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THE CRYSTAL STRUCTURE OF bis (m-BROMOBENZOYL)METHANE*

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ABSTRACT

The crystal structure of bis-(m-bromobenzoyl)methane has been determined, and the three dimensional scintillation counter data refined by anisotropic least squares. The molecule is nearly planar, with a maximum deviation of $0.12 \text{ \AA}$ from the least squares plane, and is tilted in the unit cell $\pm 29.9^\circ$ from the (010) plane. The molecule has a short intramolecular hydrogen bonded distance of $2.464 \pm .015 \text{ \AA}$, but the thermal parameters suggest an anomaly. Symmetry requires complete equivalence of the two C-O groups and the intervening C-C bonds of the enol ring, and the thermal parameters support the interpretation that this equivalence is real rather than statistical.

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INTRODUCTION

The dibenzoylmethanes have been the subject of considerable study because of their strong hydrogen bonding and their ability to chelate with a variety of metal ions. Infrared spectroscopy has been one of the principal tools used to study both the parent compounds and their chelates, along with studies of substituent effects on the ionization constants. In addition, several x-ray studies of the chelates have been made. It has been established that these β -diketones exist primarily in the enol form, but whether the enol is a resonance hybrid of

or is better represented by a single structure has remained a matter of conjecture.

Dibenzoylmethane, bis(m-chlorobenzoyl)methane, and bis (m-bromobenzoyl)methane crystallize in three different space groups, with the halogen substituted compounds having unit cells of about half the volume of the unit cell of dibenzoylmethane itself. Preliminary evidence indicated that the chloro derivative lacked a center of symmetry. Crystals of the bromo derivative were found to possess a center of symmetry, and the molecule also has twofold symmetry in the crystal, reducing the number of parameters. The bromo derivative has a sufficiently heavy atom to make the initial phases of the structure determination simple, but heavy

enough to be less than ideal for obtaining precise distances between the lighter atoms.

EXPERIMENTAL

bis (m-Bromobenzoyl)methane was prepared by reaction of m-bromoacetophenone with ethyl m-bromobenzoate in the presence of sodium amide (Borduin, 1954). Crystals suitable for x-ray analysis, in the form of thin needles, were obtained by recrystallization from chloroform. Weissenberg and precession photographs indicated the unique space group $Pnca$, with lattice constants $a = 26.48$, $b = 4.054$, and $c = 12.79$ Å. The observed flotation density was 1.8 g/cm^3 ; for four molecules in the unit cell the calculated density is 1.85 g/cm^3 .

Complete visually judged Weissenberg intensity data were taken using copper radiation, with rotation about the b (needle) axis. In addition to the usual Lorentz and polarization corrections, a beam divergence correction (Dumke, 1956) was made, but no absorption correction was made. These data were used for the structure determination; however, because of the relatively high diffracting power of bromine, they were not of sufficient quality to obtain accurate bond distances between the light atoms in this structure.

For the refinement of the atomic positions a new set of data was obtained by counter methods, using a different crystal. The crystal selected for counter measurements was a needle .24 mm in length and of equilateral trapezoidal cross section. The thickness perpendicular

to the parallel faces was .055 mm; the long parallel face measured .075 mm, and the short parallel face measured .048 mm. A General Electric XRD-5 x-ray unit equipped with a single crystal orienter and scintillation counter was used with the moving crystal-moving counter technique, a 0.3° takeoff angle and a 2.2° diffracted beam aperture. To eliminate errors involved in planimentering rate meter charts, the total count was recorded directly from the scaler. The copper radiation was filtered through nickel foil placed in the diffracted beam path. A 200 second scan, covering 3.33° in 2θ , was used for each reflection; average rate was ten reflections per hour. A standard reflection (24, 0, 0) was taken periodically and all data scaled to it. A slow variation of about 25% was observed in the standard reflection; this variation was probably caused by a faulty x-ray tube, which also showed about 25% iron radiation. Single crystal orienter settings were precalculated on the IBM 650 computer (Tulinsky, 1960). The background for each reflection was estimated from a plot of average background versus 2θ . All reciprocal lattice points up to $\theta = 77.5^\circ$ were scanned, resulting in 839 observed and 615 unobserved reflections.

The estimated error of each intensity was calculated with the formula

$$\sigma^2(I_o) = C_T + C_B + \left[.04(C_T - C_B) \right]^2 + \left[.1 C_B \right]^2,$$

where $\sigma(I_o)$ is the standard deviation of the observed intensity, C_T are the total counts, and C_B are the background counts. The first two terms in this formula represent the statistical counting error. The third term

represents errors proportional to the net count, e. g. , fluctuations in the beam intensity, errors in the absorption correction, etc. This term sets a lower limit of 4% in the estimated relative error of I_0 when statistical counting errors and background errors become negligible.

The last term adds an error contribution caused by uncertainty in the graphically estimated background count. Unobserved reflections were assigned their probable intensity value and probable error depending on the minimum intensity observable at the reciprocal lattice point in question (Hamilton, 1955). Graphical corrections were made for those reflections most seriously affected by non-characteristic radiation (streaking) or by the iron radiation component. The Lorentz and polarization corrections were made in the usual way. No extinction correction was used.

Absorption correction. With the more accurate counter data the absorption correction could not be neglected. Attempts to grind spherical or ellipsoidal crystals failed. It was decided, therefore, to carry out the necessary integration for each reflection on the Cyclone computer. An absorption correction program, designated ABCOR-I, was written for this purpose. The mathematical method used was similar to that used previously (Busing, 1957), but generalized to three dimensional data, and with the number of integration grid points, m , variable from $m = 4$ to $m = 7$. Because of memory restrictions, (only 1,024 words of memory were available on the Cyclone), it was necessary to restrict the planes bounding

the crystal to be either parallel or perpendicular to the goniometer head axis, a condition frequently met in practice, as it is indeed in this case. The crystal coordinate system was defined by taking the y axis toward the x-ray source, the z axis vertical, and the x axis toward the front of the orienter, when $\phi = \chi = \theta = 0$. The planes bounding the crystal were expressed on this basis. For a general single crystal orienter setting (ϕ, χ, θ) , the direction cosines of the incident beam vector, transformed to crystal coordinates, are:

$$p_x = \cos \phi \cos \chi \sin \theta - \sin \phi \cos \theta$$

$$p_y = \sin \phi \cos \chi \sin \theta + \cos \phi \cos \theta$$

$$p_z = \sin \chi \sin \theta$$

The direction cosines of the diffracted beam vector are:

$$p_x = \cos \phi \cos \chi \sin \theta + \sin \phi \cos \theta$$

$$p_y = \sin \phi \cos \chi \sin \theta - \cos \phi \cos \theta$$

$$p_z = \sin \chi \sin \theta$$

The incident and diffracted beam path lengths to each grid point may then be found with the formulas given in Busing's paper, and the integral evaluated. The calculated absorption coefficient of 68.1 cm^{-1} was used (International Tabellen, 1935). To check the accuracy of the integration, the absorption correction for a selected group of 11 reflections was calculated with $m = 4$, 5, and 6. The maximum difference between the $m = 4$ case and the $m = 6$ case was .96%, with an average of .22%. The maximum difference between the $m = 5$ case and the $m = 6$ case was .23%.

with an average of .15%. It was decided that $m = 4$ would provide sufficient accuracy. The value of the transmission factor varied from .45 to .72, with an average near .65. Each integration with $m = 4$ required approximately 6 seconds on the Cyclone computer. Absorption corrections for the unobserved reflections were obtained graphically.

For carbon and oxygen the scattering factors of Berghuis (1955) were used; for bromine the scattering factor of Thomas and Umeda (1957), corrected for anomalous dispersion (Dauben and Templeton, 1955), was used.

STRUCTURE DETERMINATION

The projection onto the (010) plane, which has no overlapping atoms, was solved first. The approximate bromine parameters were obtained from the two dimensional Patterson function. After improving the bromine parameters by calculation of an electron density projection, the oxygen and all carbon atoms were placed in approximate positions based on a planar molecular model with assumed distances and angles. After several cycles of structure factor calculation and electron density projection all atoms were well defined. The projection was then refined by the least squares method.

The Patterson projection onto the (001) plane indicated a bromine y parameter of $1/4$; however, a planar model based on this bromine y parameter diverged during attempted refinement by the least squares method. The situation was complicated by an ambiguity which remained from the

(010) projection, which made possible the substitution of new z parameters $z' = 1/4 - z$ without affecting the fit to the ($h0\ell$) reflections. A bounded Fourier electron density projection between $x = 0$ and $x = 1/4$ onto the (100) plane suggested that the bromine was shifted away slightly from $y = .25$ but did not indicate which way. The problem was solved by attempting to refine a large number of models having a bromine y parameter shifted by varying amounts both ways from $y = .250$, using a limited number of reflections with the ℓ index odd, and with the z transformation referred to above. Finally a model was found which would converge. The complete three dimensional film data were then refined by the least squares method (43 parameters); the final unweighted discrepancy factor was 0.155 for 587 observed reflections. The standard deviations of distances between light atoms were rather large, about $0.05 \text{ \AA}$, with the film data. It was decided to obtain more accurate intensity data using a scintillation counter.

Fourier calculations were made on the IBM 650 using the program of Fitzwater and Williams (1959); least squares calculations, primarily using only diagonal matrix elements, with individual isotropic temperature factors and layer scale factors, were also made on the IBM 650 using the program of Senko and Templeton (1956).

Refinement of the scintillation counter data.

