaining to these 8 compounds are obtained.

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