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The Crystal Structures of *trans*- and *cis*-4-Aminomethylcyclohexane-1-carboxylic Acid Hydrohalides

By Shizuo Kadoya*, Fumie Hanazaki and Yoichi Iitaka

Faculty of Pharmaceutical Sciences, University of Tokyo, Hongo, Tokyo, Japan

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The crystal structures of *trans*-4-aminomethylcyclohexane-1-carboxylic acid hydrobromide and *cis*-4-aminomethylcyclohexane-1-carboxylic acid hydrochloride have been determined by X-ray diffraction methods. The hydrobromide of the *trans* form crystallizes in the monoclinic space group $P2_1/a$, $Z=4$, with the unit-cell dimensions $a=10\cdot75$, $b=10\cdot50$, $c=10\cdot13$ Å, $\beta=117\cdot7°$. The hydrochloride of the *cis* form crystallizes in the monoclinic space group $P2_1/n$, $Z=4$, with the unit cell-dimensions $a=14\cdot52$, $b=6\cdot44$, $c=10\cdot83$ Å, $\beta=98\cdot4°$. Refinement has been carried out by the full-matrix least-squares method with three-dimensional intensity data.

In these crystals, the molecules are found to exist in the chair form with an equatorial aminomethyl group. In the *trans* form, the carboxyl group is equatorial and the plane of the carboxyl group is roughly perpendicular to the mean plane of the cyclohexane ring. In the *cis* form, the carboxyl group is axial and the orientation of the carboxyl plane is such that one of the carboxyl oxygen atoms is almost eclipsed by a carbon atom of the cyclohexane ring.

Introduction

4-Aminomethylcyclohexane-1-carboxylic acid (NH_2–CH_2–C_6H_{10}–COOH, hereafter referred to as AMCHA) was found to have a predominant inhibitory effect when used as an antiplasmin agent (Okamoto & Okamoto, 1962). Recently, Shimizu, Naito, Okano & Aoyagi (1965) separated two stereoisomers of this compound and found that one of the isomers has a potent inhibitory effect while the other exibits only a negligible activity. They also suggested, on the basis of chemical reactions, that the former takes the *trans* configuration while the latter is in the *cis* form. The present X-ray study is conducted to confirm their conclusion and to obtain a further precise knowledge of the configuration and conformation of these isomers.

Experimental

A mixture of the two isomers of AMCHA was prepared by hydrolysis of the product obtained by the high-pressure catalytic hydrogenation of *p*-(*N*-acetamidomethyl)benzoic acid over Raney nickel. The mixture was then separated into the two isomers by treatment with cupric carbonate in an aqueous solution followed by removal of the metal ion (Shimizu, Naito, Okano & Aoyagi, 1965). Various hydrohalides of AMCHA were examined by X-ray diffraction and it was found that *trans*-AMCHA . HBr and *cis*-AMCHA . HCl were the most suitable for X-ray analysis.

The crystals of *trans*-AMCHA . HBr were obtained from an aqueous solution as well developed tabular crystals and those of *cis*-AMCHA . HCl were obtained from aqueous acetone as well developed prismatic crystals.

The lattice constants were determined for both substances from *hk*0, 0*kl* and *h*0*l* precession photographs taken with Cu *Kα* radiation. Three-dimensional intensity data were collected by the multiple film equi-inclination Weissenberg method with Cu *Kα* radiation. Intensities were measured visually with the aid of a calibrated intensity scale. These values were corrected for Lorentz and polarization factors, but no corrections were made for absorption of X-rays in view of the small size of the specimens. The observed values of the structure factors were then correlated and put on a common scale. The densities were measured by the