The complete matrix program of Busing and Levy (1960), for the IBM 704, was used for refinement of the scintillation counter data, using

individual anisotropic temperature factors and a single scale factor (87 parameters). Convergence was obtained after four anisotropic cycles with a weighted discrepancy factor, including unobserved reflections, of 0.113. However, a study of the individual structure factors revealed unusually poor agreement, greater than six times the expected error, for 26 reflections. These reflections were given zero weight for the following three least squares cycles, which resulted in a drop of the weighted discrepancy factor, including unobserved reflections, to 0.068.

The intensities of the group of reflections showing poor agreement were remeasured, using a different crystal (the original crystal was accidentally lost). A marked improvement in the agreement between observed and calculated values of the intensities was noted in nearly every case. These remeasured intensities, plus the rest of the original data, were used to calculate three dimensional electron density and difference Fourier maps, using the IBM 650. These maps verified the correctness of the model by revealing no spurious holes or peaks in the electron density distribution. Both the electron density and difference maps clearly showed the presence of five of the six hydrogen atoms in the asymmetric unit, the exception being the enolic hydrogen.

For the final refinement of the revised data these hydrogens were included isotropically at calculated positions along a line parallel to the intersection of the least squares benzene ring plane and the bisector plane between the neighboring ring atoms at a distance of $1.08 \text{ \AA}$ from the attached carbon atoms. The C_8 hydrogen was placed on the twofold axis $1.08 \text{ \AA}$ from C_8 . At the end of the final two least squares refinement cycles the weighted

discrepancy factor, including unobserved reflections, was 0.071; the unweighted discrepancy factor for 839 observed reflections was 0.057.

Table I gives the final values of the parameters and their standard deviations. The quantity $\left[\sum w(F_o - F_c)^2 / (m-n) \right]^{1/2}$ was 1.48, indicating a reasonable assignment of weighting factors. All standard deviations quoted in this paper are based on the complete inverse matrix including covariances; analysis of the data was greatly facilitated by use of the IBM 704 Function and Error program of Busing (1959). Table II gives a list of the observed and calculated structure factors on a relative scale; the scale factor for conversion to absolute scale is $.3632 \pm .0013$.

DISCUSSION

The structure consists of nearly planar molecules, with their long axis along *a* and short axis along *c*, tilted $\pm 29.9^\circ$ from the (010) plane (Fig. 1). Least squares planes were fitted through the benzene ring (A), the enol ring (B), and the entire molecule (C); Table III shows the distances of the atoms from each plane and the equations of the planes in Å units. Both the benzene ring and the enol ring are planar within experimental error; the maximum deviation of the entire molecule from its least squares plane is 0.120 Å, with the bromine atom being above the plane, and C₄, C₅, and C₆ being below the plane. The inclination of the benzene ring from the molecular plane is $\pm 1.7^\circ$. The intramolecular distances and angles (Table IV) are all very close to the expected values, with an average benzene ring C-C distance of 1.394 Å. The C-O bond (1.306) is intermediate between the normal C=O (1.23) and C-O (1.43) distances, but perhaps slightly longer than expected for 50% double bond character (1.29). The C₇-C₈ distance (1.393) is the same as the C-C distances in the benzene ring within experimental error, and is considerably shorter than the normal single bond value. The C₃-C₈ distance (1.457) is also shorter than the single bond value, but in good agreement with a single bond C-C between carbons with planar trigonal coordination (Dewar and Schmeising, 1960). The short O-O distance of 2.464 Å confirms the presence of a strong hydrogen bond; the standard deviation for this distance is larger than the others because of the larger thermal motion and the twofold symmetry relationship between these atoms. The Br-C₁ distance ($1.901 \pm .007$) is longer than the corresponding

distance observed by electron diffraction methods in bromobenzene ($1.86 \pm .02$), Yuzawa and Yamaka, 1953), or in p-fluorobromobenzene ($1.87 \pm .02$, Oosaka and Akimoto, 1953), or observed crystallographically in 1,3,5-tribromobenzene ($1.86 \pm .04$, Millard and Pant, 1960). The Br-C₁ distance is especially sensitive to systematic errors, which cause ripples in the electron density map in the vicinity of the heavy atom; during the process of refining the various sets of data this effect was noticed as erratic changes in this distance until the final cycles. In view of this fact, and of the rather large standard deviations reported in the literature cited above, no significance is attached to the difference between the value found here and those cited above.

The nearest nonbonded neighbors distance (Table V), based on the calculated hydrogen positions, show that the oxygen atom is surrounded by H₂, H₄, and H₅ at 2.37, 2.49, and 2.83 Å respectively, which restrict its lateral motion. The closest intermolecular nonbonded approaches are between H₂ and H₅, at 2.38 and 2.67 Å. A close intramolecular approach occurs between H₄ and H₈, at 2.01 Å, assuming that these hydrogens lie in the planes of the benzene and enol rings respectively. The perpendicular distance between least squares molecular planes is 3.514 Å.

The thermal stereograms (Fig. II) do not show any pronounced oscillation of this rather rigid molecule about its major axes, as would have been expected. Possibly any such motion is masked by systematic errors in the observed light atom vibrations in the presence of the heavy atom, but it seems

more likely that they are masked by the peculiarities of the enol ring (see below). The standard deviations of the RMS thermal axes (including covariances) are $0.001 \text{ \AA}$ for the bromine atom and $0.01 \text{ \AA}$ for all other atoms.

The greatest thermal anisotropy is shown by the bromine and oxygen atoms. The bromine atoms has its minor thermal axis nearly parallel to the Br-C_1 bond, as might be anticipated, with the mean and major axes nearly normal to this bond. These axes are consistent with some motion of the molecule as a whole with relatively large Br-C bending amplitudes.

Of special interest is the thermal stereogram for oxygen. The enol is required by crystal symmetry to have equivalent C-O bonds, but if these were statistically equivalent due to random arrangement of

molecules within the unit cell, then the oxygen and neighboring carbon positions should show abnormally large apparent RMS amplitudes parallel to the C-O bonds. This is clearly not so, and the thermal parameters strongly suggest that the two C-O bonds are equivalent, corresponding to resonance between the two forms shown above. All sensitive distances are also more compatible with this interpretation than any other. Note that C-O is 1.306 , $\text{C}_3\text{-C}_8$ is 1.457 (trigonal single bond), and $\text{C}_7\text{-C}_8$ is 1.393 (50% double bond character).

The abnormally low thermal axes in the molecular plane may be the result of the restriction of the oxygen in this plane due to very close hydrogen neighbors (see above). The very high amplitude out of the

molecular plane is, however, unexpected and suggestive of an anomaly.

It is to be noted that $\angle C_7-O-O$ is only 89.5° , so that $\angle C_7-O-H$ would be abnormally small if H were directly on the line of centers between the oxygen atoms. It seems likely, in the circumstances, that this hydrogen bond is bent, as shown in Fig. 3a. If this is true, then the very close O-O contact of 2.46 Å, among the shortest known for hydrogen bonds, may lead to strong O-O repulsion, and a warping of the oxygen atoms out of the molecular plane as shown in Fig. 3b, so that the oxygen atoms are at random in positions m or positions n of that figure. This would lead to the apparently very high amplitude normal to the ring.

Unfortunately, the x-ray data are not sufficient to confirm this conjecture.

This suggestion does, however, have the additional merit that it would lead to some distortion or randomness in the carbon positions near the oxygens, that is, near the center of the molecule, leading to apparently high thermal parameters for the atoms and obscuring the oscillations of this rigid molecule as a whole, which are to be expected. (Possibly the single bond character of C_3-C_8 reduces the rigidity, also giving some extra torsional freedom to the enol ring which would show most clearly in the thermal parameters of the oxygen atoms.)

In spite of the fact that this structure determination seems to settle the nature of the enols, at least of the aromatic β -diketones, the interest in this point and in the short hydrogen bond has caused us to regret the uncertainties introduced by such a heavy atom as bromine. Accordingly, the structure of the corresponding (but not isomorphous) chloro-derivative is in progress.

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CAPTIONS FOR FIGURES

Fig. I. (a) Projection of the structure of the (010) plane, including hydrogens in calculated positions; (b) Projection of the structure onto the (001) plane, with hydrogens omitted for clarity. The light circles represent atoms behind the asymmetric unit, and the dotted circles represent atoms in front.

Fig. II. Thermal stereograms for the atoms, transformed so that the plane of the paper is the least squares molecular plane. The directions of the RMS thermal axes are shown stereographically, and the length of the axes are indicated in Å.

Fig. III. (a) Postulated enol ring structure with non-collinear hydrogen bond; (b) side view of oxygen atoms showing effect of O-O repulsion.

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Table I

Final values ($\times 10^5$) of the parameters and their standard deviations. The form of the temperature factor is $\exp(-\beta_{11}h^2 - \beta_{22}k^2 - \beta_{33}l^2 - 2\beta_{12}hk - 2\beta_{13}hl - 2\beta_{23}kl)$.

