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Crystal Structure of the *trans* Form of 1,4-Aminomethylcyclohexanecarboxylic Acid

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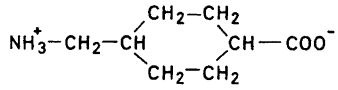
The crystals are orthorhombic with lattice parameters $a = 6.27_9$ Å, $b = 7.89_5$ Å, $c = 16.70_6$ Å. The space group is $P2_12_12_1$ and the cell contains four molecules. The phase problem was solved by a computer procedure based on direct methods. Full-matrix least squares refinement gave the R-value 4.5 % for 1070 reflections. The structure consists of zwitterions, each of which is linked to six others by approximately linear hydrogen bonds of lengths 2.79_5 Å, 2.79_4 Å, and 2.72_4 Å, respectively. The hydrogen bonding system forms infinite double layers normal to the c-axis. One oxygen atom of the COO^- group is engaged in the two longer hydrogen bonds, and the corresponding C—O distance, 1.26_1 Å, is significantly longer than the C—O distance, 1.22_8 Å, for the O-atom associated with the shorter bond. The arrangement around the nitrogen atom is approximately tetrahedral, and the C—N bond length is 1.49_4 Å.

One of the two stereo-isomers of 1,4-aminomethylcyclohexanecarboxylic acid exhibits a strong antifibrinolytic activity, the other almost none.[1] In order to establish which of the two isomers is the *cis* and which the *trans*



form, the crystal structure of the hydrobromide of the amino-acid which is "inactive" as an antifibrinolytic agent was determined.[2] It was found that the "inactive" amino-acid is the *cis* isomer with the carboxylic group in the axial position. Consequently the "active" amino-acid is the *trans* form. The X-ray crystallographic investigations[3] of *trans*-1,4-aminomethylcyclohexanecarboxylic acid hydrobromide and *cis*-1,4-aminomethylcyclohexanecarboxylic acid hydrochloride show that the "active" form of the amino-acid has the *di*-equatorial conformation, and that also the hydrochloride of the "inactive" form has the carboxylic group in the axial position.

In order to obtain more precise informations regarding the *trans* isomer of the amino-acid itself, a crystal structure determination has been carried out.

CRYSTAL DATA

1,4-Aminomethylcyclohexanecarboxylic acid belongs to the orthorhombic system. From systematic absences the space group is found to be $P2_12_12_1$. The cell parameters were found by means of *h0l*- and 0*kl*-Weissenberg photographs taken with unfiltered Cu-radiation. Powder diagrams of BaF_2 ($a = 6.2001$ Å) were superimposed on the films for calibration purpose. The 2θ-values of 139 reflections were used in a least squares refinement of the lattice parameters. The programme used has been written by R.A. Sparks at UCLA. With the wave-lengths for CuK-radiation taken as $\bar{\alpha} = 1.54178$, $\alpha_1 = 1.54051$, $\alpha_2 = 1.54433$, and $\beta = 1.39217$ Å, the following cell parameters with their estimated standard deviations resulted:

$a = 6.279$ Å	σ(Å) = 0.002
$b = 7.895$ »	σ(Å) = 0.002
$c = 16.706$ »	σ(Å) = 0.004

The number of molecules in the unit cell is $Z = 4$ ($\varrho_{calc} = 1.26$ g·cm^{-3}, $\varrho_{obs} = 1.25$ g·cm^{-3}).

The intensity material was obtained from photometric measurements of integrated Weissenberg diagrams corresponding to 0*kl*, 1*kl*, ..., 5*kl*, and *h0l*, *h1l*, ..., *h5l* (Cu$K\alpha$-radiation). The number of reflections accessible from these diagrams is 1070, 1034 of which were strong enough to be measured.

No corrections have been made for absorption or secondary extinction effects.

DETERMINATION OF THE STRUCTURE

The phase problem was solved for the 0*kl*-reflections by a computer procedure based on direct methods.[4-6] The set of programmes has been written in FORTRAN IV for UNIVAC 1107 by the author and may handle two-dimensional as well as three-dimensional data.

The $|U|$-distribution of the 0*kl*-projection (plane group *pgg*) is listed in Table 1. In order to specify the origin S(0 9 8) and S(0 7 1) were chosen to be

Table 1. $|U|$-distribution of the 0*kl*-projection.

Range of $\|U\|$	Number of reflections
0.00—0.01	8
0.01—0.02	18
0.02—0.03	6
0.03—0.04	13
0.04—0.05	11
0.05—0.10	48
0.10—0.15	17
0.15—0.20	17
0.20—0.25	14
0.25—0.30	7
0.30—0.35	4
0.35—0.40	2
0.40—0.50	2
0.50—1.00	1

Table 2. Probable sign sets produced by the permutation programme.

Signset number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
χ	0.474	0.453	0.451	0.440	0.451	0.438	0.453	0.456	0.451	0.450	0.441	0.451	0.450	0.482	0.449
ψ_0	4.964	4.044	4.153	4.400	3.996	4.280	3.887	4.402	4.296	4.375	4.091	4.349	4.301	4.279	4.410
h k l	S	S	S	S	S	S	S	S	S	S	S	S	S	S	S
0 6 4	−	+	+	−	−	−	−	−	+	+	+	−	−	−	−
0 6 8	+	−	−	+	+	−	+	+	−	−	−	+	+	−	+
0 2 18	+	−	−	−	+	+	+	−	−	−	−	+	+	+	+
0 4 10	+	+	+	−	+	+	+	−	+	+	+	+	+	+	+*
0 4 14	−	−	−	+	−	−	−	+	−	−	−	−	−	−	−*
0 8 4	−	−	−	−	−	−	−	−	−	−	−	+	−	−	−*
0 2 12	−	−	+	−	−	+	+	+	−	+	+	+	+	+	−
0 7 5	−	−	−	+	−	−	−	−	−	−	−	−	−	−	−*
0 8 11	−	−	−	+	+	+	+	+	+	+	−	−	+	+	+
0 2 19	−	−	−	+	−	−	−	+	−	−	−	−	−	−	−*
0 5 18	+	+	+	−	+	+	+	−	+	+	+	+	+	+	+*
0 8 7	+	+	+	−	−	−	−	−	−	−	−	−	−	−	−
0 6 5	+	+	+	+	+	+	+	−	−	−	+	+	+	+	+
0 2 15	−	−	−	−	−	−	−	−	+	+	+	+	+	+	+
0 9 4	−	−	−	−	−	−	−	−	−	−	−	−	−	−	−*

positive, and the programmed systematic application of Harker-Kasper inequalities gave the indication $S(0\ 2\ 9) = +$. Further, $F(0\ 0\ 4)$ being the largest structure factor of this zone and $F(0\ 0\ 2)$ very small, and taking into account the size of the molecule, the conclusion $S(0\ 0\ 4) = -$ could be drawn.

15 of the largest unitary structure factors were selected for sign permutation. Among the 19 signs thus involved in the χ-expression

$$\chi = \sum_{\mathbf{h}} \sum_{\mathbf{h}'} U_{\mathbf{h}} \cdot U_{\mathbf{h}'} \cdot U_{\mathbf{h}+\mathbf{h}'} \tag{1}$$

24 relationships could be found. 20 "small" U's ($|U| \leqq 0.04$) resulted in 80 products for the zero-check expression

$$\psi_0 = \sum_{\mathbf{k}} | \sum_{\mathbf{h}} U_{\mathbf{h}} \cdot U_{\mathbf{h}+\mathbf{k}} | \tag{2}$$

χ_e given by

$$\chi_e = \sum_{\mathbf{h}} \sum_{\mathbf{h}'} |U_{\mathbf{h}} \cdot U_{\mathbf{h}'} \cdot U_{\mathbf{h}+\mathbf{h}'}| \cdot \tanh(N \cdot |U_{\mathbf{h}} \cdot U_{\mathbf{h}'} \cdot U_{\mathbf{h}+\mathbf{h}'}|) \tag{3}$$

where N is the number of equal atoms in the cell, was calculated, and found to be $\chi_e = 0.485$. The 15 sets of signs satisfying $\chi > 0.9 \cdot \chi_e$ produced by the machine are listed in Table 2. The χ-criterion points out set number 14 as being the most probable, while the zero-check favours number 7. However, all the sets, with the exception of the less probable sets 4, 8, and 12, have 7 signs in common. Regarding these as fixed and adding 7 unknown signs, the application of the permutation programme was repeated.

Table 3. Probable sign sets produced by the second application of the permutation programme.

Sign set number	12	61
χ	0.904	0.808
ψ_0	6.282	4.586
$h\ k\ l$	S	S
0 6 4	+	+
0 6 8	−	−
0 2 18	−	−
0 2 12	+	+
0 5 13	+	+
0 5 17	−	−
0 4 18	+	+
0 8 7	−	−
0 8 11	+	−
0 8 7	+	−
0 6 5	+	+
0 2 15	+	+
0 7 2	+	+
0 7 6	−	+
0 5 10	−	−

The number of terms involved in the χ- and ψ_0-expressions were 47 and 171, respectively, and $\chi_e = 0.818$. 65 sign sets satisfying $\chi > 0.9 \cdot \chi_e$ resulted when 2^{15} combinations were tested. Number 12 was strongly indicated by the χ-criterion while number 61 was the most probable, even more expressed, according to the zero-check. The two sets are listed in Table 3, and it will be noted that they differ only in three signs.

Excluding these, 23 signs had now been obtained, and were used as basis for evaluation of 39 additional signs using the relationship

$$S(U_{\mathbf{k}}) = S(\sum_{\mathbf{h}} U_{\mathbf{h}} \cdot U_{\mathbf{h}+\mathbf{k}}) \qquad (4)$$

in a somewhat special way; the signs being accepted in the order of decreasing probabilities given by

$$P_+(\mathbf{k}) = \tfrac{1}{2} + \tfrac{1}{2} \cdot \tanh(N \cdot |U_{\mathbf{k}}| \cdot \sum_{\mathbf{h}} U_{\mathbf{h}} \cdot U_{\mathbf{h}+\mathbf{k}}) \qquad (5)$$

and being redetermined until no further sign shifts occur.

Table 4. Fractional coordinates for oxygen, nitrogen, and carbon atoms.* (Estimated standard deviations in parantheses).

	x	y	z
O_1	−0.3067 (0.0003)	−0.0081 (0.0003)	0.1133 (0.0002)
O_2	0.0013 (0.0003)	−0.0973 (0.0002)	0.0662 (0.0001)
N	0.3995 (0.0003)	0.7478 (0.0002)	0.0803 (0.0001)
C_1	0.2897 (0.0004)	0.4538 (0.0003)	0.1206 (0.0001)
C_2	0.3321 (0.0004)	0.3131 (0.0003)	0.1809 (0.0001)
C_3	0.2300 (0.0004)	0.1466 (0.0003)	0.1537 (0.0001)
C_4	−0.0097 (0.0004)	0.1651 (0.0003)	0.1394 (0.0001)
C_5	−0.0545 (0.0004)	0.3143 (0.0003)	0.0830 (0.0002)
C_6	0.0499 (0.0004)	0.4784 (0.0003)	0.1114 (0.0002)
C_7	0.4070 (0.0004)	0.6155 (0.0003)	0.1442 (0.0001)
C_8	−0.1133 (0.0004)	0.0059 (0.0003)	0.1045 (0.0001)

* For numbering of atoms, see Fig. 1.

The Fourier map corresponding to the 62 signs thus established could easily be interpreted,[7] the trial parameters gave an R_{0kl}-value of 32.8 % which was reduced to 12.1 % using a programme based upon the "minum residual method".[8]

Checking with the signs corresponding to $R_{0kl} = 12.1$ % revealed that 2 of the 62 signs had been obtained incorrectly, both of which were determined in the last step of the process.