Table 1. *Crystallographic data*

	trans–AMCHA . HBr	*cis*–AMCHA . HCl
m.p.	227–229 °C (*d*)	195–197 °C (*d*)
System	Monoclinic	Monoclinic
a	10·75 ± 0·01 Å	14·52 ± 0·02 Å
b	10·50 ± 0·01	6·44 ± 0·005
c	10·13 ± 0·01	10·83 ± 0·01
β	117·7 ± 0·2°	98·4 ± 0·2°
U	1012·4 Å^3	1003·2 Å^3
Z	4	4
Space group	$P2_1/a$	$P2_1/n$
D_m	1·554 g.cm^{-3}	1·306 g.cm^{-3}
D_x	1·559 g.cm^{-3}	1·281 g.cm^{-3}
Linear absorption coefficient	59·2 cm^{-1}	33·5 cm^{-1}
Systematic absences		
*h*0*l*	$h=2n+1$	$h+l=2n+1$
0*k*0	$k=2n+1$	$k=2n+1$

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* Permanent address: Central Research Laboratory, Daiichi Seiyaku Co. Ltd., Minamifunabori-cho, Edogawa-ku, Tokyo.

flotation method with a mixture of carbon tetrachloride and benzene. The crystallographic data are given in Table 1.

Some of the experimental details are summarized in Table 2.

For the present structure determination the following atomic scattering factors were used: for carbon, nitrogen and oxygen atoms, those of Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955), for the chlorine atom, those of Dawson (1960) and for the bromine atom, those cited as SX-71 in *International Tables for X-ray Crystallography* (1962, p. 202).

Determination and refinement of the structures

trans-AMCHA.HBr

A three-dimensional sharpened Patterson synthesis yielded the coordinates of the bromine atom. A three-dimensional Fourier map with signs determined by the bromine atom showed all eleven light atoms clearly. The structure factor calculation including all of these atoms gave the R index 0·21. The correctness of the structure was confirmed by calculating the second Fourier map. The refinement was carried out by three cycles of least-squares calculations with a diagonal approximation. The R value decreased from 0·21 to 0·16. At this point, three cycles of full-matrix least-squares refinement was started with the program ORFLS by Busing, Martin & Levy (1962) by assuming individual isotropic thermal vibrations and the equal weight of observed F's. The R index finally stands at 0·136 excluding unobserved structure factors. The final atomic parameters and their standard deviations are listed in Table 3. Observed and calculated structure factors are listed in Table 5. The mean values of the coordinate shifts and the standard deviations σ, obtained in the

Table 2. *Experimental details*

	Size of the specimens (mm) Cross-section	Length	Photographed layers	Number of independent reflexions observed ($F_o \neq 0$)
trans-AMCHA . HBr				
b-axis	0·1 × 0·2	0·2	*h*0*l* – *h*4*l*	1125
c-axis	0·1 × 0·1	0·4	*hk*0 – *hk*5	
cis-AMCHA . HCl				
a-axis	0·08 × 0·2	0·25	0*kl* – 4*kl*	1268
b-axis	0·1 × 0·3	0·15	*h*0*l* – *h*5*l*	

Table 3. *trans*-AMCHA . HBr.
Final fractional atomic coordinates and temperature factors and their standard deviations

	x/a $\sigma(x)$ (Å)	y/b $\sigma(y)$ (Å)	z/c $\sigma(z)$ (Å)	B $\sigma(B)$ (Å^2) (Å^2)
Br	0·2588 ± 0·0023	0·5336 ± 0·0021	0·9347 ± 0·0023	4·49 ± 0·06
O(1)	0·2572 ± 0·0158	0·3847 ± 0·0150	0·2068 ± 0·0158	5·28 ± 0·31
O(2)	0·4693 ± 0·0142	0·3035 ± 0·0135	0·2905 ± 0·0142	4·41 ± 0·27
N	0·4709 ± 0·0169	0·2753 ± 0·0162	1·0063 ± 0·0176	4·21 ± 0·32
C(1)	0·3472 ± 0·0204	0·2795 ± 0·0197	0·4399 ± 0·0208	3·95 ± 0·36
C(2)	0·4115 ± 0·0223	0·3897 ± 0·0214	0·5580 ± 0·0227	4·61 ± 0·41
C(3)	0·3912 ± 0·0228	0·3546 ± 0·0218	0·6951 ± 0·0230	4·79 ± 0·42
C(4)	0·4575 ± 0·0187	0·2211 ± 0·0181	0·7570 ± 0·0190	3·36 ± 0·33
C(5)	0·4029 ± 0·0232	0·1152 ± 0·0222	0·6404 ± 0·0236	4·97 ± 0·44
C(6)	0·4233 ± 0·0226	0·1512 ± 0·0218	0·5036 ± 0·0230	4·74 ± 0·42
C(7)	0·3653 ± 0·0214	0·3215 ± 0·0203	0·3034 ± 0·0204	4·18 ± 0·38
C(8)	0·4279 ± 0·0204	0·1792 ± 0·0196	0·8887 ± 0·0206	3·97 ± 0·36