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Br	3607	23057	15544	107	6945	737	-52	83	67
✓	3	26	7	1	64	6	9	2	23
O	20969	84824	20680	193	17483	232	-828	-4	-107
✓	20	189	36	9	902	27	78	12	140
C ₁	8825	39904	6843	80	5375	573	69	7	217
✓	23	190	55	8	507	47	56	15	128
C ₂	12911	55253	11662	106	4170	387	47	24	-230
✓	24	183	47	9	472	38	54	14	112
C ₃	16776	68336	5457	8	527	33	121	9	-167
✓	22	172	47	8	527	33	53	13	107
C ₄	16478	65099	94497	110	7098	396	61	3	42
✓	25	200	53	9	680	41	64	15	133
C ₅	12342	49400	90046	148	7463	443	-80	-51	41
✓	29	231	53	11	646	42	75	19	158
C ₆	8438	36621	96177	127	7155	501	-87	-59	-2
✓	26	205	55	11	684	48	67	18	144
C ₇	21006	85010	10467	131	7816	357	36	-21	-152
✓	26	210	50	10	747	41	68	16	143
C ₈	25000		5204	110	6713	280	-54		
✓			66	13	801	48	89		

Table I continued.

H ₂	13077	57358	20073	178	7606	764
H ₄	19451	74906	89620	178	7606	764
H ₅	12122	47102	81634	178	7606	764
H ₅	5240	24487	92618	178	7606	764
H ₈	25000		96760	178	7606	764

Table II. Observed and calculated structure factors.

H	K	L	OBSERVED	CALCULATED
0	2	0	46.230	-46.693
0	4	0	10.860	10.836
2	0	0	43.840	41.193
2	1	0	15.900	-14.966
2	2	0	42.500	-42.169
2	3	0	11.110	11.562
2	4	0	12.920	12.139
4	0	0	20.140	17.321
4	1	0	104.960	-114.047
4	2	0	40.560	-40.656
4	3	0	16.870	16.829
4	4	0	10.270	9.308
6	0	0	11.960	10.322
6	1	0	53.240	-53.301
6	2	0	19.670	-19.446
6	3	0	22.680	25.306
6	4	0	4.550	3.708
8	0	0	23.340	-21.051
8	1	0	56.450	-55.270
8	2	0	28.170	28.179
8	3	0	30.190	29.541
10	0	0	32.440	-30.784
10	1	0	39.520	-38.944
10	2	0	25.480	25.159
10	3	0	25.320	25.344
10	4	0	10.650	-10.129
12	0	0	60.440	-58.040
12	1	0	27.740	-27.002
12	2	0	26.530	28.728
12	3	0	8.460	7.520
12	4	0	13.840	-13.795
14	0	0	50.490	-46.441
14	2	0	33.250	33.309
14	3	0	7.590	-7.121
14	4	0	12.980	-12.677
16	0	0	54.440	-51.108
16	1	0	16.320	16.071
16	2	0	36.080	38.476
16	3	0	8.540	-8.164
16	4	0	4.260	-3.397
18	0	0	28.830	-27.218
18	1	0	27.190	27.267
18	2	0	9.790	9.351
18	3	0	12.110	-12.179
18	4	0	4.740	-4.813
20	0	0	13.640	-13.289
20	1	0	48.080	47.641
20	2	0	2.770	4.134
20	3	0	12.300	-12.111
22	0	0	8.800	5.500
22	1	0	22.350	21.705
22	2	0	3.460	-4.483
22	3	0	6.790	-12.245
24	0	0	39.410	40.065
24	1	0	19.050	18.910

Table II continued.

24	2	0	10.710	-10.792
24	3	0	9.880	-10.053
26	0	0	14.290	13.391
26	1	0	10.020	9.451
26	2	0	8.030	-14.118
26	3	0	4.180	-4.543
28	0	0	12.790	14.057
28	1	0	6.310	-6.986
28	2	0	15.090	-15.670
30	0	0	15.570	14.483
30	1	0	4.380	-4.870
30	2	0	10.580	-11.049
32	0	0	10.170	9.346
32	1	0	6.160	-7.570
0	1	1	29.030	-28.923
1	1	1	16.070	-15.596
1	2	1	8.250	-9.344
1	3	1	4.230	4.537
2	1	1	11.200	-11.093
2	3	1	5.510	-6.329
3	1	1	8.190	7.430
3	2	1	11.290	-11.953
3	4	1	5.870	5.859
4	1	1	46.040	46.837
4	2	1	7.540	8.032
4	3	1	3.300	-4.564
5	1	1	11.930	-11.531
5	2	1	5.950	6.147
5	3	1	8.990	9.114
6	4	1	2.320	4.668
7	1	1	8.950	-9.380
7	2	1	10.070	-10.760
7	3	1	9.300	9.404
8	1	1	5.080	-5.213
8	2	1	28.020	-28.583
8	4	1	6.430	5.787
9	2	1	9.060	8.905
9	3	1	2.760	4.453
9	4	1	4.970	-4.535
10	1	1	5.350	-4.924
11	1	1	9.980	-10.624
11	2	1	7.980	8.458
11	3	1	5.600	6.361
12	1	1	9.870	-9.695
12	3	1	17.990	18.769
13	1	1	3.740	4.370
13	2	1	7.430	7.710
13	4	1	4.180	-3.820
15	2	1	6.540	7.097
15	4	1	5.760	-6.058
16	2	1	13.120	13.097
16	4	1	3.910	-4.162
17	1	1	4.840	4.713
17	3	1	6.230	-5.282
17	4	1	2.480	-2.745
18	4	1	3.370	-2.978
19	1	1	3.640	3.390
19	2	1	6.440	6.390
19	3	1	5.800	-5.281

Table II continued.

20	1	1	8.840	8.832
21	3	1	3.880	-3.978
22	1	1	4.080	-4.373
23	1	1	5.700	6.240
23	2	1	3.060	-2.593
23	3	1	3.320	-3.523
24	1	1	4.350	-4.736
24	2	1	3.950	3.613
27	2	1	4.190	-3.772
28	1	1	8.090	8.453
0	0	2	10.790	11.519
0	2	2	18.790	19.741
0	4	2	7.220	-7.528
1	0	2	50.970	-48.595
1	1	2	58.470	-60.813
1	2	2	9.880	11.305
1	3	2	25.650	25.841
1	5	2	4.750	-4.386
2	0	2	23.960	-24.204
2	1	2	10.990	10.902
2	2	2	14.060	14.868
2	3	2	7.840	-8.156
2	4	2	5.780	-5.825
3	0	2	32.070	-31.182
3	1	2	63.340	-65.962
3	2	2	25.710	26.491
3	3	2	17.050	17.330
3	4	2	3.660	-6.874
3	5	2	4.720	-4.815
4	0	2	46.830	-44.717
4	1	2	4.770	5.096
4	2	2	14.230	14.607
4	3	2	9.980	-10.406
5	0	2	78.180	-77.867
5	1	2	16.320	-16.988
5	2	2	36.140	36.916
5	3	2	10.660	10.790
5	4	2	11.060	-10.739
5	5	2	4.130	-3.577
6	0	2	10.740	-10.536
6	1	2	17.380	18.423
6	2	2	5.470	-5.909
6	3	2	8.960	-9.958
7	0	2	68.560	-69.207
7	1	2	8.660	-8.045
7	2	2	42.090	43.514
7	4	2	12.700	-12.302
8	0	2	5.600	5.039
8	1	2	46.680	46.766
8	3	2	5.120	-5.938
9	0	2	51.750	-49.963
9	1	2	33.690	33.003
9	2	2	32.500	33.390
9	3	2	7.140	-6.821
9	4	2	5.830	-11.369
10	0	2	7.530	7.454
10	1	2	8.260	8.996
10	2	2	8.760	-10.108
11	0	2	46.890	-44.927

Table II continued.

11	1	2	33.040	33.087
11	2	2	25.870	25.650
11	3	2	20.800	-21.029
11	4	2	4.190	-4.196
12	0	2	54.580	52.864
12	1	2	6.680	6.849
12	2	2	15.450	-16.472
12	3	2	4.790	-4.469
13	1	2	44.190	43.423
13	2	2	4.080	5.319
13	3	2	21.420	-21.576
13	4	2	3.420	-3.861
14	0	2	8.590	9.157
14	2	2	11.130	-11.281
15	1	2	45.880	45.666
15	2	2	5.790	-6.367
15	3	2	6.290	-12.303
16	0	2	11.430	11.220
16	1	2	19.170	-19.870
16	2	2	7.380	-7.610
16	4	2	5.610	5.705
17	0	2	26.420	25.977
17	1	2	26.010	26.110
17	2	2	20.360	-20.142
17	3	2	12.170	-11.788
17	4	2	4.650	4.609
18	0	2	6.300	5.861
18	1	2	8.850	-8.874
18	2	2	7.630	-7.453
18	3	2	6.150	5.992
19	0	2	36.630	37.044
19	1	2	16.760	16.199
19	2	2	17.240	-16.994
19	3	2	7.320	-7.698
19	4	2	6.730	6.329
20	0	2	6.880	-3.936
20	1	2	7.510	-6.636
20	3	2	7.510	7.690
21	0	2	31.540	31.185
21	1	2	6.180	-4.875
21	2	2	20.460	-20.105
22	0	2	6.970	-3.977
22	1	2	9.780	-9.995
22	2	2	3.940	3.531
22	3	2	5.790	5.261
23	0	2	27.190	25.798
23	1	2	7.630	-7.908
23	2	2	17.560	-17.540
23	3	2	5.000	5.017
24	1	2	7.900	-7.225
24	2	2	6.500	5.392
25	0	2	6.140	6.265
25	1	2	16.840	-16.943
25	2	2	10.410	-10.371
25	3	2	4.310	7.651
26	0	2	10.170	-9.798
26	2	2	5.280	5.606
27	0	2	9.330	8.300
27	1	2	18.740	-18.555