Using the established z-parameters, approximate x-coordinate values were obtained by allowing the *h0l*-projection of the molecule (determined from a model) to move in small steps parallel to the x-axis and calculating the *R*-factor for each step. The parameters corresponding to the minimum *R*-value (32.0 %) were chosen as starting coordinates for a full-matrix least squares refinement.

REFINEMENT OF THE STRUCTURE

With the coordinates obtained by the two-dimensional analysis as starting parameters, a three-dimensional full-matrix least squares refinement was

Table 5. Anisotropic thermal vibration parameters. (Estimated standard deviations in parantheses).

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
O_1	0.0180 (0.0005)	0.0136 (0.0003)	0.0070 (0.0001)	−0.0133 (0.0008)	0.0024 (0.0004)	−0.0047 (0.0003)
O_2	0.0198 (0.0005)	0.0106 (0.0002)	0.0047 (0.0001)	0.0041 (0.0007)	−0.0042 (0.0004)	−0.0048 (0.0002)
N	0.0151 (0.0005)	0.0079 (0.0003)	0.0035 (0.0001)	−0.0045 (0.0006)	0.0007 (0.0003)	−0.0010 (0.0002)
C_1	0.0145 (0.0005)	0.0081 (0.0003)	0.0024 (0.0001)	−0.0056 (0.0007)	−0.0001 (0.0003)	0.0006 (0.0003)
C_2	0.0177 (0.0006)	0.0103 (0.0004)	0.0029 (0.0001)	−0.0054 (0.0009)	−0.0040 (0.0004)	0.0010 (0.0003)
C_3	0.0164 (0.0006)	0.0083 (0.0003)	0.0033 (0.0001)	−0.0032 (0.0008)	−0.0025 (0.0004)	0.0014 (0.0003)
C_4	0.0137 (0.0005)	0.0079 (0.0003)	0.0026 (0.0001)	−0.0057 (0.0007)	0.0009 (0.0003)	−0.0001 (0.0003)
C_5	0.0146 (0.0006)	0.0073 (0.0003)	0.0037 (0.0001)	−0.0039 (0.0008)	−0.0044 (0.0004)	0.0007 (0.0003)
C_6	0.0171 (0.0006)	0.0067 (0.0003)	0.0039 (0.0001)	−0.0049 (0.0008)	−0.0031 (0.0004)	0.0001 (0.0003)
C_7	0.0196 (0.0006)	0.0094 (0.0003)	0.0029 (0.0001)	−0.0066 (0.0009)	−0.0024 (0.0004)	−0.0008 (0.0003)
C_8	0.0147 (0.0005)	0.0067 (0.0003)	0.0030 (0.0001)	−0.0020 (0.0008)	−0.0009 (0.0003)	0.0004 (0.0003)

carried out using a programme written by Gantzel, Sparks and Trueblood [9] (revised for UNIVAC 1107 by cand.real. Christian Rømming at this university). The weighting scheme No. 1:

$$\text{for } F_0 \leqq \text{FB}, \qquad W = \text{A1}(F_0)^{\text{B1}}$$

$$\text{for } F_0 > \text{FB}, \qquad W = \text{A2}(F_0)^{\text{B2}}$$

was adapted by taking

Table 6. Fractional coordinates and isotropic thermal vibration parameters for hydrogen atom.* (Estimated standard deviations in parantheses).

	x	y	z	B (Å^2)
H_{1a}	0.342 (0.004)	0.419 (0.003)	0.069 (0.001)	1.8 (0.5)
H_{2e}	0.493 (0.004)	0.293 (0.003)	0.188 (0.001)	1.3 (0.5)
H_{2a}	0.270 (0.003)	0.353 (0.003)	0.234 (0.001)	0.4 (0.4)
H_{3e}	0.253 (0.004)	0.057 (0.003)	0.196 (0.001)	1.2 (0.5)
H_{3a}	0.300 (0.004)	0.102 (0.003)	0.104 (0.001)	1.0 (0.5)
H_{4a}	−0.080 (0.003)	0.190 (0.003)	0.194 (0.001)	0.2 (0.4)
H_{5e}	−0.212 (0.004)	0.328 (0.003)	0.074 (0.001)	0.5 (0.4)
H_{5a}	0.014 (0.004)	0.289 (0.003)	0.025 (0.001)	1.6 (0.5)
H_{6e}	0.025 (0.005)	0.573 (0.004)	0.072 (0.002)	3.2 (0.6)
H_{6a}	−0.010 (0.004)	0.521 (0.003)	0.165 (0.001)	1.0 (0.5)
$H_{7,1}$	0.341 (0.004)	0.674 (0.003)	0.197 (0.001)	2.1 (0.6)
$H_{7,2}$	0.565 (0.004)	0.589 (0.003)	0.151 (0.001)	1.0 (0.5)
H_{N1}	0.430 (0.004)	0.692 (0.003)	0.031 (0.001)	1.9 (0.5)
H_{N2}	0.515 (0.004)	0.841 (0.003)	0.095 (0.001)	1.1 (0.5)
H_{N3}	0.255 (0.004)	0.808 (0.003)	0.075 (0.001)	2.0 (0.6)

* Referring to Fig. 1, the hydrogen atoms H_{ne} and H_{na} are, respectively, equatorially and axially bonded to C_n. $H_{7,1}$ and $H_{7,2}$ are bonded to C_7, and H_{N1}, H_{N2} and H_{N3} to N.

Table 7. Calculated and observed (and unobserved) structure factors. The unobserved F-values correspond to I_{min}.