Table 4. *cis*-AMCHA . HCl.
Final fractional atomic coordinates and temperature factors and their standard deviations

	x/a $\sigma(x)$ (Å)	y/b $\sigma(y)$ (Å)	z/c $\sigma(z)$ (Å)	B $\sigma(B)$ (Å^2) (Å^2)
Cl	0·2348 ± 0·0031	0·1707 ± 0·0035	0·4011 ± 0·0031	3·99 ± 0·07
O(1)	0·5391 ± 0·0093	0·4821 ± 0·0101	0·8612 ± 0·0092	5·34 ± 0·21
O(2)	0·5954 ± 0·0105	0·7855 ± 0·0112	0·9183 ± 0·0103	6·43 ± 0·25
N	0·2794 ± 0·0093	0·6466 ± 0·0103	0·3885 ± 0·0091	3·68 ± 0·19
C(1)	0·4317 ± 0·0116	0·7694 ± 0·0125	0·8587 ± 0·0114	3·64 ± 0·23
C(2)	0·3577 ± 0·0121	0·6120 ± 0·0129	0·8027 ± 0·0119	3·94 ± 0·25
C(3)	0·3629 ± 0·0119	0·5659 ± 0·0130	0·6634 ± 0·0119	3·95 ± 0·24
C(4)	0·3592 ± 0·0113	0·7728 ± 0·0124	0·5904 ± 0·0112	3·58 ± 0·23
C(5)	0·4379 ± 0·0123	0·9173 ± 0·0132	0·6421 ± 0·0121	4·02 ± 0·25
C(6)	0·4301 ± 0·0128	0·9692 ± 0·0140	0·7801 ± 0·0126	4·47 ± 0·26
C(7)	0·5261 ± 0·0127	0·6856 ± 0·0140	0·8807 ± 0·0122	4·25 ± 0·25
C(8)	0·3670 ± 0·0119	0·7315 ± 0·0127	0·4510 ± 0·0116	3·87 ± 0·24

last least-squares cycle, were as follows: for bromine, shifts $\simeq 0{\cdot}0004$ Å, $\sigma \simeq 0{\cdot}0022$ Å; for carbon, nitrogen and oxygen, shifts $\simeq 0{\cdot}0017$ Å, $\sigma \simeq 0{\cdot}0197$ Å. The superimposed electron density map illustrating the structure of *trans*-AMCHA . HBr is shown in Fig. 1.

cis-AMCHA . HCl

A three-dimensional sharpened Patterson synthesis yielded the five sets of possible positions for chlorine atoms. The possibilities were reduced to two from stereochemical considerations as well as the several two-dimensional Fourier syntheses calculated by assuming the contributions of the chlorine atoms. These considerations suggested the most probable coordinates of the chlorine atom as $x=0{\cdot}24$, $y=0{\cdot}17$, $z=0{\cdot}40$. A subsequent three-dimensional Fourier synthesis using the signs calculated on the basis of the chlorine atom indicated twenty-five peaks of height 4 to 6 e.Å^{-3}. Here again, structural considerations served for locating all the eleven light atoms, and made it possible to prepare the second three-dimensional Fourier map. The R values at this stage were 0·31 including unobserved structure factors and 0·25 excluding them. An approximate structure of *cis*-AMCHA . HCl was thus established.