Table II continued. 24

27	2	2	3.780	-2.848
28	0	2	11.490	-11.659
28	2	2	6.220	5.786
29	0	2	5.210	-3.877
29	1	2	11.790	-12.164
29	2	2	3.660	3.572
30	0	2	5.340	-4.726
30	1	2	4.750	4.208
31	0	2	8.450	-8.507
31	1	2	6.100	-10.736
32	1	2	7.350	7.769
33	0	2	9.790	-10.424
0	1	3	11.840	-14.780
0	3	3	21.020	21.007
1	1	3	5.290	-4.789
2	1	3	5.190	-4.998
2	2	3	3.840	4.953
2	3	3	5.600	5.083
3	1	3	4.720	4.479
4	1	3	9.780	-9.256
4	2	3	23.240	22.895
4	4	3	8.270	-7.262
5	1	3	3.940	-3.718
6	1	3	2.800	-1.711
6	4	3	7.690	-6.884
7	2	3	3.130	-3.855
7	3	3	3.370	3.657
8	1	3	20.180	20.791
8	2	3	5.690	6.289
8	4	3	5.600	-4.599
9	1	3	7.180	-7.835
10	1	3	4.550	-4.739
10	2	3	4.780	5.404
10	3	3	6.100	-5.748
10	4	3	4.670	-3.937
11	2	3	3.820	4.474
12	3	3	6.380	-5.804
15	4	3	4.060	-4.464
13	2	3	4.540	4.390
14	3	3	6.680	-6.401
15	1	3	3.890	4.029
16	1	3	14.260	13.733
16	3	3	6.780	-6.361
18	4	3	5.120	4.107
20	2	3	12.810	-12.486
20	4	3	4.730	4.544
22	2	3	4.390	-3.879
24	1	3	5.610	-4.015
24	3	3	8.320	7.525
28	2	3	4.100	3.341
0	0	4	65.550	-65.748
0	2	4	23.230	21.905
0	4	4	10.610	-10.147
1	0	4	17.800	19.307
1	1	4	41.640	42.570
1	2	4	8.240	-8.668
1	3	4	18.710	-18.651
2	0	4	48.840	-46.453
2	1	4	16.040	15.629

Table II continued. 25

2	2	4	26.170	26.802
2	3	4	10.310	-10.728
2	4	4	9.410	-8.924
3	0	4	32.330	32.712
3	1	4	34.260	36.671
3	2	4	16.080	-16.528
3	3	4	11.130	-11.310
3	4	4	7.310	6.827
4	0	4	16.800	-17.025
4	1	4	31.700	31.201
4	2	4	28.790	29.495
4	3	4	13.510	-12.899
5	0	4	40.650	40.004
5	1	4	11.430	11.787
5	2	4	32.220	-33.077
5	3	4	6.840	-6.333
5	4	4	8.000	7.232
6	0	4	16.240	-15.104
6	1	4	40.720	40.775
6	2	4	5.200	6.048
6	3	4	14.900	-14.079
7	0	4	50.440	50.225
7	2	4	22.010	-22.635
7	4	4	7.490	6.890
8	0	4	8.100	-7.071
8	1	4	44.270	43.412
8	2	4	11.870	-12.010
8	3	4	15.300	-15.529
9	0	4	31.190	31.336
9	1	4	24.280	-24.007
9	2	4	21.830	-22.408
9	3	4	9.350	9.172
9	4	4	6.250	5.879
10	0	4	22.710	22.813
10	1	4	26.810	27.501
10	2	4	14.500	-14.138
10	3	4	13.910	-14.298
10	4	4	5.000	4.385
11	0	4	29.830	29.541
11	1	4	25.590	-25.838
11	2	4	11.070	-11.180
11	3	4	8.160	8.209
11	4	4	6.030	5.971
12	0	4	53.450	51.365
12	1	4	15.640	15.811
12	2	4	16.410	-16.106
12	3	4	6.120	-5.483
12	4	4	6.780	6.354
13	0	4	9.270	-8.131
13	1	4	30.290	-30.731
13	3	4	12.680	12.043
14	0	4	30.990	30.850
14	1	4	4.280	3.956
14	2	4	22.430	-22.284
14	4	4	7.180	6.505
15	0	4	6.310	-6.793
15	1	4	27.210	-26.347
15	2	4	5.220	4.810
15	3	4	13.440	13.552

Table II continued.

16	0	4	20.420	19.813
16	1	4	14.720	-14.034
16	2	4	21.050	-21.076
16	4	4	4.740	4.486
17	0	4	21.850	-21.860
17	1	4	13.180	-13.118
17	2	4	12.810	12.467
17	3	4	8.480	8.518
17	4	4	4.210	-4.163
18	0	4	18.400	18.605
18	1	4	17.660	-17.666
18	2	4	12.590	-12.438
18	3	4	6.830	5.991
18	4	4	4.990	4.201
19	0	4	11.670	-19.729
19	1	4	8.970	-8.400
19	2	4	18.220	18.569
19	4	4	4.810	-4.715
20	0	4	10.800	10.797
20	1	4	18.850	-18.218
20	3	4	9.550	9.348
21	0	4	19.550	-19.373
21	1	4	3.230	3.215
21	2	4	13.640	13.256
22	0	4	5.660	-4.140
22	1	4	17.260	-17.183
22	3	4	10.260	10.221
23	0	4	16.060	-16.425
23	1	4	10.330	10.370
23	2	4	9.760	9.055
23	3	4	5.470	-5.118
24	0	4	12.450	-11.670
24	1	4	13.810	-13.574
24	3	4	6.200	5.333
25	0	4	9.970	-9.341
25	1	4	13.160	12.769
25	2	4	4.790	3.822
25	3	4	6.590	-6.456
26	0	4	11.120	-10.808
26	1	4	7.710	-7.809
26	2	4	9.220	9.308
27	1	4	12.020	12.155
28	0	4	11.670	-11.021
28	2	4	10.540	10.777
29	0	4	5.660	5.362
29	1	4	10.000	10.084
29	2	4	5.110	-4.486
30	0	4	10.720	-11.142
30	1	4	3.850	2.792
31	0	4	7.990	8.532
31	1	4	2.720	4.642
32	0	4	8.130	-8.527
0	1	5	19.170	18.903
1	1	5	5.870	-6.215
1	2	5	10.270	10.544
1	3	5	4.730	-4.285
1	4	5	4.820	-3.405
2	1	5	1.920	-1.157
3	1	5	6.960	6.239

Table II continued.

3	2	5	4.670	4.971
3	3	5	7.020	-3.654
3	4	5	6.840	-6.721
4	1	5	12.720	-13.439
4	2	5	3.480	-3.447
4	3	5	3.030	-3.730
5	1	5	5.550	5.864
5	2	5	2.840	3.085
5	3	5	4.190	-7.077
7	1	5	9.770	9.290
7	3	5	7.790	-7.244
8	1	5	8.090	7.733
9	2	5	2.770	-3.205
9	3	5	8.800	-6.931
11	1	5	5.250	5.321
11	4	5	5.910	5.002
12	1	5	7.900	-8.282
13	2	5	7.430	-7.544
13	4	5	5.430	4.956
15	2	5	6.010	-5.899
15	3	5	5.140	4.567
15	4	5	3.980	3.391
16	1	5	4.690	4.914
17	1	5	6.550	-6.467
17	2	5	4.770	-4.665
17	3	5	4.770	3.051
19	1	5	3.940	-3.133
19	3	5	5.540	4.391
21	1	5	4.410	-3.930
21	3	5	4.270	4.068
23	2	5	4.210	2.966
23	3	5	3.960	3.904
24	1	5	5.050	4.505
25	2	5	4.470	3.139
27	2	5	2.740	1.888
28	1	5	4.160	-3.655
0	0	6	21.980	21.793
0	2	6	33.480	-34.257
0	4	6	10.540	10.298
1	0	6	4.140	-3.066
1	1	6	22.710	22.415
1	2	6	3.230	-1.909
1	3	6	10.380	-10.415
2	0	6	50.500	51.786
2	1	6	23.320	-24.291
2	2	6	20.950	-29.337
2	3	6	9.680	8.804
2	4	6	8.440	7.864
3	0	6	28.850	27.626
3	1	6	13.630	13.562
3	2	6	7.890	-7.071
4	0	6	39.230	39.705
4	1	6	23.520	-24.343
4	2	6	14.470	-14.789
4	3	6	15.960	16.086
4	4	6	6.540	5.456
5	0	6	13.460	13.085
5	1	6	13.580	13.752
5	2	6	15.340	-15.511

Table II continued. 28

6	0	6	9.080	8.346
6	1	6	42.070	-43.569
6	3	6	16.910	16.925
7	0	6	19.800	19.222
7	1	6	5.780	-4.746
7	2	6	10.310	-10.168
8	0	6	13.920	-13.438
8	1	6	40.000	-41.012
8	3	6	14.630	14.272
8	4	6	4.620	-3.870
9	0	6	20.940	20.494
9	1	6	4.950	-3.691
9	2	6	11.780	-11.345
10	0	6	29.620	-30.070
10	1	6	25.950	-26.376
10	2	6	16.980	17.031
10	3	6	10.040	9.600
10	4	6	4.280	-4.461
11	0	6	11.480	10.661
11	1	6	8.460	-8.047
11	2	6	8.470	-8.182
11	3	6	6.200	5.933
12	0	6	35.740	-35.881
12	1	6	11.480	-11.279
12	2	6	24.710	24.898
12	3	6	7.240	6.796
12	4	6	6.130	-5.515
13	0	6	6.550	6.711
13	1	6	12.270	-11.578
13	2	6	7.320	-7.530
13	3	6	5.890	5.621
14	0	6	33.190	-32.941
14	2	6	22.710	22.683
14	4	6	6.360	-6.216
15	0	6	4.960	3.346
15	1	6	15.390	-14.572
15	3	6	6.630	6.285
16	0	6	24.720	-24.453
16	1	6	16.130	16.006
16	2	6	15.810	14.550
16	3	6	6.430	-6.047
16	4	6	7.530	-7.807
17	0	6	5.500	-2.940
17	1	6	12.590	-13.009
17	3	6	4.650	4.029
18	0	6	16.420	-15.755
18	1	6	21.460	21.066
18	2	6	11.990	11.684
18	3	6	10.790	-10.258
19	0	6	8.820	-8.157
19	1	6	7.830	-7.550
19	2	6	9.290	9.075
19	3	6	4.820	4.649
20	1	6	18.460	17.388
20	3	6	11.790	-11.653
21	0	6	14.420	-14.233
21	1	6	6.010	-5.132
21	2	6	5.900	4.182
22	0	6	9.280	8.406