h	k	l	|Fo|	|Fc|	cosα	sinα
0	0	2	29.4	29.5	1.0000	-.0000
0	0	4	145.8	148.1	-1.0000	.0000
0	0	6	35.5	35.8	-1.0000	.0000
0	0	8	3.4	3.0	1.0000	-.0000
0	0	10	5.3	5.6	1.0000	.0000
0	0	12	5.4	5.5	1.0000	-.0000
0	0	14	4.2	4.0	1.0000	-.0000
0	0	16	3.0	2.9	1.0000	-.0000
0	0	18	3.1	3.2	-1.0000	.0000
0	1	1	8.9	8.8	-.0000	1.0000
0	1	2	14.5	13.1	-.0000	1.0000
0	1	3	44.8	46.7	-.0000	-1.0000
0	1	4	24.8	23.0	.0000	1.0000
0	1	5	21.4	20.4	-.0000	1.0000
0	1	7	23.6	23.1	.0000	1.0000
0	1	8	8.7	7.5	.0000	-1.0000
0	1	9	2.3	2.3	.0000	1.0000
0	1	10	5.1	4.6	-.0000	-1.0000
0	1	11	1.5	1.2	-.0000	1.0000
0	1	12	3.7	3.1	.0000	-1.0000
0	1	13	5.7	6.2	-.0000	-1.0000
0	1	14	2.2	2.0	.0000	1.0000
0	1	15	3.6	3.1	-.0000	-1.0000
0	1	17	1.6	1.6	.0000	1.0000
0	1	18	3.7	4.2	-.0000	-1.0000
0	1	19	1.5	1.2	-.0000	-1.0000
0	1	20	1.2	1.1	.0000	1.0000
0	1	21	1.4	1.5	.0000	1.0000
0	2	0	20.5	20.4	1.0000	.0000
0	2	1	3.9	4.2	-1.0000	.0000
0	2	2	8.7	8.1	1.0000	-.0000
0	2	3	26.5	25.5	1.0000	.0000
0	2	4	39.1	39.0	-1.0000	.0000
0	2	5	52.2	50.7	1.0000	-.0000
0	2	6	15.2	14.5	-1.0000	.0000
0	2	7	8.1	7.8	-1.0000	.0000
0	2	8	37.0	36.9	1.0000	-.0000
0	2	9	31.5	31.2	-1.0000	.0000
0	2	10	10.8	10.7	1.0000	-.0000
0	2	11	2.6	2.4	1.0000	-.0000
0	2	12	20.3	19.6	-1.0000	.0000
0	2	13	5.9	6.2	1.0000	-.0000
0	2	14	12.2	12.9	-1.0000	-.0000
0	2	15	10.7	10.9	-1.0000	.0000
0	2	16	3.8	3.4	1.0000	-.0000
0	2	17	3.1	3.0	1.0000	.0000
0	2	18	10.4	11.0	1.0000	-.0000
0	2	19	7.6	8.3	1.0000	-.0000
0	2	20	2.3	2.6	1.0000	-.0000
0	3	1	2.9	2.6	-.0000	-1.0000
0	3	2	8.7	9.6	.0000	1.0000
0	3	3	2.1	2.0	-.0000	-1.0000
0	3	4	8.1	8.3	.0000	1.0000
0	3	5	15.0	14.0	-.0000	-1.0000
0	3	6	11.9	10.5	.0000	1.0000
0	3	7	1.4	1.3	-.0000	1.0000
0	3	8	16.8	16.5	-.0000	-1.0000
0	3	9	17.2	16.7	.0000	1.0000
0	3	10	8.4	8.0	-.0000	-1.0000
0	3	11	4.8	4.6	-.0000	1.0000
0	3	12	14.1	13.7	.0000	1.0000
0	3	13	3.8	4.2	-.0000	-1.0000
0	3	14	3.7	3.0	-.0000	-1.0000
0	3	15	3.5	3.4	-.0000	-1.0000
0	3	16	3.4	3.1	-.0000	-1.0000
0	3	17	1.0	.5	.0000	1.0000
0	3	19	.7	.1	.0000	1.0000
0	3	20	2.1	2.6	-.0000	-1.0000
0	4	0	12.5	12.0	1.0000	-.0000
0	4	1	6.5	6.6	1.0000	-.0000
0	4	2	12.3	11.6	1.0000	-.0000
0	4	3	15.5	15.3	1.0000	.0000
0	4	4	14.5	15.1	-1.0000	.0000
0	4	5	9.9	8.8	-1.0000	.0000
0	4	6	25.0	25.1	-1.0000	.0000
0	4	7	9.4	8.9	-1.0000	.0000
0	4	8	10.4	10.3	1.0000	-.0000
0	4	9	17.4	17.0	1.0000	-.0000
0	4	10	26.7	27.3	1.0000	-.0000
0	4	11	4.1	4.0	1.0000	-.0000
0	4	12	3.1	3.0	-1.0000	-.0000
0	4	13	11.7	12.0	-1.0000	.0000
0	4	14	15.4	15.3	-1.0000	.0000
0	4	15	3.3	2.8	-1.0000	-.0000
0	4	16	1.1	1.3	1.0000	-.0000
0	4	18	4.6	5.2	1.0000	-.0000
0	4	19	1.7	1.9	1.0000	-.0000
0	5	1	12.2	11.6	-.0000	-1.0000
0	5	2	1.1	.9	.0000	-1.0000
0	5	3	4.9	5.3	-.0000	1.0000
0	5	4	9.8	9.5	-.0000	-1.0000
0	5	5	1.3	1.2	-.0000	-1.0000
0	5	6	22.7	21.6	.0000	-1.0000
0	5	7	4.4	4.2	.0000	1.0000
0	5	8	3.3	3.5	.0000	1.0000
0	5	9	14.2	14.1	.0000	1.0000
0	5	10	14.7	15.5	-.0000	1.0000
0	5	11	1.9	1.6	-.0000	-1.0000
0	5	13	12.4	12.3	-.0000	-1.0000
0	5	15	1.7	1.5	-.0000	-1.0000
0	5	16	1.1	.6	.0000	1.0000
0	5	17	5.6	5.6	.0000	1.0000
0	5	18	4.7	5.3	-.0000	-1.0000
0	6	0	20.4	20.2	1.0000	-.0000
0	6	1	16.8	18.4	1.0000	.0000
0	6	2	9.4	9.0	-1.0000	-.0000
0	6	3	11.5	11.3	1.0000	-.0000
0	6	4	19.7	19.6	-1.0000	.0000
0	6	5	17.3	17.6	-1.0000	-.0000
0	6	6	6.5	6.3	1.0000	.0000
0	6	7	4.2	4.1	-1.0000	.0000
0	6	8	13.8	13.7	1.0000	-.0000
0	6	9	7.4	7.9	1.0000	-.0000
0	6	10	7.3	7.4	1.0000	-.0000
0	6	11	2.0	2.0	1.0000	-.0000
0	6	12	2.5	2.6	-1.0000	.0000
0	6	13	1.3	1.3	-1.0000	.0000
0	6	14	7.0	7.3	-1.0000	.0000
0	6	15	1.3	1.5	-1.0000	-.0000
0	6	16	2.3	2.4	-1.0000	.0000
0	7	1	27.8	28.3	.0000	1.0000
0	7	2	16.9	16.5	.0000	1.0000
0	7	3	15.0	14.3	-.0000	-1.0000
0	7	5	15.6	15.7	-.0000	-1.0000
0	7	6	10.9	10.6	-.0000	-1.0000
0	7	7	3.9	3.7	.0000	-1.0000
0	7	8	1.1	1.2	-.0000	-1.0000
0	7	9	1.0	1.5	-.0000	-1.0000
0	7	10	1.1	1.1	.0000	1.0000
0	7	11	3.1	2.8	.0000	1.0000
0	7	12	2.8	2.6	.0000	1.0000
0	7	13	4.3	3.8	-.0000	1.0000
0	7	14	3.0	2.9	.0000	1.0000
0	7	15	3.0	3.7	.0000	1.0000
0	8	0	7.5	7.3	1.0000	-.0000
0	8	2	3.6	3.7	1.0000	-.0000
0	8	4	9.0	8.6	-1.0000	.0000
0	8	5	1.5	2.1	-1.0000	-.0000
0	8	6	6.7	6.3	-1.0000	.0000
0	8	7	8.2	8.0	-1.0000	.0000
0	8	8	5.4	5.7	1.0000	-.0000
0	8	10	1.6	1.3	1.0000	.0000
0	8	11	9.1	8.4	1.0000	-.0000
0	8	12	1.6	1.4	1.0000	.0000
0	8	13	2.4	2.5	1.0000	-.0000
0	9	2	4.2	3.9	.0000	1.0000
0	9	3	1.8	1.3	-1.0000	.0000
0	9	4	9.0	8.2	.0000	1.0000
0	9	5	1.9	1.7	-.0000	-1.0000
0	9	6	.9	.9	.0000	1.0000
0	9	7	6.5	5.8	.0000	1.0000
0	9	8	10.4	9.9	-.0000	-1.0000
0	9	9	2.8	2.6	.0000	1.0000
0	10	0	9.5	8.6	2.9	-.0000
0	10	1	2.1	.7	-1.0000	-.0000
1	0	1	15.6	15.4	.0000	1.0000
1	0	2	37.2	41.8	-1.0000	-.0000
1	0	3	41.3	44.6	.0000	1.0000
1	0	4	26.5	29.5	1.0000	-.0000
1	0	5	17.6	17.4	.0000	1.0000
1	0	6	8.9	8.9	-1.0000	.0000
1	0	7	13.0	12.3	-.0000	-1.0000
1	0	8	18.0	18.0	-1.0000	.0000
1	0	9	3.6	3.7	.0000	-1.0000
1	0	10	8.1	7.6	1.0000	.0000
1	0	12	7.9	7.4	1.0000	-.0000
1	0	13	3.8	3.5	.0000	-1.0000
1	0	16	2.7	2.3	-1.0000	.0000
1	0	17	1.3	1.1	-.0000	-1.0000
1	0	18	3.1	3.1	-1.0000	.0000
1	0	19	.9	.7	-.0000	1.0000
1	0	20	.8	.7	1.0000	.0000
1	0	21	2.5	2.5	-.0000	1.0000
1	1	0	58.3	62.1	-.0000	-1.0000
1	1	1	26.0	26.9	.8280	-.5607
1	1	2	40.6	44.5	-.9944	-.1054
1	1	3	22.2	22.0	-.4806	.8769
1	1	4	42.0	44.6	-.2779	.9606
1	1	5	22.9	24.3	.1156	.9933
1	1	6	24.5	25.1	.8100	.5864
1	1	7	11.2	10.9	.0964	-.9953
1	1	8	22.2	22.0	.1173	-.9931
1	1	9	16.3	16.4	-.8869	-.4984
1	1	10	13.7	13.9	-.2245	-.9745
1	1	11	8.4	8.4	-.9504	-.3109
1	1	12	11.6	11.6	.4900	.8717
1	1	13	5.7	6.1	.9091	-.4165
1	1	14	10.4	10.6	-.5925	.8055
1	1	15	8.0	8.2	.6646	.7472
1	1	16	11.0	11.0	-.8840	-.4675
1	1	17	2.6	2.6	-.4972	.8677
1	1	18	4.1	4.3	.7225	-.6914
1	1	19	2.3	2.2	-.1976	-.9803
1	1	20	4.8	4.6	.9355	.3534
1	1	21	2.1	2.3	.9333	-.3591
1	2	0	25.1	25.0	-.0000	-1.0000
1	2	1	17.9	17.7	-.4701	.8826
1	2	2	37.5	38.6	.7486	-.6630
1	2	3	22.3	22.4	.3854	.9228
1	2	4	4.5	4.4	.8400	.5425
1	2	5	12.6	12.3	.3090	.9511
1	2	6	21.8	21.8	-.1240	.9922
1	2	7	11.0	10.2	-.9251	-.3798
1	2	8	13.6	13.0	-.4787	.8780
1	2	9	16.1	15.6	.3759	-.9267
1	2	10	8.5	7.9	-.9275	.3731
1	2	11	4.7	4.4	.9735	.2286
1	2	12	7.3	6.9	.0831	-.7304
1	2	13	11.7	11.0	-.8444	.5357
1	2	14	7.1	7.2	.6584	-.7527
1	2	15	4.5	4.3	.0803	-.9982
1	2	16	.9	1.5	-.7860	.6183
1	2	17	7.7	7.0	.9277	-.3734
1	2	18	1.2	1.2	-.9913	.1319
1	2	19	3.6	3.6	-.7577	.6526
1	2	20	1.0	1.0	-.9720	-.2348
1	3	0	35.6	36.7	-.0000	-1.0000
1	3	1	22.4	22.1	-.7118	-.7024
1	3	2	22.2	22.3	.7011	-.7130
1	3	3	36.1	35.4	.8016	-.5975
1	3	4	52.3	53.0	.7164	.6977
1	3	5	5.4	4.4	-.9484	-.3170
1	3	6	25.2	24.8	-.7166	.6981
1	3	7	21.3	20.8	-.8198	.5727
1	3	8	23.1	22.8	-.5796	-.8148
1	3	9	4.9	4.5	.8137	.5812
1	3	10	15.4	15.4	-.9367	-.3500
1	3	11	9.2	9.0	.9785	-.2065
1	3	12	5.9	5.4	-.8090	.4949
1	3	13	1.6	1.3	.0861	.7275
1	3	14	2.4	2.0	.3853	.9228
1	3	15	4.9	4.8	-.9991	-.0429
1	3	16	4.4	4.3	.7270	.6866
1	3	17	1.7	1.4	-.2676	-.9635
1	3	18	4.9	5.1	.6543	-.7563
1	3	19	2.4	2.4	.7882	-.7060
1	3	20	1.4	1.5	.4217	-.9067
1	4	0	10.1	16.1	-.0000	-1.0000
1	4	1	9.4	8.4	.9861	-.1659
1	4	2	19.4	20.0	.9541	.2995
1	4	3	11.3	10.9	.1026	-.9947
1	4	4	12.0	11.4	-.7409	.6716
1	4	5	20.8	21.3	-.6564	-.7544
1	4	6	16.2	16.2	-.8063	-.5916
1	4	7	5.5	5.4	.5401	-.8416
1	4	8	5.1	4.3	.9833	.1819
1	4	9	10.6	10.6	.5046	.8634
1	4	10	10.0	9.6	.5917	.8062
1	4	11	11.7	11.5	-.3183	.9480
1	4	12	4.1	3.9	-.1975	.9803
1	4	13	4.4	4.0	.2885	.9633
1	4	14	2.7	2.3	.7819	.6234
1	4	15	2.2	3.8	-.0587	-.9983
1	4	16	3.4	3.4	-.4064	-.9137
1	4	17	5.5	5.6	-.0968	-.9953
1	4	18	4.2	4.1	-.9928	-.1198
1	4	19	2.3	2.1	.8908	-.4545
1	5	0	20.9	19.4	-.0000	-1.0000
1	5	1	20.2	18.3	-.9996	.0294
1	5	2	3.7	3.7	.8622	.5067
1	5	3	4.9	4.8	-.5576	-.8301
1	5	4	14.9	14.0	-.4914	.8710
1	5	5	15.1	14.5	.9773	.2121
1	5	6	3.9	3.8	-.9412	.3378
1	5	7	11.9	11.1	.6214	.7835
1	5	8	11.4	10.7	.9247	-.3800
1	5	9	6.5	6.0	.5821	-.8131
1	5	10	10.2	10.0	.4725	-.8813
1	5	11	10.4	9.9	.2438	-.9698
1	5	12	7.6	7.1	-.9328	.3603
1	5	13	7.2	7.1	-.8227	.5684
1	5	14	8.6	8.4	-.2649	.9643
1	5	15	7.0	6.3	-.5747	.8184
1	5	16	3.3	3.3	.8387	-.5446
1	5	17	1.0	1.0	.3841	-.9233
1	5	18	2.9	2.9	-.3559	-.9345
1	6	0	5.0	4.4	.0000	1.0000
1	6	1	14.3	14.6	.6246	.7809
1	6	2	11.1	11.3	.9537	-.3008
1	6	3	17.4	17.5	-.6940	.7200
1	6	4	14.9	14.7	.9908	-.1354
1	6	5	9.9	9.5	-.2543	-.9671
1	6	6	8.5	8.9	-.8068	.5909
1	6	7	13.5	14.1	.5408	-.8412
1	6	8	11.0	11.2	-.9878	-.1555
1	6	9	1.4	1.0	-.2212	.9752
1	6	10	4.9	4.9	.4686	-.8834
1	6	11	2.3	2.2	-.7418	.6706
1	6	12	2.0	2.3	.9812	-.1932
1	6	13	2.7	2.2	-.6754	.7375
1	6	14	2.3	2.2	-.0317	.9995
1	6	15	5.2	5.1	.0280	.9996
1	6	16	2.3	2.1	.3935	.9193
1	7	0	2.8	2.7	.0000	-1.0000
1	7	1	10.4	10.3	-.0792	-.9969
1	7	2	8.8	8.5	-.9126	-.4088
1	7	3	5.1	5.0	-.3471	-.9378

Table 7. Continued.