Refinement of the structure was then carried out by five cycles of diagonal least-squares calculations. The R value decreased from 0·25 to 0·153. Refinement was further continued by two cycles of full-matrix least-squares calculations with the program ORFLS. Individual isotropic thermal parameters were included for this calculation and equal weight was given to each of the observed F's. The R value finally stands at 0·152 excluding unobserved structure factors. The final atomic parameters and their standard deviations are listed in Table 4. Observed and calculated structure factors are listed in Table 6. The mean values of the coordinate shifts and the standard deviations obtained in the least-squares cycle were: for chlorine, shifts $\simeq 0{\cdot}0010$ Å, $\sigma \simeq 0{\cdot}0032$ Å; for carbon, nitrogen and oxygen, shifts $\simeq 0{\cdot}0033$ Å, $\sigma \simeq 0{\cdot}0117$ Å. The superimposed electron density map illustrating the structure of *cis*-AMCHA . HCl is shown in Fig. 2.

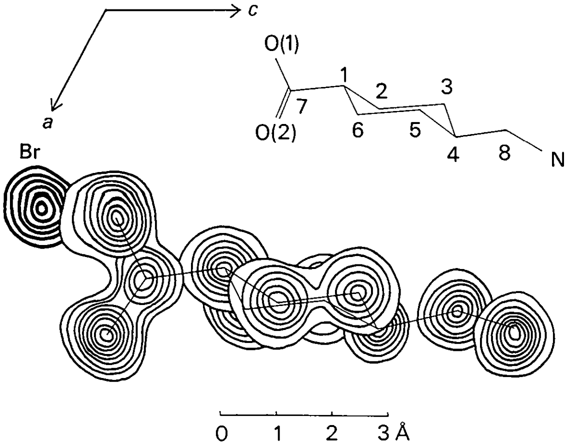


Fig. 1. *trans*-AMCHA . HBr. Composite electron density map in the **b** direction. Contours are drawn for light atoms at 1, 2, 3 e.Å^{-3}..., and for bromine at 10, 20, 30 e.Å^{-3}....

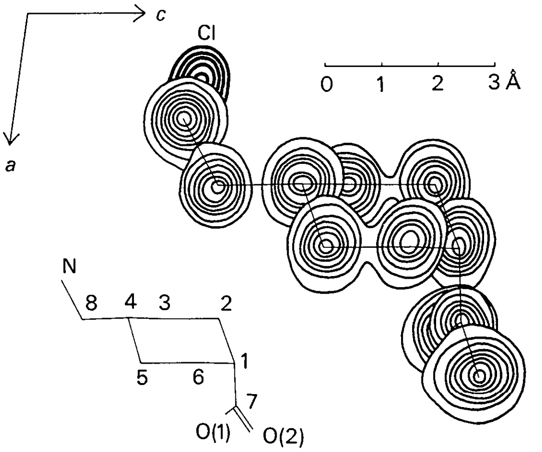
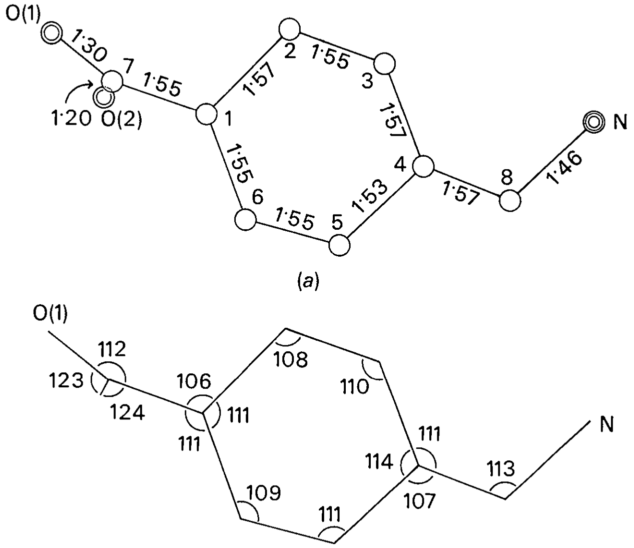


Fig. 2. *cis*-AMCHA . HCl. Composite electron density map in the **b** direction. Contours are drawn for light atoms at 1, 2, 3 e.Å^{-3}..., and for chlorine at 5, 10, 15 e.Å^{-3}.