Table II continued. 29

22	1	6	20.550	20.478
22	2	6	6.850	-5.595
22	3	6	8.600	-8.236
23	0	6	8.880	-8.924
23	2	6	8.270	7.465
24	0	6	8.480	6.514
24	1	6	12.190	11.963
24	2	6	10.350	-10.155
24	3	6	4.420	-4.645
25	0	6	9.110	-8.500
25	1	6	5.530	3.333
25	2	6	6.270	5.889
26	0	6	18.210	18.380
26	1	6	4.460	3.319
26	2	6	10.490	-10.821
27	1	6	5.740	5.887
28	0	6	15.430	16.583
28	2	6	7.110	-8.143
29	0	6	3.190	-3.020
29	1	6	5.770	6.026
30	0	6	8.900	9.203
30	1	6	7.150	-7.501
0	1	7	6.930	6.159
0	3	7	10.050	-10.337
1	1	7	2.320	-3.298
1	4	7	4.620	4.196
2	1	7	10.250	10.584
2	2	7	5.150	-4.755
2	3	7	5.340	-4.283
3	1	7	4.120	-3.709
3	3	7	6.700	6.152
4	1	7	6.610	-6.274
4	2	7	9.140	-8.858
4	4	7	4.970	4.242
5	1	7	3.350	-3.854
6	2	7	8.650	-9.567
6	4	7	5.490	4.915
7	2	7	7.360	7.343
8	1	7	3.240	-3.046
8	2	7	4.570	4.653
10	2	7	7.870	-7.958
10	3	7	7.310	6.409
10	4	7	4.380	4.400
11	1	7	4.200	4.345
12	1	7	4.780	5.135
14	1	7	6.430	-6.393
14	3	7	7.580	7.004
16	1	7	7.510	-7.032
16	3	7	4.570	4.118
17	2	7	5.690	3.763
18	2	7	6.800	6.050
19	1	7	5.040	4.140
20	2	7	7.880	7.077
21	3	7	3.730	-2.728
0	0	8	15.920	-14.870
1	0	8	4.360	3.174
1	1	8	32.300	-33.817
1	3	8	15.430	14.830
1	4	8	5.650	-4.672

Table II continued. 30

2	0	8	8.600	8.275
3	0	8	27.480	-28.247
3	1	8	21.400	-21.491
3	2	8	16.640	16.772
3	3	8	13.830	14.088
3	4	8	6.240	-5.695
4	0	8	5.170	1.957
4	1	8	10.400	10.459
4	2	8	6.830	-7.504
5	0	8	27.010	-27.906
5	1	8	22.540	-23.711
5	2	8	20.860	21.008
5	4	8	7.610	-6.797
7	0	8	33.110	-34.582
7	1	8	5.790	4.349
7	2	8	25.720	26.650
7	4	8	6.610	-6.207
8	0	8	12.310	12.744
8	1	8	10.090	-9.788
9	0	8	40.560	-43.405
9	1	8	9.140	8.040
9	2	8	18.440	18.499
9	3	8	7.420	-6.278
9	4	8	5.450	-5.411
10	0	8	5.500	2.695
11	0	8	13.660	-13.678
11	1	8	28.590	29.335
11	2	8	7.660	10.447
11	3	8	9.150	-8.320
11	4	8	4.830	-4.485
12	0	8	15.090	-15.783
12	1	8	5.660	-3.248
13	0	8	11.570	-11.150
13	1	8	27.990	28.525
13	2	8	6.070	5.752
13	3	8	10.210	-9.851
14	1	8	8.220	-7.783
15	0	8	19.040	19.043
15	1	8	19.720	19.713
15	2	8	6.970	-4.244
15	3	8	12.120	-11.908
16	0	8	7.850	5.697
17	0	8	14.180	13.651
17	1	8	18.190	18.010
17	2	8	11.420	-10.749
17	3	0	0.820	-8.765
18	0	8	7.520	-7.597
18	2	8	7.050	6.226
19	0	8	17.510	16.770
19	1	8	5.800	3.228
19	2	8	14.180	-14.241
19	3	8	4.730	-4.264
20	0	8	8.390	-7.185
20	1	8	6.640	-6.015
21	0	8	18.870	18.404
21	2	8	13.760	-13.396
22	2	8	5.350	4.323
23	0	8	12.960	12.879
23	1	8	8.810	-7.623

Table II continued. 31

23	2	8	9.180	-8.798
24	0	8	8.180	-7.939
24	1	8	5.710	4.414
24	2	8	4.590	3.935
25	0	8	12.220	11.860
25	1	8	10.550	-10.017
25	2	8	6.050	-6.431
26	1	8	4.490	3.697
27	1	8	10.600	-11.016
28	1	8	4.140	5.532
0	3	9	8.140	-7.843
1	1	9	5.480	3.415
1	2	9	8.630	-7.931
2	1	9	6.180	-4.387
2	2	9	5.890	3.893
2	3	9	8.990	7.853
2	4	9	5.370	-5.270
3	1	9	6.700	-5.234
3	3	9	7.190	5.874
4	2	9	7.660	-7.832
4	3	9	7.290	5.089
5	1	9	7.560	-5.611
6	2	9	11.270	10.290
7	2	9	7.420	5.766
8	1	9	11.500	-11.598
8	2	9	8.100	6.815
8	4	9	3.520	-3.480
10	1	9	8.270	7.763
11	1	9	7.360	4.914
12	1	9	8.590	8.106
12	3	9	5.600	-4.579
13	1	9	7.160	-7.042
14	1	9	6.230	4.286
16	1	9	9.310	-8.965
16	2	9	5.870	-4.807
17	2	9	6.710	6.386
18	2	9	6.640	-5.254
19	1	9	4.690	3.724
20	2	9	5.760	5.001
22	2	9	4.260	-3.169
23	2	9	4.200	-2.899
0	0	10	22.440	-22.698
0	2	10	19.270	20.091
0	4	10	3.720	-4.000
1	1	10	11.980	11.781
2	0	10	26.920	-27.683
2	1	10	10.830	10.667
2	2	10	16.420	16.633
2	4	10	3.280	-3.204
3	0	10	11.820	11.697
3	2	10	6.630	-6.207
3	3	10	5.830	-4.179
4	0	10	13.310	-12.270
4	1	10	17.650	18.620
4	3	10	7.810	-7.704
5	0	10	12.700	12.749
5	2	10	4.960	-3.179
5	3	10	4.340	-3.336
6	0	10	8.530	-7.816

Table II continued.

6	1	10	25.730	26.479
6	2	10	8.460	8.468
6	3	10	9.760	-9.413
7	0	10	8.140	6.270
7	1	10	7.210	-6.554
7	2	10	6.540	-5.100
8	0	10	9.710	8.424
8	1	10	8.810	7.703
8	3	10	10.550	-10.523
9	2	10	6.960	-5.827
9	3	10	4.640	3.460
10	0	10	22.830	22.503
10	1	10	21.120	22.684
10	2	10	10.170	-8.905
10	3	10	7.980	-7.423
11	0	10	3.650	-4.570
11	1	10	8.170	-6.683
11	3	10	5.530	4.195
12	0	10	5.870	-4.605
12	1	10	9.120	8.110
12	2	10	13.130	-12.356
13	0	10	7.040	5.215
13	1	10	6.600	-5.304
13	3	10	4.940	3.838
14	0	10	27.530	28.226
14	2	10	14.060	-14.133
15	0	10	3.000	-3.308
15	1	10	6.650	-3.376
15	2	10	2.460	5.645
16	0	10	18.950	19.202
16	2	10	9.600	-9.284
16	3	10	4.470	3.658
17	0	10	8.030	-7.123
17	1	10	6.480	-4.789
17	2	10	4.680	3.373
18	0	10	10.310	10.137
18	1	10	13.880	-13.879
18	2	10	5.510	-5.206
19	0	10	9.140	-9.211
19	2	10	4.850	3.584
20	1	10	13.060	-13.888
20	2	10	5.600	-6.187
21	0	10	7.570	-6.662
21	2	10	4.360	4.205
22	0	10	4.670	-2.829
22	1	10	11.380	-11.494
23	1	10	7.390	7.192
24	0	10	5.960	-7.073
24	1	10	6.320	-6.951
25	1	10	5.070	5.866
26	0	10	7.930	-8.547
0	3	11	5.000	-4.771
2	3	11	3.500	3.263
3	3	11	4.010	-2.965
5	2	11	8.730	8.704
7	3	11	4.760	-3.291
8	2	11	3.280	4.689
9	1	11	9.310	8.918
9	3	11	5.140	-3.984