h	k	l	|Fo|	|Fc|	cosα	sinα	h	k	l	|Fo|	|Fc|	cosα	sinα	h	k	l	|Fo|	|Fc|	cosα	sinα
1	7	4	9.6	8.9	-.9608	.2774	2	3	8	5.3	5.5	-.5546	.8321	3	0	7	7.2	6.7	-.0000	-1.0000
1	7	5	7.2	7.1	-.1356	.9908	2	3	9	10.2	10.0	-.6989	.7152	3	0	9	3.9	3.8	.0000	-1.0000
1	7	6	8.8	8.4	.2465	.9691	2	3	10	8.4	8.2	-.0851	-.7407	3	0	11	1.7	1.9	-.0000	-1.0000
1	7	7	3.3	3.3	.9665	.2567	2	3	11	5.4	5.2	-.3747	.9272	3	0	12	3.1	3.0	1.0000	-.0000
1	7	8	5.4	5.4	.8205	-.5716	2	3	12	3.6	3.5	.2974	-.9547	3	0	13	3.5	3.6	-.0000	-1.0000
1	7	9	1.5	1.7	.5980	-.8015	2	3	13	7.8	7.7	.8831	-.4691	3	0	14	1.1	1.0	1.0000	.0000
1	7	10	6.4	5.9	-.1494	-.9888	2	3	14	5.4	5.4	.0933	.9956	3	0	15	3.5	3.5	.0000	-1.0000
1	7	11	1.9	1.4	-.3989	-.9170	2	3	15	4.5	4.4	.2053	-.9787	3	0	16	2.2	2.4	-1.0000	.0000
1	7	12	2.4	1.8	.3580	.9337	2	3	16	1.6	1.6	.7752	.6317	3	0	17	7.0	7.3	.0000	1.0000
1	7	13	3.4	2.8	.9897	.1428	2	3	17	2.4	2.2	-.9307	-.3659	3	0	18	.9	.9	1.0000	.0000
1	7	14	2.8	2.7	.4430	.8965	2	3	18	2.2	2.3	.0949	-.9955	3	0	19	2.4	2.7	-.0000	1.0000
1	7	15	2.9	2.6	.0287	.9996	2	3	19	1.6	1.5	-.9996	-.0272	3	1	0	14.4	14.2	-.0000	-1.0000
1	8	0	8.8	8.9	.0000	1.0000	2	4	0	9.8	9.9	-1.0000	.0000	3	1	1	27.1	26.6	.2186	.9758
1	8	1	2.7	2.3	.4119	-.9112	2	4	1	2.7	2.9	.3213	-.9470	3	1	2	7.5	7.5	-.9669	.2551
1	8	2	3.8	3.5	.8619	.5071	2	4	2	12.6	12.2	-.5599	.8286	3	1	3	24.8	24.2	.3563	.9344
1	8	3	5.2	4.8	.1209	-.9927	2	4	3	7.9	7.5	-.2026	-.9649	3	1	4	15.7	16.0	.7924	.6101
1	8	4	4.3	4.1	-.4474	-.8944	2	4	4	7.2	6.9	.9656	-.2600	3	1	5	8.3	8.4	-.8317	-.5553
1	8	5	4.2	3.9	-.8785	-.4777	2	4	5	6.8	6.7	.8563	.5164	3	1	6	7.5	8.1	.8764	-.4817
1	8	6	2.7	2.2	-.9153	.4028	2	4	6	5.9	6.1	.9886	.1503	3	1	7	6.5	6.9	-.8234	-.5675
1	8	7	1.3	1.1	-.9960	-.0898	2	4	7	13.3	13.7	.5241	.8516	3	1	8	3.8	4.0	-.9144	-.4048
1	8	8	3.3	2.9	-.9119	-.4104	2	4	8	1.7	1.6	-.8216	-.5701	3	1	9	5.5	5.8	-.8888	-.4583
1	8	9	5.5	4.8	.9987	-.0507	2	4	9	2.6	2.2	-.6545	.7560	3	1	10	4.3	4.0	-.9795	.2016
1	8	10	7.3	6.6	.4408	-.8976	2	4	10	7.1	7.2	.3209	-.9471	3	1	11	8.2	8.0	-.5780	.8160
1	8	11	5.8	5.5	.0763	.9971	2	4	11	6.6	7.0	-.2752	-.9614	3	1	12	5.2	5.3	-.8539	-.5204
1	8	12	6.6	6.9	.9999	.0135	2	4	12	4.8	5.1	.8567	.5159	3	1	13	4.5	4.0	-.9859	-.1673
1	9	0	4.9	4.5	-.0000	-1.0000	2	4	13	3.0	3.5	-.8358	-.5491	3	1	14	2.3	1.9	.9734	-.2291
1	9	1	3.3	3.4	.8156	-.5786	2	4	14	4.7	4.7	-.7915	.6111	3	1	15	0.3	8.0	.5499	.8353
1	9	2	7.9	7.5	-.9872	-.1596	2	4	15	3.4	3.0	-.6744	.7383	3	1	16	4.9	4.8	.0344	.9994
1	9	3	3.5	3.1	.7267	-.6870	2	4	16	4.7	4.5	-.9584	-.2853	3	1	17	3.1	3.4	-.6054	.7959
1	9	4	4.4	4.3	-.5285	.8489	2	4	17	1.4	1.7	.9895	-.1444	3	1	18	2.2	2.1	-.9999	-.0166
1	9	5	4.9	4.6	-.6748	.7380	2	4	18	1.3	1.5	1.0000	-.0074	3	1	19	2.8	3.2	-.2845	-.9587
1	9	6	2.3	2.1	.6598	.7515	2	5	0	4.8	5.3	-1.0000	-.0000	3	2	0	21.6	21.0	-.0000	-1.0000
1	9	7	6.1	5.9	-.8980	.4400	2	5	1	3.8	3.7	-.2073	-.9783	3	2	1	5.6	5.6	-.6509	.7591
1	9	8	.9	1.0	.6992	-.7149	2	5	2	13.7	13.5	-.3695	-.9292	3	2	2	8.1	8.6	.1235	-.9923
1	9	9	4.9	4.5	-.2349	-.9720	2	5	3	3.9	3.6	.6351	-.7725	3	2	3	12.3	12.5	-.2036	.9790
1	10	0	4.3	4.2	-.0000	-1.0000	2	5	4	21.5	20.5	-.0413	-.9991	3	2	4	6.8	7.1	.9887	.1499
2	0	0	26.0	26.4	1.0000	-.0000	2	5	5	6.3	6.2	-.5250	.8511	3	2	5	5.8	6.1	.9652	-.3266
2	0	1	36.8	41.8	-.0000	-1.0000	2	5	6	10.7	10.0	.9697	-.2445	3	2	6	9.1	9.3	.2993	.9542
2	0	2	30.4	32.0	1.0000	.0000	2	5	7	5.7	5.4	-.9039	.4277	3	2	7	11.1	11.3	.3252	-.9456
2	0	3	20.2	20.7	.0000	1.0000	2	5	8	12.8	13.0	.6193	.7852	3	2	8	13.9	13.7	-.3396	.9406
2	0	4	2.7	2.3	-1.0000	.0000	2	5	9	5.8	7.0	-.9636	-.2672	3	2	9	6.2	6.2	-.4842	.8750
2	0	5	10.7	11.1	.0000	1.0000	2	5	10	7.1	6.9	-.7678	.6406	3	2	10	3.0	3.2	-.8914	-.4533
2	0	6	22.5	22.2	-1.0000	-.0000	2	5	11	3.4	3.5	.5643	.8256	3	2	11	6.2	6.3	-.0609	.9981
2	0	7	13.0	12.9	.0000	1.0000	2	5	12	6.2	6.2	-.9987	-.0518	3	2	12	4.7	4.3	.3746	-.9272
2	0	8	14.6	14.7	-1.0000	.0000	2	5	13	3.2	3.3	-.9297	.3684	3	2	13	3.7	3.5	-.3123	-.9500
2	0	9	4.9	5.2	.0000	1.0000	2	5	14	.9	.5	-.4714	-.8819	3	2	14	2.7	2.5	.2734	.9619
2	0	10	6.1	6.2	-1.0000	.0000	2	5	15	3.9	4.5	.2116	-.9773	3	2	15	5.1	5.1	-.4466	-.8947
2	0	11	10.2	10.1	.0000	-1.0000	2	5	16	1.1	1.1	.9820	.1762	3	2	16	3.7	3.8	-.0290	-.9996
2	0	12	5.3	5.5	1.0000	.0000	2	5	17	2.5	2.4	-.9790	-.2037	3	2	17	2.5	2.4	.5057	-.8627
2	0	13	5.3	5.5	.0000	-1.0000	2	6	0	6.7	7.0	-1.0000	-.0000	3	2	18	3.3	3.2	.4039	-.9148
2	0	14	10.3	10.8	1.0000	-.0000	2	6	1	6.9	7.0	-.8374	.5465	3	2	19	3.0	4.3	.7050	.7092
2	0	15	1.5	1.8	-.0000	-1.0000	2	6	2	5.1	5.3	-.3968	-.9179	3	3	0	6.3	6.2	-.0000	1.0000
2	0	16	1.0	.7	-1.0000	.0000	2	6	3	4.9	4.5	-.9995	.0331	3	3	1	5.2	4.8	-.1667	.9860