(*a*)

(*b*)

Fig. 3. *trans*-AMCHA . HBr. (*a*) Bond lengths (Å) and (*b*) angles (°) of the *trans*-AMCHA molecule found in the hydrobromide.

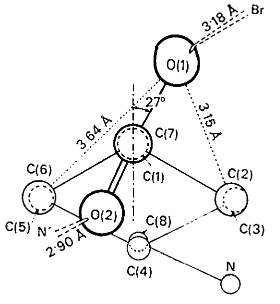


Fig. 4. *trans*-AMCHA . HBr. Projection of the molecule along the C(7)–C(1) bond showing the orientation of the carboxyl group and the aminomethyl group.

Table 5. *Observed and calculated structure factors for trans-*AMCHA . HBr

H	K	L	$\|F_o\|$	F_c
2	0	0	46.71	-49.91
4	0	0	89.46	77.57
5	0	0	11.51	0.00
6	0	0	71.51	-71.47
8	0	0	28.86	32.57
10	0	0	18.75	-20.86
1	1	0	18.57	17.94
2	1	0	121.77	122.30
3	1	0	28.04	-24.67
4	1	0	51.07	55.35
5	1	0	23.08	22.96
6	1	0	6.86	5.70
7	1	0	11.78	-9.82
8	1	0	10.80	10.25
9	1	0	13.13	14.76
0	2	0	6.92	2.78
1	2	0	6.05	-6.89
2	2	0	132.03	-153.22
3	2	0	21.85	21.14
4	2	0	67.34	65.32
5	2	0	24.33	-25.71
6	2	0	51.35	-53.02
7	2	0	3.07	11.17
8	2	0	24.70	27.74
12	2	0	3.86	8.89
1	3	0	12.90	-14.39
2	3	0	7.07	-7.96
3	3	0	1.82	-1.63
4	3	0	3.32	5.61
5	3	0	3.56	3.71
6	3	0	23.32	-23.05
7	3	0	21.01	-26.46
8	3	0	6.92	-11.09
0	4	0	23.24	29.17
1	4	0	75.71	-75.99
2	4	0	37.86	-35.75
3	4	0	51.87	48.90
4	4	0	55.10	55.53
5	4	0	25.27	-25.17
6	4	0	3.44	-1.41
7	4	0	17.46	18.95
8	4	0	10.85	12.76
9	4	0	17.99	-22.89
10	4	0	11.17	-14.10
1	5	0	15.46	17.54
2	5	0	33.28	-27.49
3	5	0	9.10	-4.76
5	5	0	10.65	13.11
7	5	0	10.68	7.03
8	5	0	16.00	19.48
0	6	0	24.82	25.25
1	6	0	58.75	-61.31
2	6	0	12.82	-11.21
3	6	0	63.01	60.48
5	6	0	45.91	-42.95
6	6	0	11.85	-12.44
7	6	0	27.94	31.02
1	7	0	10.30	-10.46
0	8	0	4.96	-1.44
1	8	0	41.57	-45.49
3	8	0	37.02	32.51
5	8	0	27.44	-29.60
7	8	0	14.58	14.82
0	10	0	9.27	-5.86
1	10	0	16.91	-17.28
2	10	0	10.61	13.79
3	10	0	22.82	17.42
5	10	0	14.32	-12.01
0	12	0	15.53	-15.92
1	12	0	4.25	-7.45
2	12	0	5.81	9.82
3	12	0	6.65	6.73
4	12	0	10.35	-10.81
0	0	1	71.09	73.75
2	0	1	123.28	-121.47
4	0	1	95.10	86.78
6	0	1	43.96	-40.78
7	0	1	6.15	0.00
8	0	1	29.67	36.82
10	0	1	6.46	-13.15
-2	0	1	71.41	-85.73
-4	0	1	142.98	151.45
-5	0	1	7.48	0.00
-6	0	1	45.62	-42.31
-8	0	1	10.14	12.48
-9	0	1	11.19	0.00
-10	0	1	18.17	-20.37