Table II continued. 33

12	3	11	4.260	-3.603
13	2	11	5.910	-4.784
15	1	11	6.060	-4.989
15	3	11	3.050	2.615
16	1	11	5.330	-3.589
0	2	12	7.740	-6.697
1	1	12	12.580	13.759
2	0	12	16.260	17.120
2	1	12	9.120	-8.690
2	2	12	8.060	-7.199
3	0	12	11.150	12.078
3	1	12	7.510	7.466
3	2	12	5.730	-5.283
3	3	12	6.030	-6.302
4	0	12	6.720	6.057
4	2	12	5.860	-4.485
4	3	12	4.990	4.141
5	0	12	11.500	11.607
5	1	12	6.660	5.758
5	2	12	6.090	-5.954
5	3	12	3.710	-3.541
6	1	12	12.590	-12.591
6	3	12	5.600	5.856
7	0	12	8.350	8.544
7	2	12	9.970	-10.507
8	1	12	9.740	-9.347
8	3	12	4.710	4.089
9	0	12	11.130	11.571
9	2	12	6.990	-6.742
10	0	12	8.550	-8.507
10	1	12	7.710	-6.814
10	2	12	6.930	7.059
11	0	12	5.420	4.568
11	1	12	8.160	-7.482
11	2	12	5.380	-4.875
11	3	12	3.230	3.350
12	0	12	10.670	-9.726
12	2	12	7.780	7.600
13	0	12	9.480	9.615
13	1	12	7.980	-7.900
14	0	12	11.600	-11.210
14	2	12	6.570	6.101
15	1	12	6.820	-7.290
16	0	12	5.470	-4.417
16	1	12	6.650	6.357
17	1	12	9.720	-10.292
18	1	12	8.310	8.244
18	2	12	4.110	4.154
19	0	12	7.110	-7.016
19	1	12	3.980	-4.542
21	0	12	8.470	-9.330
22	0	12	5.410	5.807
3	1	13	5.570	-4.245
6	2	13	6.190	-5.273
10	1	13	4.870	-2.718
0	2	14	4.570	-4.773
1	1	14	9.130	-9.122
3	0	14	3.830	-6.934
3	1	14	6.120	-4.698

Table II continued.

3	2	14	5.330	4.918
4	0	14	6.640	6.476
5	0	14	9.250	-8.801
5	1	14	5.800	-4.380
5	2	14	6.060	5.811
7	0	14	11.120	-10.971
9	0	14	6.570	-5.570
9	2	14	6.410	7.326
10	1	14	5.270	-4.789
11	1	14	7.150	6.610
13	1	14	7.260	7.373
14	0	14	5.050	-4.456
15	1	14	5.410	5.961
16	0	14	5.830	-6.915
0	0	16	4.560	-5.115
2	0	16	5.170	-5.761
4	0	16	4.430	-5.352
2	5	0	3.660	-2.167
4	5	0	3.940	-2.259
6	5	0	4.270	-7.336
8	4	0	2.540	2.040
14	1	0	2.270	-2.046
20	4	0	1.860	-2.346
0	3	1	2.330	-1.343
0	5	1	2.200	2.468
1	4	1	1.020	5.217
1	5	1	2.230	-1.114
2	2	1	1.940	-1.820
2	4	1	2.540	3.292
2	5	1	2.240	2.918
3	3	1	2.360	3.404
3	5	1	2.530	-2.726
4	4	1	2.460	1.876
4	5	1	2.710	1.908
5	4	1	2.330	2.320
5	5	1	2.790	-3.271
6	1	1	1.830	-1.029
6	2	1	1.840	.934
6	3	1	2.240	.292
6	5	1	2.610	-2.373
7	4	1	2.380	-1.321
7	5	1	2.570	-2.077
8	3	1	2.500	-3.665
9	1	1	1.850	.313
10	2	1	1.980	-4.068
10	3	1	2.370	-.481
10	4	1	2.300	-2.029
11	4	1	2.400	-1.753
12	2	1	2.140	.715
12	4	1	2.080	2.163
13	3	1	2.540	-2.836
14	1	1	2.210	-3.624
14	2	1	2.300	1.884
14	3	1	2.420	.169
14	4	1	1.960	3.619
15	1	1	1.980	1.015
15	3	1	2.340	.627
16	1	1	2.100	-.985
16	3	1	2.340	-.637

Table II continued.

17	2	1	2.420	-1.613
18	1	1	2.220	-.993
18	2	1	2.390	-1.791
18	3	1	2.440	2.446
19	4	1	1.900	-.326
20	2	1	2.410	-2.457
20	3	1	2.270	.512
20	4	1	1.790	-1.099
21	1	1	2.460	-1.604
21	2	1	2.570	-2.707
22	2	1	2.450	2.898
22	3	1	2.210	-1.568
24	3	1	1.900	.460
25	1	1	2.220	.466
25	2	1	2.320	-2.885
25	3	1	1.750	-.253
26	1	1	2.300	.741
26	2	1	2.110	.861
26	3	1	1.880	-2.619
27	1	1	2.180	.527
27	3	1	1.560	-.644
28	2	1	1.980	2.548
29	1	1	2.130	-2.485
29	2	1	1.790	-1.560
30	1	1	1.840	-.348
30	2	1	1.540	-.853
31	1	1	1.730	-1.199
32	1	1	1.500	-.523
1	4	2	2.410	-1.612
2	5	2	1.650	.628
4	4	2	2.370	-.826
4	5	2	2.090	3.177
6	4	2	2.380	-.163
6	5	2	1.710	1.868
7	3	2	2.350	2.575
8	2	2	2.170	2.157
8	4	2	2.480	3.414
10	3	2	2.560	-2.892
10	4	2	2.320	1.936
12	4	2	2.220	1.151
13	0	2	2.060	-2.698
14	1	2	2.080	-.583
14	3	2	2.440	-1.213
14	4	2	2.180	2.701
15	0	2	2.120	1.801
15	4	2	2.140	2.761
16	3	2	2.390	2.144
18	4	2	1.890	1.896
20	2	2	2.370	.637
20	4	2	1.740	.840
21	3	2	2.230	-1.062
24	0	2	2.660	.496
24	3	2	2.020	2.112
26	1	2	2.410	-1.023
26	3	2	1.780	-.838
28	1	2	2.220	-1.047
30	2	2	1.740	1.026
32	0	2	1.760	-1.454
0	5	3	2.020	-3.396

Table II continued.

36

1	2	3	2.060	-2.957
1	3	3	2.430	-.489
1	4	3	2.490	1.672
1	5	3	1.880	-.605
2	4	3	2.490	-.097
2	5	3	2.000	-2.843
3	2	3	2.030	-1.109
3	3	3	2.440	1.636
3	4	3	2.610	1.970
3	5	3	1.850	-1.600
4	3	3	2.630	2.791
4	5	3	1.750	-2.122
5	2	3	2.080	-.478
5	3	3	2.590	2.255
5	4	3	2.550	.940
6	2	3	2.210	2.399
6	3	3	2.440	1.465
7	1	3	1.970	1.088
7	4	3	2.410	-1.472
8	3	3	2.600	-3.004
9	2	3	2.210	.788
9	3	3	2.410	-.100
9	4	3	2.430	-2.464
11	1	3	2.080	1.087
11	3	3	2.600	2.631
11	4	3	2.390	2.508
12	1	3	2.050	-.587
12	2	3	2.330	2.778
12	4	3	2.260	-2.109
13	1	3	2.080	-1.447
13	3	3	2.490	-1.622
13	4	3	2.080	.533
14	1	3	2.150	1.354
14	2	3	2.350	-.382
14	4	3	2.060	.942
15	2	3	2.420	-1.305
15	3	3	2.590	2.879
16	2	3	2.530	-1.424
16	4	3	2.140	2.232
17	1	3	2.340	.786
17	2	3	2.430	-1.385
17	3	3	2.420	-1.318
17	4	3	1.890	-1.515
18	1	3	2.360	.604
18	2	3	2.550	-2.405
18	3	3	2.470	-2.394
19	1	3	2.430	-1.832
19	2	3	2.550	3.758
19	3	3	2.370	-2.076
19	4	3	1.790	.312
20	1	3	2.460	-1.781
20	3	3	2.260	-1.443
21	1	3	2.430	-2.333
21	2	3	2.470	1.011
21	3	3	2.200	-1.480
22	1	3	2.420	-.180
22	3	3	2.150	1.160
23	1	3	2.600	4.448
23	2	3	2.370	-.390