2	0	17	2.6	2.8	.0000	1.0000	2	6	4	4.1	4.0	-.5351	.8448	3	3	2	7.9	7.6	.6755	-.7374
2	0	18	4.9	5.1	-1.0000	.0000	2	6	5	7.2	7.6	.5431	-.8397	3	3	3	9.7	9.8	.4278	-.9039
2	0	19	4.5	4.7	.0000	1.0000	2	6	6	1.2	.9	.8480	.5300	3	3	4	7.7	7.9	.6723	-.7403
2	0	20	.7	.6	1.0000	-.0000	2	6	7	1.2	.9	-.5611	.8278	3	3	5	16.9	16.7	.5231	-.8523
2	1	0	3.5	3.6	-1.0000	.0000	2	6	8	8.7	9.1	.9361	-.3519	3	3	6	17.9	18.4	.5282	.8491
2	1	1	20.2	20.2	-.7424	-.6700	2	6	9	1.5	1.2	-.9822	.1879	3	3	7	5.4	5.3	-.8785	.4778
2	1	2	15.5	15.5	-.6638	-.7479	2	6	10	3.7	3.7	.8530	.5218	3	3	8	5.5	5.5	.6216	.7833
2	1	3	7.3	6.9	-.5238	.8519	2	6	11	2.9	2.7	.3295	-.9442	3	3	9	14.3	14.4	-.3761	.9266
2	1	4	11.9	11.7	.3762	.9266	2	6	12	3.6	3.8	-.8497	.5272	3	3	10	13.8	14.7	.5308	-.8472
2	1	5	10.2	10.0	.9951	-.0987	2	6	13	3.9	3.6	.3507	.9365	3	3	11	8.1	8.1	.9532	.3024
2	1	6	17.0	17.8	.3861	.9225	2	6	15	2.7	2.6	.6026	.7980	3	3	12	5.2	5.2	-.8202	-.5721
2	1	7	8.9	8.6	-.7433	.6689	2	6	16	2.0	1.7	-.3578	-.9338	3	3	13	5.3	4.8	.1377	-.9905
2	1	8	3.8	3.2	-.9865	.1636	2	7	0	15.2	15.9	1.0000	-.0000	3	3	14	5.5	5.6	.1195	.9928
2	1	9	11.4	11.1	-.5461	.8377	2	7	1	11.5	12.5	.1571	.9876	3	3	15	4.1	4.0	-.7879	-.6158
2	1	10	6.0	6.5	.7612	-.6485	2	7	2	7.7	7.8	.1198	-.9928	3	3	16	1.0	1.1	.5904	.8071
2	1	11	5.5	5.3	.9318	-.3630	2	7	3	4.4	4.1	.9565	-.2919	3	3	17	1.3	1.2	.3696	-.9292
2	1	12	6.1	6.1	-.3086	-.9512	2	7	4	7.6	8.4	-.9999	.0131	3	3	18	1.0	1.3	.1693	-.9856
2	1	13	5.5	5.3	.9071	-.4210	2	7	5	9.6	10.7	-.1548	-.9880	3	4	0	9.7	9.5	-.0000	-1.0000
2	1	14	9.5	9.3	-.7646	-.6445	2	7	6	4.8	4.2	-.5149	.8572	3	4	1	6.0	5.5	.8860	.4634
2	1	15	2.1	2.0	-.7662	.6426	2	7	7	4.4	4.7	-.7021	-.7121	3	4	2	9.6	10.5	-.8312	-.5560
2	1	16	3.8	3.8	.9548	.2973	2	7	8	3.5	3.3	-.7944	-.6074	3	4	3	5.0	5.3	.9171	.3987
2	1	17	4.8	4.8	-.8292	-.5589	2	7	9	4.4	3.9	-.9673	-.2536	3	4	4	11.1	10.9	-.5056	.8628
2	1	18	5.1	5.2	.3793	.9253	2	7	10	1.9	1.5	.2972	-.9548	3	4	5	8.3	8.4	-.6941	-.7199
2	1	19	1.9	1.5	.0704	-.9975	2	7	11	3.0	3.4	.8966	-.4427	3	4	6	5.8	5.4	-.1895	.9819
2	1	20	1.5	1.5	-.9532	-.3025	2	7	12	3.0	3.0	.9939	-.0136	3	4	7	11.3	11.5	-.8462	-.5329
2	2	0	10.5	10.0	-1.0000	-.0000	2	7	13	6.7	6.2	-.4914	.8709	3	4	8	10.4	10.6	-.3882	-.9218
2	2	1	25.8	24.7	-.0563	-.9984	2	7	14	3.0	2.9	.8468	-.5318	3	4	9	3.3	3.1	.9431	.3324
2	2	2	5.7	5.1	-.9758	-.2189	2	8	0	.9	.4	1.0000	-.0000	3	4	10	6.7	7.0	.7976	.6032
2	2	3	16.4	16.7	.8867	-.4624	2	8	1	2.5	2.5	-.9046	-.4263	3	4	11	7.9	8.2	.7274	.6863
2	2	4	15.2	14.8	.9910	-.1339	2	8	2	1.3	1.0	-.9583	.2857	3	4	12	8.0	8.7	.0554	.9985
2	2	5	23.6	22.5	.9249	-.3801	2	8	3	4.7	4.0	-.8852	-.4651	3	4	13	3.5	3.3	-.0616	.9981
2	2	6	10.6	9.7	.7117	-.7024	2	8	4	1.4	1.4	-.3293	.9442	3	4	14	5.0	5.2	-.6049	-.7969
2	2	7	14.1	13.2	.3455	-.9384	2	8	5	4.1	4.4	-.5665	.8241	3	4	15	2.6	2.7	-.6462	.7631
2	2	8	12.3	12.2	-.9135	-.4068	2	8	6	.9	1.0	-.1197	-.9928	3	4	16	2.9	2.9	-.4350	-.9004
2	2	9	14.6	14.1	-.9660	-.2586	2	8	7	1.3	1.2	.6802	.7511	3	4	17	1.7	1.9	-.5121	-.8589
2	2	10	9.7	9.6	-.4907	.8713	2	8	8	2.5	2.2	-.0438	-.9990	3	5	0	2.1	2.1	.0000	1.0000
2	2	11	13.0	12.8	-.7721	.6355	2	8	9	.7	.8	-.9690	-.2470	3	5	1	9.1	9.6	-.9782	-.2076
2	2	12	5.7	5.7	.6141	-.7892	2	8	10	2.9	2.6	.9231	.3845	3	5	2	3.2	3.3	.9517	-.3072
2	2	13	4.9	4.8	.6536	.7568	2	8	11	1.4	.9	-.2356	.9718	3	5	3	5.0	5.0	-.1666	.9871
2	2	14	3.2	2.8	-.8577	-.5142	2	9	0	9.1	9.1	-1.0000	-.0000	3	5	4	2.0	2.3	.3296	.9440
2	2	15	4.1	4.0	.9054	.4245	2	9	1	1.5	1.0	.9998	.0299	3	5	5	7.4	7.7	.1161	.9932
2	2	16	2.7	2.6	-.3597	.9331	2	9	2	6.2	5.9	-.1848	-.9828	3	5	6	3.7	3.5	.7971	.6039
2	2	17	3.3	3.3	-.9527	-.3038	2	9	3	2.8	2.8	.9276	.3737	3	5	7	11.0	11.3	.8971	-.4418
2	2	18	4.3	4.4	.7526	-.6584	2	9	4	4.9	4.9	.7929	.6093	3	5	8	1.0	1.1	.8436	-.5370
2	2	19	4.6	4.5	.2532	-.9674	2	9	5	1.8	1.5	.9574	.2888	3	5	9	7.5	7.6	.6589	-.7522
2	2	20	2.8	2.2	.9891	-.1471	2	9	6	6.8	7.0	.2939	.9558	3	5	10	5.7	5.2	-.5607	-.8280
2	3	0	6.3	6.2	1.0000	-.0000	2	9	7	2.6	2.5	-.9694	-.2454	3	5	11	8.7	8.9	-.8924	.4512
2	3	1	28.4	28.4	.6065	-.7951	2	9	8	4.1	3.9	.9262	-.3771	3	5	12	3.0	2.7	-.8081	.5891
2	3	2	17.9	18.0	.6526	-.7577	3	0	1	43.7	45.6	.0000	1.0000	3	5	13	.8	.4	.9991	.0432
2	3	3	9.9	9.8	.9398	.3418	3	0	2	1.6	1.4	1.0000	.0000	3	5	14	5.7	5.4	.0256	.9997
2	3	4	2.6	2.3	-.1392	.9903	3	0	3	43.6	43.6	.0000	1.0000	3	5	15	2.6	2.7	.2290	-.9734
2	3	5	8.0	7.6	-.4806	.8770	3	0	4	11.2	10.1	-1.0000	-.0000	3	5	16	2.4	2.6	-.9972	-.0753
2	3	6	16.6	16.4	-.9261	.3774	3	0	5	3.1	2.9	-.0000	-1.0000	3	5	0	7.4	8.9	-.0000	-1.0000
2	3	7	5.4	4.9	.3188	.9478	3	0	6	1.6	1.3	-1.0000	.0000	3	6	1	5.4	5.9	.0596	.9982