0	1	1	7.90	-17.73
1	1	1	15.58	-18.28
2	1	1	2.71	-2.92
3	1	1	21.21	21.42
4	1	1	11.39	-15.80
5	1	1	6.15	5.60
10	1	1	9.56	4.43
-1	1	1	19.29	19.99
-2	1	1	89.30	93.67
-3	1	1	47.13	-46.03
-4	1	1	42.14	-36.87
-5	1	1	38.25	34.43
-6	1	1	20.43	-20.80
-7	1	1	34.57	-33.36
-8	1	1	19.62	-18.88
-9	1	1	15.80	17.59
-11	1	1	6.75	-11.74
0	2	1	87.69	97.67
1	2	1	72.33	-80.76
2	2	1	114.60	-114.39
3	2	1	21.50	18.59
4	2	1	53.32	56.30
5	2	1	22.75	-21.14
6	2	1	32.32	-33.75
7	2	1	10.75	14.55
8	2	1	19.70	23.66
10	2	1	11.82	-16.82
-1	2	1	12.53	11.51
-2	2	1	108.29	-105.00
-3	2	1	31.63	-29.07
-4	2	1	49.39	37.82
-5	2	1	2.28	6.90
-6	2	1	40.11	-37.83
-7	2	1	10.80	-11.71
-8	2	1	28.66	27.91
-9	2	1	4.09	8.68
-10	2	1	8.55	-10.14
-12	2	1	5.32	5.78
0	3	1	13.25	-17.50
1	3	1	51.54	-49.63
2	3	1	20.53	18.11
3	3	1	3.10	-4.52
4	3	1	40.11	-45.74
5	3	1	20.37	-20.89
8	3	1	7.57	5.50
-1	3	1	66.09	74.95
-2	3	1	76.16	66.28
-3	3	1	45.64	-38.92
-4	3	1	26.91	-23.64
-5	3	1	48.05	45.15
-6	3	1	33.92	31.81
-7	3	1	16.21	-14.79
-8	3	1	16.70	-18.79
-9	3	1	19.45	22.34
-10	3	1	10.11	13.38
-11	3	1	6.07	-11.55
0	4	1	81.10	83.30
1	4	1	13.60	-14.40
2	4	1	7.17	-8.67
3	4	1	67.67	60.17
4	4	1	39.17	38.54
5	4	1	36.14	-37.13
6	4	1	34.03	-40.10
7	4	1	20.07	23.78
8	4	1	7.72	10.38
9	4	1	10.10	-15.59
-1	4	1	81.86	85.55
-2	4	1	39.85	-37.89
-3	4	1	42.32	-38.44
-4	4	1	30.50	23.51
-5	4	1	40.39	43.50
-6	4	1	27.58	-23.53
-7	4	1	14.63	-16.79
-8	4	1	16.18	15.69
0	5	1	29.62	-25.42
1	5	1	16.22	-13.87
2	5	1	26.56	22.00
3	5	1	48.66	39.32
4	5	1	14.68	12.85
7	5	1	11.21	8.17
-1	5	1	16.34	12.04
-2	5	1	18.59	14.33
-3	5	1	34.09	-34.99
-4	5	1	32.58	-29.98
-5	5	1	16.67	15.07
-6	5	1	24.70	25.31
-7	5	1	20.07	-25.57
-8	5	1	9.14	-14.57
0	6	1	8.56	12.48
1	6	1	50.12	-82.64
2	6	1	22.47	-16.46
3	6	1	42.32	37.52
4	6	1	11.58	9.41
5	6	1	31.36	-31.34
7	6	1	20.21	21.14
-1	6	1	44.37	37.92
-2	6	1	25.89	-22.60
-3	6	1	53.83	-50.81
-5	6	1	26.64	27.01
-6	6	1	10.86	-10.53
-7	6	1	18.29	-23.00
-9	6	1	11.85	13.61
0	7	1	25.96	-26.12
3	7	1	8.55	-15.93
5	7	1	9.11	-5.98
-1	7	1	7.80	8.20
-2	7	1	7.96	4.79
-3	7	1	11.63	3.19