Table II-continued. 37

23	3	3	1.910	-.363
24	2	3	2.320	-1.299
25	1	3	2.420	1.706
25	2	3	2.170	-.843
25	3	3	1.860	-1.228
26	1	3	2.410	-2.815
26	2	3	2.050	-.552
26	3	3	1.720	1.806
27	1	3	2.230	.678
27	2	3	1.970	-.886
28	1	3	2.120	-1.485
29	1	3	2.190	-2.526
29	2	3	1.850	-1.827
30	1	3	1.880	-.908
31	1	3	1.830	.505
32	1	3	1.660	1.319
1	4	4	2.450	1.492
4	4	4	2.570	-2.705
6	4	4	2.500	-1.970
7	1	4	1.980	1.601
7	3	4	2.600	1.601
8	4	4	2.270	.145
13	2	4	2.550	-3.420
13	4	4	2.070	-.385
14	3	4	2.500	.324
15	4	4	1.980	-1.308
16	3	4	2.600	3.241
19	3	4	2.310	2.304
20	2	4	2.400	-.133
21	3	4	2.130	-2.127
22	2	4	2.410	.050
24	2	4	2.340	3.708
27	0	4	2.400	2.366
27	2	4	1.970	.754
28	1	4	2.180	-1.529
0	3	5	2.550	3.360
2	2	5	2.190	2.456
2	3	5	2.630	-.845
2	4	5	2.490	1.385
4	4	5	2.410	-.172
5	4	5	2.480	-2.991
6	1	5	2.030	.785
6	2	5	2.340	-2.393
6	3	5	2.500	-.789
6	4	5	2.360	-.337
7	2	5	2.200	1.407
7	4	5	2.260	.923
8	2	5	2.320	1.472
8	3	5	2.580	4.112
8	4	5	2.200	.868
9	1	5	2.100	-.402
9	4	5	2.260	2.268
10	1	5	2.070	1.331
10	2	5	2.360	.618
10	3	5	2.600	2.110
10	4	5	2.270	2.467
11	3	5	2.610	-3.228
12	2	5	2.340	-.334
12	3	5	2.510	-3.200

Table II continued. 38

12	4	5	2.100	-.870
13	1	5	2.210	1.091
13	3	5	2.510	-1.351
14	1	5	2.270	-.364
14	2	5	2.400	-1.154
14	3	5	2.410	1.807
14	4	5	2.020	-3.017
15	1	5	2.350	.734
16	2	5	2.420	1.313
16	3	5	2.380	2.625
16	4	5	1.900	.080
17	4	5	1.850	2.616
18	1	5	2.510	-1.203
18	2	5	2.530	3.073
18	3	5	2.260	-1.311
18	4	5	1.540	.311
19	2	5	2.500	-.855
20	1	5	2.580	-2.761
20	2	5	2.390	1.030
20	3	5	2.170	-2.435
21	2	5	.500	1.551
22	1	5	2.490	1.607
22	2	5	2.290	-1.023
22	3	5	2.000	-.930
23	1	5	2.430	.707
24	2	5	2.170	-1.081
24	3	5	1.800	.633
25	1	5	2.340	-2.068
25	3	5	1.570	.095
26	1	5	2.190	-.681
26	2	5	1.950	.070
27	1	5	2.050	.479
28	2	5	1.810	-1.325
29	1	5	1.830	.259
29	2	5	1.610	1.645
30	1	5	1.830	.939
31	1	5	1.640	1.240
1	4	6	2.380	-1.204
3	3	6	2.700	-2.944
3	4	6	2.410	2.727
5	3	6	2.700	-3.362
5	4	6	2.240	2.839
6	2	6	2.400	-1.513
6	4	6	2.280	1.877
7	3	6	2.840	-3.824
8	2	6	2.310	1.778
9	3	6	2.490	1.342
9	4	6	2.290	3.441
11	4	6	2.180	3.801
13	4	6	1.900	.750
14	1	6	2.410	2.714
14	3	6	2.410	1.125
15	2	6	2.420	.582
15	4	6	1.860	.401
17	2	6	2.470	1.438
20	0	6	2.560	.037
20	2	6	2.500	2.564
21	3	6	2.170	2.716
23	1	6	2.570	1.587

Table II continued.

23	3	6	1.910	-2.329
27	0	6	2.190	-2.695
27	2	6	1.930	2.847
28	1	6	1.930	-.571
31	0	6	1.620	1.542
1	3	7	2.570	-1.037
2	4	7	2.150	-1.295
3	2	7	2.430	-3.093
3	4	7	2.130	-1.162
4	3	7	2.510	-.912
5	2	7	2.420	-1.911
5	3	7	2.590	2.389
5	4	7	2.130	.244
6	1	7	2.200	1.472
6	3	7	2.570	-3.518
7	1	7	2.180	.157
7	3	7	2.490	1.722
7	4	7	2.020	.679
8	3	7	2.520	1.939
8	4	7	2.200	2.509
9	1	7	2.340	-2.347
9	2	7	2.450	1.446
9	3	7	2.510	1.228
9	4	7	2.000	-.764
10	1	7	2.400	-2.583
11	3	7	2.490	.588
11	4	7	1.960	-2.748
12	2	7	2.580	-3.283
12	3	7	2.380	-.914
12	4	7	1.840	1.006
13	1	7	2.510	-2.480
13	2	7	2.540	.383
13	3	7	2.340	.214
13	4	7	1.910	-2.297
14	2	7	2.620	2.431
14	4	7	1.800	-1.469
15	1	7	2.580	.543
15	2	7	2.580	2.759
15	3	7	2.360	-1.103
15	4	7	1.630	-.337
16	2	7	2.610	-4.151
17	1	7	2.560	-1.801
17	3	7	2.240	-1.929
18	1	7	2.540	.984
18	3	7	2.190	1.711
19	2	7	2.460	-1.360
19	3	7	2.060	-1.704
20	1	7	2.500	-2.462
20	3	7	1.970	1.232
21	1	7	2.500	2.247
21	2	7	2.320	-.642
22	1	7	2.590	2.750
22	2	7	2.360	2.861
22	3	7	1.770	-.947
23	1	7	2.330	.675
23	2	7	2.210	-2.209
23	3	7	1.550	-.118
24	1	7	2.410	2.216
24	2	7	2.070	.010

Table II continued.

25	1	7	2.240	-1.486
25	2	7	1.990	-2.007
26	1	7	2.230	2.570
26	2	7	1.830	.268
27	1	7	1.940	-.721
27	2	7	1.670	-1.709
28	1	7	1.900	-1.571
29	1	7	1.630	-.310
0	2	8	2.620	3.696
0	4	8	2.150	2.694
1	2	8	2.590	2.541
2	1	8	2.470	-2.468
2	2	8	2.510	-1.552
2	3	8	2.730	3.757
2	4	8	2.040	1.096
4	3	8	2.550	1.348
4	4	8	2.120	-2.578
5	3	8	2.740	4.310
6	0	8	2.670	3.112
6	1	8	2.540	-3.193
6	2	8	2.760	3.354
6	3	8	2.670	-1.938
6	4	8	1.980	.948
7	3	8	2.590	-1.993
8	2	8	2.640	-1.483
8	3	8	2.540	-1.086
8	4	8	1.860	.277
10	1	8	2.500	.193
10	2	8	2.770	-3.371
10	3	8	2.580	1.569
10	4	8	1.900	1.140
12	2	8	2.690	-2.472
12	3	8	2.520	2.155
12	4	8	1.660	1.457
14	0	8	2.750	3.573
14	2	8	2.610	1.473
14	3	8	2.470	2.892
16	1	8	2.610	1.860
16	2	8	2.580	2.585
16	3	8	2.320	2.814
18	1	8	2.650	-2.508
18	3	8	1.980	1.927
20	2	8	2.330	-.736
20	3	8	1.850	-1.975
21	1	8	2.520	1.866
21	3	8	1.680	1.211
22	0	8	2.600	-2.762
22	1	8	2.610	4.017
26	0	8	2.180	.511
26	2	8	1.530	-.036
27	0	8	2.040	1.382
28	0	8	1.850	2.264
29	0	8	1.630	-2.607
0	1	9	2.470	.606
1	3	9	2.600	1.154
1	4	9	2.000	1.791
3	2	9	2.670	-.159
3	4	9	2.000	1.974
4	1	9	2.530	1.021

Table II continued.

4	4	9	1.890	.266
5	2	9	2.670	-1.232
5	3	9	2.700	1.632
5	4	9	1.890	1.843
6	1	9	2.620	2.167
6	3	9	2.620	-1.356
6	4	9	1.940	-1.776
7	1	9	2.600	-1.203
7	3	9	2.540	1.325
7	4	9	1.800	-.127
8	3	9	2.500	-1.492
9	1	9	2.590	.939
9	2	9	2.620	-1.484
9	3	9	2.610	3.077
9	4	9	1.700	-.865
10	2	9	2.660	.872
10	3	9	2.400	-2.102
11	2	9	2.760	.345
11	3	9	2.430	1.566
12	2	9	2.510	-.362
13	2	9	2.510	.821
13	3	9	2.220	1.541
14	2	9	2.510	-.146
14	3	9	2.260	-2.447
15	1	9	2.630	-2.217
15	2	9	2.520	1.595
15	3	9	2.110	-.936
16	3	9	1.990	-.879
17	1	9	2.560	.964
17	3	9	1.890	.324
18	1	9	2.650	3.006
18	3	9	1.900	-1.891
19	2	9	2.240	1.268
19	3	9	1.780	-1.671
20	1	9	2.370	1.792
21	1	9	2.390	3.007
22	1	9	2.200	-1.802
23	1	9	2.110	-.379
24	1	9	2.010	-.110
24	2	9	1.740	-2.242
25	1	9	1.860	.932
26	1	9	1.790	-1.291
27	1	9	1.510	-.628
1	0	10	2.580	-1.081
1	2	10	2.620	-2.055
1	3	10	2.390	-.643
1	4	10	1.640	-.203
2	3	10	2.460	-1.616
3	1	10	2.660	2.793
3	4	10	1.610	-.444
4	2	10	2.690	2.903
5	1	10	2.560	.833
7	3	10	2.440	.836
8	2	10	2.590	-2.374
9	0	10	2.660	.741
9	1	10	2.660	-3.151
11	2	10	2.610	-1.717
12	3	10	2.230	-3.484
13	2	10	2.560	2.782