Table 7. Continued.

h	k	l	|F₀|	|Fc|	cos α	sin α
3	0	2	10.0	11.9	.9948	.1059
3	0	3	3.6	3.1	-.7985	-.6021
3	0	4	7.4	8.3	.5445	.8388
3	0	5	10.7	11.0	.0048	-1.0000
3	0	6	1.0	1.4	-.3831	-.9237
3	0	7	3.4	3.2	.7989	-.6014
3	0	8	4.4	4.8	-.4766	-.8791
3	0	9	5.1	4.3	.3810	.9246
3	0	10	6.2	6.5	-.9054	-.4247
3	0	11	4.3	4.3	-.3486	.9372
3	0	12	3.6	3.6	-.6893	.7244
3	0	13	1.3	1.3	-.9996	.0279
3	0	14	5.4	5.6	.8208	.5712
3	7	0	9.0	9.4	-.0000	-1.0000
3	7	1	.9	.7	.8683	.4960
3	7	2	12.5	13.9	-.9994	-.0348
3	7	3	2.8	2.6	-.9600	-.2801
3	7	4	8.3	8.6	-.4077	.9131
3	7	5	1.0	1.3	-.7258	-.6879
3	7	6	.9	1.1	.9754	-.2205
3	7	7	2.3	2.6	.8923	-.4513
3	7	8	3.9	3.7	.3274	-.9449
3	7	9	2.0	1.8	1.0000	-.0057
3	7	10	3.4	3.2	.9785	.2065
3	7	11	3.3	3.1	-.0807	.9967
3	7	12	1.7	1.6	.9995	.0301
3	7	13	.8	.6	-.8193	.5733
3	8	0	1.7	1.6	-.0000	1.0000
3	8	1	4.5	5.4	.8412	-.5408
3	8	2	7.3	8.3	-.9567	.2912
3	8	3	4.3	4.9	-.9901	.1406
3	8	4	4.2	4.1	-.9224	.3863
3	8	5	3.6	3.7	-.8017	.5977
3	8	6	2.1	2.3	.9883	-.4182
3	8	7	4.0	4.2	.7587	-.6514
3	8	8	4.3	4.6	.5698	-.8218
3	8	10	3.0	4.3	.3578	-.9338
3	9	0	6.3	7.0	-.0000	-1.0000
3	9	1	2.7	3.6	.5937	.8047
3	9	2	2.3	2.7	.8690	-.4948
3	9	3	1.6	1.8	.2645	.9644
3	9	4	4.4	6.0	-.4362	.8998
3	9	5	1.7	2.7	-.3095	-.9509
4	0	0	16.8	16.5	1.0000	-.0000
4	0	1	11.5	13.2	-.0000	-1.0000
4	0	2	2.8	2.7	1.0000	.0000
4	0	3	2.4	2.4	-.0000	1.0000
4	0	4	6.8	6.1	-1.0000	.0000
4	0	5	13.5	13.8	.0000	1.0000
4	0	6	2.7	2.4	1.0000	-.0000
4	0	7	1.8	1.3	.0000	1.0000
4	0	8	2.5	2.5	1.0000	-.0000
4	0	9	.9	1.1	-.0000	1.0000
4	0	10	10.8	11.2	-1.0000	.0000
4	0	12	5.7	5.5	-1.0000	.0000
4	0	13	11.2	11.5	.0000	-1.0000
4	0	14	7.0	6.6	1.0000	-.0000
4	0	15	.9	.6	-.0000	-1.0000
4	0	16	4.3	4.0	1.0000	.0000
4	0	17	7.7	8.7	-.0000	1.0000
4	1	0	6.9	6.9	-1.0000	.0000
4	1	1	20.1	20.5	.8764	.4816
4	1	2	7.4	6.8	.2050	.9788
4	1	3	19.1	19.3	.8177	-.5757
4	1	4	3.1	2.6	.7651	-.6439
4	1	5	11.3	11.6	-.8966	-.4428
4	1	6	5.9	6.1	-.2828	.9592
4	1	7	15.4	15.9	-.8382	.5453
4	1	8	10.5	10.6	.0476	.9989
4	1	9	.9	.7	.9011	.4337
4	1	10	6.2	6.5	-.2839	-.9589
4	1	11	11.4	11.6	.8967	-.4426
4	1	12	11.5	11.6	.1083	-.9941
4	1	13	6.5	6.7	.3452	.9385
4	1	14	2.7	2.7	.9307	.3657
4	1	15	7.2	7.5	-.9258	.3779
4	1	16	6.3	6.5	-.4741	.8804
4	1	17	5.8	5.8	-.2524	-.9676
4	2	0	6.6	6.9	1.0000	.0000
4	2	1	7.3	7.2	.0920	.9958
4	2	2	12.1	11.7	.2454	.9694
4	2	3	10.5	10.4	.9651	.2619
4	2	4	9.7	9.2	-.0336	-.9994
4	2	5	15.5	16.2	-.8452	-.5345
4	2	6	6.3	5.8	-.6715	-.7410
4	2	7	5.4	5.2	-.6913	-.7225
4	2	8	10.0	9.8	-.6025	.7981
4	2	9	6.3	6.3	-.9779	.2089
4	2	10	3.7	3.5	.1181	.9930
4	2	11	1.1	.5	-.4681	-.8837
4	2	12	1.7	1.3	.5715	-.8206
4	2	13	3.4	3.2	-.5287	.8488
4	2	14	3.1	3.1	.1104	-.9939
4	2	15	2.4	2.2	-.7553	.6554
4	2	16	3.6	3.6	.9590	-.2833
4	2	17	1.6	1.6	.8137	-.5812
4	3	0	0.6	0.2	-1.0000	.0000
4	3	1	13.5	13.7	.5946	-.8040
4	3	2	23.9	24.9	.0401	-.9992
4	3	3	24.8	24.6	.9102	-.4142
4	3	4	9.7	9.5	.9372	.3487
4	3	5	8.6	8.7	.0652	.9979
4	3	6	13.8	14.1	.0133	.9999
4	3	7	25.2	25.7	-.7866	.6175
4	3	8	9.8	10.1	-.9203	-.3912
4	3	9	4.1	3.6	-.1617	.9868
4	3	10	3.4	3.1	-.1783	-.9840
4	3	11	8.9	8.8	.8732	-.4873
4	3	12	5.1	5.1	.9539	.3000
4	3	13	3.5	3.4	.2073	-.9783
4	3	14	.9	.6	-.1784	-.9840
4	3	15	2.6	2.6	-.2796	-.9601
4	3	16	1.3	1.3	-.9988	-.0802
4	3	17	1.0	1.3	-.9581	-.2865
4	4	0	16.0	16.2	-1.0000	.0000
4	4	1	11.3	11.2	.9629	-.2699
4	4	2	7.8	7.5	-.6383	.5452
4	4	3	9.3	9.7	.9327	-.3607
4	4	4	12.0	12.1	.5161	.8565
4	4	5	9.7	8.8	-.8987	.4380
4	4	6	10.9	10.0	.8435	-.5371
4	4	7	7.8	7.4	-.0743	.9972
4	4	8	8.5	8.7	.6305	-.7762
4	4	9	6.0	5.8	.9607	-.2776
4	4	10	3.7	3.3	-.0612	.9981
4	4	11	4.8	4.5	-.3045	-.9525
4	4	12	5.8	5.5	-.9999	-.0109
4	4	13	3.5	3.6	-.9948	.1021
4	4	14	2.0	2.0	-.9918	-.1280
4	4	15	1.0	1.5	-.8724	.4888
4	4	16	1.7	1.6	.9904	.1382
4	5	0	13.2	13.2	-1.0000	-.0000
4	5	1	10.8	11.0	.9804	-.1973
4	5	2	10.6	11.5	-.2846	-.9587
4	5	3	8.9	8.8	.5499	.8353
4	5	4	14.4	14.5	.7533	-.6576
4	5	5	10.2	10.1	-.9724	-.2332
4	5	6	6.4	5.6	.9610	.2760
4	5	7	10.3	9.9	-.2767	-.9609
4	5	8	6.5	6.4	-.7461	.6659
4	5	9	5.0	4.9	.7525	.6586
4	5	10	2.6	2.4	-.9912	.1328
4	5	11	8.6	8.7	.6383	.7698
4	5	12	1.6	1.6	.3961	.9182
4	5	13	2.5	2.7	-.0554	-.9985
4	5	14	.6	.5	-.5041	.8636
4	5	15	3.9	4.0	-.9915	-.1304
4	6	0	3.4	4.1	1.0000	-.0000
4	6	1	4.2	4.3	.9315	-.9021
4	6	2	3.4	3.6	-.6522	.7581
4	6	3	3.5	3.3	.9535	.3012
4	6	4	4.5	5.1	-.9986	-.0530
4	6	5	5.5	5.8	-.4726	.8813
4	6	6	4.1	4.0	.9323	-.3616
4	6	7	5.1	4.7	-.9314	-.3640
4	6	8	4.2	4.7	.8196	-.5729
4	6	9	3.5	3.3	.7063	-.7079
4	6	10	5.1	4.8	-.8929	.4503
4	6	11	4.5	4.1	.9230	.3849
4	6	12	4.8	5.1	.2179	.9760
4	7	1	4.5	4.3	.9622	.2722
4	7	2	2.9	2.9	.9700	.2432
4	7	3	6.5	6.3	.9962	.0876
4	7	4	4.9	4.8	.0551	-.9985
4	7	5	1.0	.6	-.0967	-.9953
4	7	6	3.7	4.1	-.8058	-.5921
4	7	7	4.2	4.1	-.9731	.2303
4	7	8	6.1	6.6	-.4695	.8830
4	7	9	1.5	1.5	-.9796	-.2008
4	7	10	2.0	2.4	-.9673	.2539
4	7	11	3.3	3.1	.1343	-.9909
4	8	0	5.8	6.3	-1.0000	.0000
4	8	1	3.7	4.7	-.5157	-.8568
4	8	2	4.0	4.5	-.6372	.7707
4	8	3	4.9	5.2	-.3012	.9536
4	8	4	4.5	4.5	.9948	-.1019
4	8	5	1.4	1.5	.5873	.8094
4	8	6	5.8	4.9	.8234	-.5675
5	0	1	1.3	1.3	.0000	1.0000
5	0	2	4.5	5.3	-1.0000	.0000
5	0	3	4.6	4.7	-.0000	1.0000
5	0	4	1.3	1.4	-1.0000	.0000
5	0	5	4.7	4.6	.0000	1.0000
5	0	6	9.3	9.5	1.0000	.0000
5	0	7	11.7	12.1	.0000	1.0000
5	0	9	4.0	3.9	.0000	1.0000
5	0	10	9.6	9.9	-1.0000	-.0000
5	0	11	18.0	19.0	-.0000	-1.0000
5	0	12	.7	.5	-1.0000	.0000
5	0	13	7.9	8.2	-.0000	-1.0000
5	0	14	2.0	2.1	1.0000	.0000
5	0	15	10.1	11.1	.0000	1.0000
5	0	16	2.8	3.2	1.0000	-.0000
5	1	0	2.6	2.7	.0000	1.0000
5	1	1	3.5	3.3	-.1079	.9942
5	1	2	8.8	9.1	.9986	-.0488
5	1	3	4.9	4.6	.6383	.7698
5	1	4	7.8	8.4	.9897	.1426
5	1	5	6.0	5.4	.8890	.4579
5	1	6	5.0	5.1	.9485	.3167
5	1	7	3.1	3.3	-.9019	.4320
5	1	8	9.0	9.5	-.7850	-.6195
5	1	9	8.7	8.8	-.7916	-.6111
5	1	10	6.6	6.7	-.9834	-.1815
5	1	11	3.0	2.9	-.9222	-.3867
5	1	12	4.5	4.7	.4170	.9089
5	1	13	2.0	2.2	.7352	.6779
5	1	15	3.0	4.0	.9895	-.1445
5	1	16	2.0	2.1	.3665	-.9304
5	2	0	11.7	11.7	.0000	1.0000
5	2	1	13.3	13.3	-.4496	-.8932
5	2	2	16.6	17.5	-.8801	-.4747
5	2	3	19.0	19.2	.2579	-.9662
5	2	4	13.2	13.1	-.2543	-.9671
5	2	5	4.4	4.4	.2143	.9768
5	2	6	12.3	12.5	.4658	.8849
5	2	7	14.5	14.4	.0603	.9982
5	2	8	11.5	11.6	.5145	.8575
5	2	9	4.0	3.9	.9960	-.0898
5	2	10	3.5	3.4	-.0933	-.9956
5	2	11	6.0	5.9	-.6317	-.7753
5	2	12	5.3	5.5	-.9115	-.4114
5	2	13	4.0	3.9	-.9562	-.2927
5	2	14	1.7	1.8	.8697	.4941
5	2	15	.9	.8	.8711	-.4911
5	2	16	2.3	2.4	.8263	-.5632
5	3	0	10.8	10.3	-.0000	-1.0000
5	3	1	11.0	12.0	-.8745	-.4850
5	3	2	5.1	4.9	.9863	.1647
5	3	3	10.0	10.8	.9290	-.3701
5	3	4	6.1	5.9	.2608	.9654
5	3	5	6.0	6.8	.8722	.4891
5	3	6	2.8	2.4	-.9144	-.4047
5	3	7	3.1	2.8	-.8007	.7995
5	3	8	4.1	4.1	.7215	.6924
5	3	9	2.5	2.4	-.7856	.6187
5	3	10	3.7	3.7	.9840	-.1783
5	3	11	2.4	2.4	-.9489	-.3150
5	3	12	4.5	4.4	-.6413	-.7673
5	3	13	1.9	2.0	.2071	-.9783
5	3	14	3.3	3.5	-.9703	.2420
5	3	15	1.1	1.4	.9910	.1341
5	4	0	5.0	5.3	-.0000	-1.0000
5	4	1	13.4	13.1	.5009	-.8655
5	4	2	4.9	4.7	-.9997	.0246
5	4	3	11.0	10.6	-.2972	-.9548
5	4	4	4.7	4.6	-.9971	-.0762
5	4	5	10.0	9.6	-.2275	.9738
5	4	6	4.6	4.4	.9538	-.3005
5	4	7	5.8	5.4	-.4921	.8705
5	4	8	8.4	8.4	.7659	.6429
5	4	9	7.0	6.6	-.2881	-.9576
5	4	10	3.8	3.6	-.7276	.6860
5	4	11	4.5	4.7	.9361	-.3518
5	4	12	5.7	5.9	-.8724	-.4888
5	4	13	2.5	2.7	.1627	.9867
5	4	14	2.2	2.3	.6255	-.7802
5	5	0	3.8	3.9	.0000	1.0000
5	5	1	7.7	7.7	-.9240	-.3823
5	5	2	9.8	9.9	.9998	-.0212
5	5	3	5.9	6.0	-.5728	-.8197
5	5	4	4.0	3.9	.9712	-.2388
5	5	5	8.3	8.4	1.0000	-.0020
5	5	6	4.4	4.6	-.9591	-.2831
5	5	7	8.1	7.8	.7976	.6032
5	5	8	3.8	4.3	-.1231	-.9924
5	5	9	3.6	3.6	-.8139	.5811
5	5	10	1.9	2.2	.1717	.9851
5	5	11	4.2	4.0	-.4881	-.8726
5	5	12	4.1	4.7	-.9439	.8695
5	5	13	1.6	1.6	.9030	-.4297
5	6	0	3.0	3.1	.0000	1.0000
5	6	1	4.8	5.0	.0456	-.9990
5	6	2	2.6	2.3	-.5605	.8281
5	6	3	9.8	9.8	-.2066	-.9784
5	6	4	1.9	1.6	-.3302	-.9439
5	6	5	6.9	6.9	-.2069	-.9784
5	6	6	6.4	6.6	.6903	-.7235
5	6	7	6.3	6.4	.7752	.6318
5	6	8	1.0	1.1	.9986	-.0531
5	6	9	8.2	9.1	.2210	.9753
5	6	10	5.4	5.4	-.6322	.7748
5	6	11	3.9	4.1	-.9898	-.1425
5	7	0	1.2	.6	-.0000	1.0000
5	7	1	4.1	4.0	-.9999	-.0152
5	7	2	0.1	0.1	-.9959	-.0906
5	7	3	1.5	1.5	.6155	-.7881
5	7	4	3.7	4.0	-.9096	-.4154
5	7	5	5.1	5.9	.9467	.3221
5	7	6	1.5	1.6	.3985	.9172
5	7	7	4.1	4.0	.3242	.9460
5	7	8	2.6	2.5	-.7973	.6036
6	0	1	0.5	0.6	.0000	1.0000
6	0	3	4.9	4.7	-.0000	-1.0000
6	0	4	3.4	3.0	1.0000	-.0000
6	0	5	4.8	4.6	-.0000	-1.0000
6	0	6	3.0	3.3	1.0000	-.0000
6	0	7	2.4	2.3	.0000	1.0000
6	0	8	4.2	4.0	-1.0000	-.0000
6	0	9	1.2	1.2	.0000	1.0000
6	0	10	1.8	1.7	-1.0000	.0000
6	0	11	1.8	1.4	.0000	1.0000
6	0	12	2.9	2.6	-1.0000	.0000
6	1	0	6.1	8.3	1.0000	-.0000
6	1	1	7.5	7.3	-.8956	.4449
6	1	2	8.1	8.2	.4007	.9162
6	1	3	9.3	9.4	-.8015	-.5980
6	1	4	7.0	7.0	-.5376	.8432
6	1	5	2.1	2.0	.8887	.4585
6	1	6	6.9	7.0	-.8752	-.4837
6	1	7	5.9	5.9	.8346	.5508
6	1	8	1.9	1.7	-.8031	-.5958
6	1	9	1.1	1.1	.3069	-.9517
6	1	10	2.3	2.3	.7102	.7040
6	1	11	3.0	2.9	-.9996	-.0454
6	1	12	3.5	3.5	.1997	-.9799
6	1	13	.7	.7	-.9525	-.3046
6	1	14	2.5	2.8	.9307	-.3658
6	2	0	2.1	2.1	1.0000	-.0000
6	2	1	9.1	8.0	.6275	.7786
6	2	2	8.1	7.3	.7035	-.7107

Table 7. Continued.

h	k	l	|F_o|	|F_c|	cos α	sin α
0	2	3	3.9	3.5	.5977	-.8017
0	2	5	7.3	6.7	-.0782	-.9969
0	2	6	7.6	7.6	-.9875	.1578
0	2	7	5.8	5.8	.9927	-.1207
0	2	8	2.5	2.3	-.9997	.0225
0	2	9	5.8	5.3	-.1887	.9820
0	2	10	2.2	2.2	-.0008	1.0000
0	2	11	4.7	4.5	-.9243	.3818
0	2	12	2.1	2.5	.9074	.4203
0	2	13	2.9	2.7	-.2426	-.9701
0	3	0	1.0	.9	-1.0000	-.0000
0	3	1	9.6	6.5	-.3293	-.9442
0	3	2	2.5	2.6	-.8256	-.5643
0	3	3	3.9	3.4	-.8666	-.4990
0	3	4	4.8	4.6	-.0860	-.9963
0	3	5	4.9	4.8	.8759	.4825
0	3	6	5.0	4.5	.7723	.6352
0	3	7	8.4	8.3	.5599	.8286
0	3	8	3.7	3.6	.9566	.2913
0	3	9	4.7	4.6	-.7741	.6330
0	3	10	2.3	2.3	-.6014	-.7989
0	3	11	4.7	5.5	-.8337	-.5522
0	3	12	4.4	5.4	-.7090	.7052
0	4	0	3.4	3.1	-1.0000	.0000
0	4	1	7.2	6.6	-.0186	.9998
0	4	2	5.6	4.9	-.9279	.3729
0	4	3	4.2	4.6	.9673	-.2537
0	4	4	2.6	2.1	-.0388	.9992
0	4	5	8.9	8.7	.2197	-.9756
0	4	6	8.1	7.7	.9435	.3315
0	4	7	4.8	4.5	-.5555	-.8315
0	4	8	4.3	4.1	.9106	-.4134
0	4	9	8.5	6.6	.3534	.9355
0	4	10	4.4	4.6	-.6094	-.7928
0	4	11	4.1	4.2	-.4708	.8822
0	5	0	3.5	3.3	1.0000	-.0000
0	5	1	3.4	3.6	-.9619	.2735
0	5	2	1.7	2.1	.3117	-.9502
0	5	3	5.6	5.8	-.9227	.3856
0	5	4	3.2	3.6	-.8450	.5347
0	5	5	2.6	2.4	-.4595	-.8882
0	5	6	4.1	4.6	-.0101	-.9999
0	5	7	5.3	5.4	.6471	-.7624
0	5	8	2.6	2.5	.3189	-.9478
0	5	9	3.4	3.7	.8942	-.1071
0	7	4	1.3	1.5	-.0000	-1.0000
0	8	1	1.2	.6	-1.0000	-.0000
0	8	3	1.2	.2	1.0000	.0000
0	8	9	1.0	.3	-1.0000	.0000
0	9	1	1.0	.6	-.0000	1.0000
7	0	1	4.1	4.2	.0000	1.0000
7	0	2	5.6	4.9	1.0000	-.0000
7	0	3	6.9	6.7	.0000	1.0000
7	0	4	3.3	3.6	1.0000	-.0000
7	0	5	1.5	1.5	-.0000	-1.0000
7	0	6	2.2	2.0	-1.0000	.0000
7	0	7	4.1	4.1	-.0000	-1.0000
7	0	8	1.6	1.3	1.0000	.0000
7	0	9	4.5	5.0	.0000	1.0000
7	0	10	2.4	2.4	-1.0000	-.0000
7	1	0	3.6	3.6	.0000	-1.0000
7	1	1	4.6	4.6	.8872	-.4614
7	1	2	5.0	5.1	.9708	.2400
7	1	3	1.7	1.4	.7904	-.6126
7	1	4	4.0	3.8	.6751	.7378
7	1	5	3.5	3.6	-.9985	-.0556
7	1	6	2.5	2.4	.8468	-.5319
7	1	7	3.9	4.0	-.9872	-.1596
7	1	8	2.4	2.2	-.5934	-.8050
7	1	9	3.2	3.2	.0384	.9993
7	1	10	5.5	5.4	-.9914	-.1311
7	2	1	5.5	5.3	.5826	.8267
7	2	2	7.2	6.5	-.9860	-.1565
7	2	3	7.7	7.2	-.8571	.5152
7	2	4	7.4	7.1	-.9591	-.2831
7	2	5	2.5	2.4	.6096	-.7927
7	2	6	3.3	3.1	.9413	.3376
7	2	7	5.7	5.4	.9732	-.2299
7	2	8	4.6	4.7	.9138	.4061
7	2	9	1.6	1.6	-.9799	-.1993
7	3	0	1.0	1.0	.0000	1.0000
7	3	1	1.3	1.4	-.9982	.0596
7	3	2	3.2	2.7	.4129	-.9106
7	3	3	1.1	.6	.8319	.5549
7	3	4	1.9	1.5	.8970	.4420
7	3	5	2.6	2.6	.2556	.9668
7	3	6	3.7	3.9	.2716	.9624
7	3	7	1.8	1.7	.2967	.9550
7	3	8	2.2	2.2	.7194	-.6946
7	4	0	7.5	7.5	-.0000	-1.0000
7	4	1	1.4	1.1	.9828	.1847
7	4	2	3.1	3.2	-.7771	-.6294
7	4	3	2.6	2.8	.9972	.0743
7	4	4	5.3	5.4	.5812	.8409
7	4	5	3.8	3.4	-.9529	-.3032
7	4	6	4.7	4.5	.8364	.5482
7	5	0	2.7	2.7	.0000	-1.0000
7	5	1	3.9	3.5	.6553	-.7553
8	1	0	3.7	3.2	.0000	1.0000
8	1	0	7.1	7.2	1.0000	-.0000
0	0	20	.9	.9	-1.0000	.0000
0	1	6	.7	.4	-.0000	1.0000
0	1	16	1.1	.6	-.0000	1.0000
0	3	18	1.6	.3	-.0000	1.0000
0	4	17	1.0	.1	-1.0000	.0000
0	5	12	1.1	.9	.0000	-1.0000
0	5	14	1.0	.1	.0000	1.0000
0	0	17	.8	.7	1.0000	.0000

UNOBSERVED REFLECTIONS

1	0	11	1.1	1.6	-.0000	-1.0000
1	0	14	1.3	.5	1.0000	.0000
1	0	15	1.3	.5	.0000	-1.0000
1	0	17	.5	1.4	.9652	.2618
1	8	13	.5	4.7	-.7542	.6567
2	0	14	.7	.5	-.7987	.6017
3	0	8	.9	.7	-1.0000	.0000
3	0	10	1.0	.3	1.0000	-.0000
3	0	15	.4	.8	-.1063	-.9943
3	8	9	.5	.2	.7420	.6704
4	0	11	1.1	.0	.0000	-1.0000
4	0	16	.7	.4	-1.0000	.0000
4	1	18	.7	.7	.1422	-.9898
4	0	13	.6	.4	-.5110	-.8596
4	7	0	.9	.0	1.0000	.0000
5	0	8	1.0	.0	-1.0000	-.0000
5	1	14	.6	.0	.2563	.9661
0	0	0	1.2	.0	1.0000	.0000
0	0	2	1.2	.0	-1.0000	-.0000
0	0	13	.7	.2	-.0000	-1.0000
0	2	4	1.0	.0	-.2560	.9667
7	6	0	.6	.4	-.0000	1.0000
0	0	0	.6	.2	1.0000	.0000

A1 = 10.0, A2 = 15.0, B1 = 0.0, B2 = −0.5, and FB = 2.0.
The form factors calculated by Hanson, Herman, Lea and Skillman were used.[10]

After 3 cycles of isotropic refinement anisotropic temperature factors were introduced for the oxygen, nitrogen, and carbon atoms. The C-bonded hydrogen atom positions had been calculated assuming tetrahedral C—H bonds of lengths 1.05 Å. The H-atoms of the NH_3^+-group were localized from a difference Fourier map, and reflections corresponding to $\sin\theta/\lambda < 0.45$ were included in the refinement of hydrogen atoms.

The R-value arrived at for all data (the 36 accidentally absent reflections included with $F_u = \frac{1}{2}(F_o)\text{min}$) was 4.5 %.

A final difference Fourier map, calculated with the observed data and with phases determined by the parameters corresponding to $R = 4.5$ % contained no larger density fluctuations than 0.23 e·Å^{-3}, the E.S.D. of the electron density [11] being $\sigma(\varrho) = 0.06$ e·Å^{-3}.

The fractional atomic coordinates and the thermal vibration parameters arrived at are given in Tables 4, 5, and 6. The expressions for anisotropic and isotropic vibrations, respectively, are:

$$\exp[-B_{11}h^2 + B_{22}k^2 + B_{33}l^2 + B_{12}hk + B_{13}hl + B_{23}kl]$$

and $\exp(-\text{B}\ \sin^2\theta/\lambda^2)$.

A comparison between calculated and observed (and unobserved) data is presented in Table 7 (the unobserved F-values correspond to I_{min}).*

* Eight unobserved reflections have by accident been placed above the heading.

THERMAL MOTIONS

The principal axes of the thermal vibration ellipsoids for the oxygen, nitrogen, and carbon atoms were calculated from the temperature parameters given in Table 5. Root mean square amplitudes for the atomic anisotropic thermal vibrations along the principal axes as well as the components of these axes along the crystal axes are given in Table 8.

Table 8. The principal axes of the thermal vibration ellipsoids given by the components of a unit vector in fractional coordinates, e_x, e_y, e_z; the corresponding r.m.s. amplitudes, and the B-values.