Table II continued. 42

14	1	10	2.660	-2.943
14	3	10	1.940	-.809
15	3	10	2.050	3.013
16	1	10	2.540	1.598
17	3	10	1.660	-.393
19	1	10	2.310	1.423
20	0	10	2.490	3.554
21	1	10	2.240	3.765
22	2	10	1.740	1.471
23	0	10	2.040	-.420
23	2	10	1.490	1.400
25	0	10	1.490	1.054
0	1	11	2.560	.416
4	2	11	2.470	-4.236
1	1	11	2.550	-3.126
1	2	11	2.510	.598
1	3	11	2.160	2.652
2	1	11	2.530	-.555
2	2	11	2.520	2.477
3	1	11	2.610	1.623
3	2	11	2.430	1.093
4	1	11	2.480	-1.969
4	3	11	2.170	2.408
5	1	11	2.520	-.668
5	3	11	2.170	-1.857
6	1	11	2.610	2.350
6	2	11	2.440	1.933
6	3	11	2.120	.091
7	1	11	2.590	1.274
7	2	11	2.590	-3.504
8	1	11	2.590	-4.922
8	3	11	2.010	.503
9	2	11	2.490	-.263
10	1	11	2.520	1.026
10	2	11	2.400	.891
10	3	11	2.000	.221
11	1	11	2.660	-2.073
11	2	11	2.350	-4.255
11	3	11	1.880	-.557
12	1	11	2.670	3.123
12	2	11	2.300	.090
13	1	11	2.480	.740
13	3	11	1.780	-.751
14	1	11	2.530	3.002
14	2	11	2.240	1.351
14	3	11	1.660	.287
15	2	11	2.160	-1.143
16	2	11	2.150	-2.267
17	1	11	2.370	.130
17	2	11	2.100	-1.902
18	1	11	2.260	1.837
18	2	11	1.950	-.851
19	1	11	2.120	.069
19	2	11	2.100	3.912
20	1	11	2.170	-.341
20	2	11	1.740	2.408
21	1	11	1.960	-1.367
22	1	11	1.830	1.212
23	1	11	1.680	.382

Table II continued. 43

0	0	12	2.730	-1.489
1	0	12	2.710	2.530
1	2	12	2.380	-.263
1	3	12	2.120	-2.867
2	3	12	2.000	1.394
4	1	12	2.640	-2.315
6	0	12	2.560	-.300
6	2	12	2.430	.269
7	1	12	2.640	-1.716
7	3	12	1.870	-.795
8	0	12	2.630	-2.567
8	2	12	2.340	.498
9	1	12	2.410	-.544
9	3	12	1.800	1.926
10	3	12	1.760	1.581
12	1	12	2.370	-.667
13	2	12	2.150	-3.360
14	1	12	2.340	2.776
15	0	12	2.460	-2.354
15	2	12	1.920	-.393
16	2	12	1.920	1.168
17	0	12	2.310	-1.415
17	2	12	1.830	3.230
18	0	12	2.140	-1.488
20	0	12	1.940	2.240
20	1	12	2.000	3.357
21	1	12	1.770	-2.710
0	1	13	2.490	2.665
1	1	13	2.370	.086
1	2	13	2.230	-1.058
1	3	13	1.650	.523
2	1	13	2.530	3.280
2	2	13	2.170	-.549
2	3	13	1.750	-2.618
3	2	13	2.170	.555
3	3	13	1.590	-1.301
4	1	13	2.470	-3.654
4	2	13	2.120	-1.412
4	3	13	1.570	-1.539
5	1	13	2.510	2.074
5	2	13	2.140	.924
6	1	13	2.400	1.525
7	1	13	2.430	1.433
7	2	13	2.140	1.098
8	1	13	2.300	1.957
8	2	13	2.130	.514
9	1	13	2.320	.142
9	2	13	2.010	.130
10	2	13	2.020	-1.273
11	1	13	2.330	-1.446
11	2	13	1.890	-.339
12	1	13	2.200	-2.189
12	2	13	1.830	-.740
13	1	13	2.110	1.794
13	2	13	1.770	-.308
14	1	13	1.990	-.670
14	2	13	1.750	.279
15	1	13	1.930	.089
15	2	13	1.490	-.685

Table II continued. 44

16	1	13	1.860	1.105
17	1	13	1.820	.126
18	1	13	1.660	-.778
0	0	14	2.350	2.529
1	0	14	2.390	3.354
1	2	14	1.980	2.887
2	0	14	2.460	3.565
2	1	14	2.220	-1.258
2	2	14	2.000	-2.546
4	1	14	2.310	-2.997
4	2	14	2.020	-1.082
6	0	14	2.330	2.867
6	1	14	2.230	-2.887
6	2	14	2.080	-1.660
7	1	14	2.170	1.380
7	2	14	2.020	3.325
8	0	14	2.340	-2.621
8	1	14	2.330	-4.567
8	2	14	1.870	-2.649
9	1	14	2.240	3.621
10	0	14	2.220	-.413
10	2	14	1.630	1.590
11	0	14	2.130	-2.687
12	0	14	1.990	-.631
12	1	14	2.060	-3.491
13	0	14	2.060	-1.806
14	1	14	1.760	-1.155
15	0	14	1.820	1.141
0	1	15	2.060	.689
1	1	15	1.930	-.383
2	1	15	1.970	-.214
3	1	15	2.010	-1.856
4	1	15	1.960	-.695
5	1	15	1.940	1.555
6	1	15	1.800	-.862
7	1	15	1.830	-1.338
8	1	15	1.710	1.700
9	1	15	1.670	-.980
10	1	15	1.570	.875
1	0	16	1.620	-.403
3	0	16	1.630	-1.079
5	0	16	1.530	-.546

Table III. Distances from the least squares planes and equations of the planes in Å units.

<u>Atom</u>	<u>A</u>	<u>B</u>	<u>C</u>
Br	.014	.124	.120
O	-.041	-.001	-.001
C ₁	.001	.026	.022
C ₂	-.005	.026	.023
C ₃	.005	-.026	-.028
C ₄	-.002	-.100	-.102
C ₅	-.002	-.104	-.108
C ₆	.003	-.038	-.042
C ₇	.025	.001	.000
C ₈	.082	.000	.000

$$(A) \quad -1.9794 x + 3.5972 y - .1270 z = 1$$

$$(B) \quad -2.3866 x + 4.1438 y + .0000 z = 1$$

$$(C) \quad -2.2797 x + 3.9642 y + .0000 z = 1$$

Table IV. Intramolecular bond distances in Å and bond angles in degrees.

<u>Atoms</u>	<u>Distance</u>	<u>Atoms</u>	<u>Angle</u>
Br-C ₁	1.901 ± .007 Å	Br-C ₁ -C ₂	117.8 ± .5°
C ₁ -C ₂	1.392 ± .009	C ₆ -C ₁ -C ₂	122.7 ± .7
C ₂ -C ₃	1.400 ± .009	C ₆ -C ₁ -Br	119.5 ± .6
C ₃ -C ₄	1.410 ± .008	C ₁ -C ₂ -C ₃	119.1 ± .6
C ₄ -C ₅	1.389 ± .010	C ₂ -C ₃ -C ₇	119.3 ± .6
C ₅ -C ₆	1.397 ± .010	C ₇ -C ₃ -C ₄	121.6 ± .6
C ₆ -C ₁	1.375 ± .009	C ₂ -C ₃ -C ₄	119.2 ± .6
C ₃ -C ₇	1.457 ± .009	C ₃ -C ₄ -C ₅	119.6 ± .7
C ₇ -C ₈	1.393 ± .008	C ₄ -C ₅ -C ₆	121.6 ± .6
C ₇ -O	1.306 ± .008	C ₅ -C ₆ -C ₁	117.8 ± .7
O-O	2.464 ± .015	C ₃ -C ₇ -O	115.6 ± .6
		C ₈ -C ₇ -O	119.4 ± .7
		C ₃ -C ₇ -C ₈	125.0 ± .6
		C ₇ -C ₈ -C ₇	122.2 ± .8
		C ₇ -O-O	89.5 ± .8

Table V. Nearest nonbonded neighbor distances less than 3 Å.

<u>Atoms</u>	<u>Distance</u>	<u>Atoms</u>	<u>Distance</u>	<u>Atoms</u>	<u>Distance</u>
Br-Br	3.689 Å	C ₂ -C ₄	2.42 Å	C ₅ -H ₄	2.15 Å
-C ₂	2.83	-C ₅	2.78	-H ₆	2.16
-C ₆	2.84	-C ₆	2.43	C ₆ -H ₅	2.14
-H ₂	2.93	-C ₇	2.46	C ₇ -C ₇	2.44
-H ₆	2.96	C ₃ -C ₅	2.42	-H ₂	2.68
O-C ₂	2.71	-C ₆	2.82	-H ₄	2.73
-C ₃	2.34	-C ₈	2.53	-H ₈	2.14
-C ₈	2.33	-H ₂	2.16	C ₈ -H ₄	2.68
-H ₂	2.37	-H ₄	2.16	H ₂ -H ₅	2.38
-H ₄	2.49	-H ₈	2.76	-H ₅	2.67
-H ₅	2.83	C ₄ -C ₆	2.43	H ₄ -H ₈	2.01
C ₁ -C ₃	2.41	-C ₇	2.50	H ₅ -H ₆	2.48
-C ₄	2.76	-C ₈	2.99		
-C ₅	2.37	-H ₅	2.14		
-H ₂	2.15	-H ₈	2.68		
-H ₆	2.15

Figure I (a)

Figure I(b)

Figure II

Figure III