Atom	e_x	e_y	e_z	$(\overline{u^2})^{\frac{1}{2}}$ (Å)	B (Å^2)
	0.025	−0.036	0.057	0.324	8.28
O_1	0.101	−0.089	−0.019	0.226	4.03
	0.120	0.083	0.004	0.149	1.75
	0.050	0.046	−0.052	0.277	6.04
O_2	0.151	−0.009	0.019	0.188	2.80
	0.009	−0.118	−0.022	0.164	2.11
	0.021	−0.021	0.059	0.223	3.94
N	0.134	−0.064	−0.012	0.182	2.62
	0.083	0.108	0.004	0.145	1.67
	0.093	−0.068	0.036	0.188	2.79
C_1	0.085	−0.038	−0.047	0.182	2.63
	0.097	0.099	0.007	0.141	1.56
	0.096	−0.044	−0.043	0.227	4.08
C_2	0.039	−0.099	0.035	0.179	2.53
	0.121	0.066	0.023	0.159	1.99
	0.062	−0.031	−0.053	0.224	3.96
C_3	0.135	−0.036	0.027	0.175	2.42
	0.057	0.118	−0.006	0.155	1.91
	0.060	−0.031	0.053	0.193	2.95
C_4	0.104	−0.077	−0.027	0.180	2.56
	0.104	0.095	−0.004	0.137	1.49
	0.062	−0.015	−0.055	0.241	4.57
C_5	0.111	−0.077	0.022	0.165	2.15
	0.096	0.099	0.009	0.141	1.56
	0.053	−0.008	−0.056	0.242	4.61
C_6	0.136	−0.052	0.020	0.184	2.68
	0.064	0.115	0.005	0.136	1.46
	0.117	−0.032	−0.037	0.218	3.75
C_7	0.066	−0.071	0.043	0.198	3.09
	0.085	0.100	0.018	0.152	1.83
	0.028	−0.010	−0.059	0.209	3.44
C_8	0.151	−0.032	0.011	0.172	2.34
	0.042	0.122	−0.002	0.143	1.62

Since the oscillations of the whole molecule are dependent on the hydrogen bonding system, a rigid-body analysis of translational and librational motion has not been carried out.

DISCUSSION

Interatomic distances and angles of the zwitterion may be found in Fig. 1. The distances and angles between carbon atoms and hydrogen atoms, and those concerning the hydrogen bonding system are presented in Tables 9 and 10. Standard deviations have been calculated from the E.S.D.'s given in

Table 9. Interatomic distances and angles between carbon and hydrogen atoms with their estimated standard deviations (Fig. 1).

Bond	(Å)	σ (Å)
C_1-H_{1a}	0.95	0.02
C_2-H_{2e}	1.03	0.03
C_2-H_{2a}	1.02	0.02
C_3-H_{3e}	1.01	0.02
C_3-H_{3a}	1.00	0.02
C_4-H_{4a}	1.03	0.02
C_5-H_{5e}	1.00	0.03
C_5-H_{5a}	1.07	0.02
C_6-H_{6e}	1.01	0.03
C_6-H_{6a}	1.03	0.02
$C_7-H_{7,1}$	1.08	0.02
$C_7-H_{7,2}$	1.02	0.03

Angle	(°)	σ (°)
$C_7-C_1-H_{1a}$	108	1
$C_2-C_1-H_{1a}$	109	1
$C_6-C_1-H_{1a}$	106	1
$C_1-C_2-H_{2e}$	111	1
$C_1-C_2-H_{2a}$	106	1
$H_{2e}-C_2-H_{2a}$	109	1
$H_{2e}-C_2-C_3$	108	1
$H_{2a}-C_2-C_3$	111	1
$C_2-C_3-H_{3e}$	109	1
$C_2-C_3-H_{3a}$	111	1
$H_{3e}-C_3-H_{3a}$	106	2
$H_{3e}-C_3-C_4$	108	1
$H_{3a}-C_3-C_4$	110	1
$C_3-C_4-H_{4a}$	108	1
$C_8-C_4-H_{4a}$	108	1
$C_5-C_4-H_{4a}$	109	1
$C_4-C_5-H_{5e}$	111	1
$C_4-C_5-H_{5a}$	109	1
$H_{5e}-C_5-H_{5a}$	107	2
$H_{5e}-C_5-C_6$	112	1
$H_{5a}-C_5-C_6$	105	1
$C_5-C_6-H_{6e}$	111	2
$C_5-C_6-H_{6a}$	113	1
$H_{6e}-C_6-H_{6a}$	106	2
$H_{6e}-C_6-C_1$	108	2
$H_{6a}-C_6-C_1$	108	1
$C_1-C_7-H_{7,1}$	109	1
$C_1-C_7-H_{7,2}$	113	1
$H_{7,1}-C_7-H_{7,2}$	111	2
$H_{7,1}-C_7-N$	105	1
$H_{7,2}-C_7-N$	106	1

Tables 4 and 6 without taking into account the standard deviations of the cell parameters.

Fig. 1 shows that all C—C distances are equal within probable limits of error, the average value being 1.529 Å. Regarding the distances as independently determined, the corresponding estimated standard deviation is 0.0011 Å. The angles $C_2-C_3-C_4$ and $C_4-C_5-C_6$ are significantly larger than the four other angles of the six-membered ring.

The $C_4C_8O_1O_2^-$ group is almost planar. Perpendicular distances from the least-squares plane through these atoms are:

C_4	−0.015 Å
C_8	0.003 »
O_1	0.005 »
O_2	0.006 »

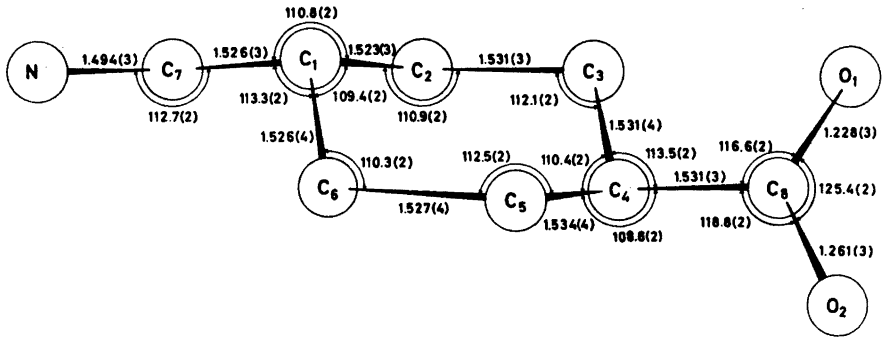


Fig. 1. Schematical drawing of the zwitterion.

The least squares plane defined by the atoms C_2, C_3, C_5, C_6 gives the following fit:

C_2	−0.004 Å
C_3	0.002 »
C_5	−0.002 »
C_6	0.002 »

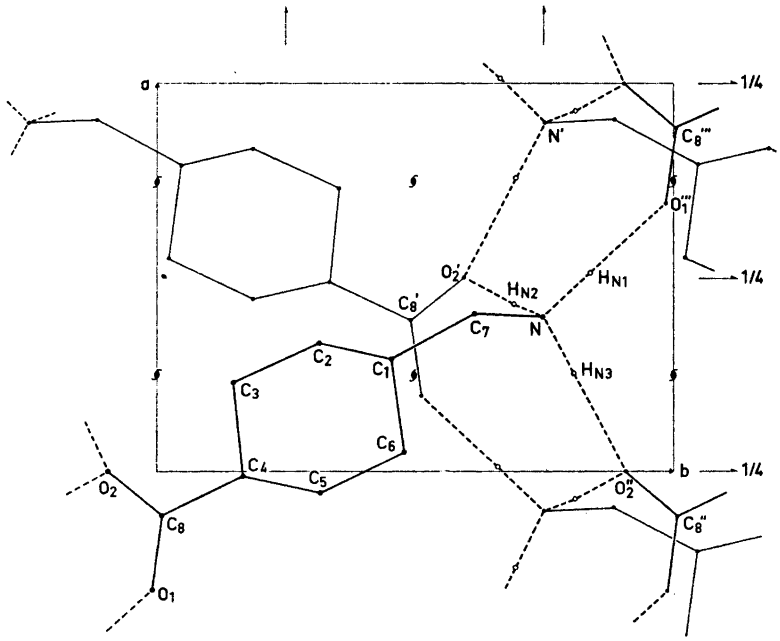


Fig. 2. Part of the structure viewed along [001].

The angle between these two planes is 51.5°, corresponding closely to the value obtained for the hydrobromide.[3]

The significant difference between the two C—O bond lengths may possibly be explained[12] by the fact that O_1 is engaged in one, and O_2 in two hydrogen bonds. The C—N bond length, 1.49_4 Å, agrees with the standard value, found in the terminal C—NH_3^+ bond.[13]

Each zwitterion is linked to six others by hydrogen bonds from N to O forming infinite double layers normal to the *c*-axis. A fragment of one such layer is shown in Fig. 2, where the structure is viewed along [001]. The two hydrogen bonds in which O_2 is engaged do not differ significantly in length (2.79_5 Å and 2.79_4 Å), while the single hydrogen bond to O_1 is considerably shorter (2.72_4 Å). The arrangement around the nitrogen atom is approximately

Table 10. Interatomic distances and angles concerning the hydrogen bonding system, and their estimated standard deviations (Fig. 2).

Bond	(Å)	σ (Å)
$N-O_2'$	2.795	0.002
$N-O_2''$	2.794	0.003
$N-O_1'''$	2.724	0.003
$N-N_{N1}$	0.95	0.02
$N-H_{N2}$	1.06	0.02
$N-H_{N3}$	1.03	0.02

Angle	(°)	σ (°)
C_7-N-O_2'	108.7	0.1
C_7-N-O_2''	113.3	0.1
C_7-N-O_1'''	109.2	0.1
$O_2'-N-O_2''$	108.5	0.1
$O_2'-N-O_1'''$	108.9	0.1
$O_2''-N-O_1'''$	108.3	0.1
$N-O_2'-C_8'$	126.0	0.2
$N-O_2''-C_8''$	138.6	0.1
$N-O_1'''-C_8'''$	135.1	0.2
$N-O_2'-N'$	95.3	0.1

Angle	(°)	σ (°)
C_7-N-H_{N1}	106	1
C_7-N-H_{N2}	107	1
C_7-N-H_{N3}	114	1
$H_{N1}-N-H_{N2}$	113	2
$H_{N1}-N-H_{N3}$	109	2
$H_{N2}-N-H_{N3}$	107	2
$N-H_{N1}\cdots O_1'''$	176	2
$N-H_{N2}\cdots O_2'$	175	2
$N-H_{N3}\cdots O_2''$	177	2

tetrahedral and the hydrogen bonds nearly linear, the N—H---O angles being 176°, 175°, and 177°, respectively.

The hydrogen atom, H_{N1}, associated with the shorter hydrogen bond, seems to be situated closer to the nitrogen atom than the H-atoms of the two longer bonds. According to the large standard deviations, this cannot, however, be stated with confidence.

REFERENCES

1. Melander, B., Gliniecki, G., Granstrand, B. and Hanshoff, G. *Acta Pharmacol. Toxicol.* **22** (1965) 340.
2. Groth, P. and Hassel, O. *Acta Chem. Scand.* **19** (1965) 1709.
3. Kadoya, S., Hanazaki, F. and Iitaka, Y. *Acta Cryst.* **21** (1966) 38.
4. Cochran, W. and Douglas, A. S. *Proc. Roy Soc. (London)* **227** (1954) 486.
5. Cochran, W. and Douglas, A. S. *Proc. Roy. Soc. (London)* **243** (1958) 281.

6. Hughes, E. W. *Acta Cryst.* **6** (1953) 871.
7. Groth, P. *Acta Chem. Scand.* **20** (1966) 1421.
8. Stanley, E. *Acta Cryst.* **17** (1964) 1028.
9. Gantzel, P. K., Sparks, R. A. and Trueblood, K. N. *IUCr World List of Crystallographic Computer Programs*, No. 384.
10. Hanson, H. P., Herman, F., Lea, J. D. and Skillman, S. *Acta Cryst.* **17** (1964) 1040.
11. Cruickshank, D. W. J. *Acta Cryst.* **2** (1949) 65.
12. Hvoslef, J. *Acta Cryst.* **B 24** (1968) 23.
13. Hahn, T. *Z. Krist.* **109** (1957) 438.

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