-4	7	1	20.96	-20.49
-6	7	1	19.37	17.69
0	8	1	10.48	-8.56
1	8	1	27.41	-24.32
3	8	1	32.53	35.91
5	8	1	20.35	-25.92
7	8	1	11.28	15.39
-1	8	1	44.57	41.71
-2	8	1	10.61	9.26
-3	8	1	31.86	-28.83
-5	8	1	25.07	26.51
-7	8	1	13.80	-13.18
-9	8	1	8.22	9.05
1	9	1	6.42	9.61
-1	9	1	9.06	-7.57
-2	9	1	23.23	21.43
-3	9	1	11.21	11.08
-4	9	1	11.19	-13.29
-6	9	1	10.57	14.03
-7	9	1	7.96	2.78
0	10	1	6.42	-11.78
1	10	1	24.85	-18.81
2	10	1	15.53	12.67
3	10	1	17.51	15.96
5	10	1	9.46	-11.13
-1	10	1	22.32	18.25
-2	10	1	11.10	8.50
-3	10	1	21.97	-20.02
-2	11	1	11.88	9.72
1	12	1	8.67	-9.75
2	12	1	12.63	11.21
-4	12	1	10.68	-9.57
-5	12	1	9.15	9.43
0	0	2	64.02	55.78
2	0	2	50.96	-60.57
4	0	2	41.50	42.81
6	0	2	31.58	-39.91
8	0	2	6.09	8.07
10	0	2	6.50	-10.14
-2	0	2	51.39	-51.58
-4	0	2	25.54	21.60
-6	0	2	15.74	-14.39
-8	0	2	20.70	16.37
0	1	2	6.26	-5.09
1	1	2	70.80	-73.16
2	1	2	21.25	21.97
3	1	2	45.79	44.85
4	1	2	13.82	-9.84
5	1	2	20.07	-18.96
7	1	2	9.09	10.69
-1	1	2	68.00	70.14
-2	1	2	33.36	36.23
-3	1	2	83.11	-77.21
-4	1	2	21.45	-16.34
-5	1	2	63.98	57.03
-6	1	2	34.85	29.17
-7	1	2	42.76	-40.89
-8	1	2	3.54	-8.67
-9	1	2	27.44	29.35
-11	1	2	10.72	-14.03
0	2	2	67.69	71.99
1	2	2	59.39	-58.01
2	2	2	31.96	-28.76
3	2	2	26.75	23.30
4	2	2	45.59	50.51
5	2	2	22.47	-19.57
6	2	2	28.36	-31.48
7	2	2	20.00	22.07
8	2	2	15.43	21.47
-1	2	2	59.96	60.09
-2	2	2	75.00	-73.85
-3	2	2	33.48	-28.47
-4	2	2	35.51	33.85
-5	2	2	31.79	30.21
-6	2	2	30.08	-25.17
-7	2	2	3.14	-6.19
-9	2	2	3.94	6.85
0	3	2	96.01	-90.35
1	3	2	39.86	-33.86
2	3	2	28.82	29.28
3	3	2	35.23	29.41
5	3	2	30.67	-31.55
6	3	2	12.42	18.33
7	3	2	12.90	11.88
-1	3	2	87.38	84.49
-2	3	2	46.78	40.10
-3	3	2	74.66	-63.04
-4	3	2	55.64	-46.53
-5	3	2	55.24	50.94
-6	3	2	39.78	34.42
-7	3	2	38.78	-40.85
-8	3	2	21.60	-21.58
-9	3	2	17.75	19.36
-10	3	2	12.55	14.21
-11	3	2	9.68	-14.78
0	4	2	47.00	50.89
1	4	2	42.99	-38.11
2	4	2	71.83	-70.04
3	4	2	47.39	50.50
4	4	2	26.36	26.52
5	4	2	28.61	-31.38
6	4	2	12.10	-13.25
7	4	2	3.36	8.13
8	4	2	13.28	20.69
9	4	2	6.46	-12.12
-1	4	2	34.63	31.76
-2	4	2	37.50	-29.57
-3	4	2	53.39	-44.50
-4	4	2	40.19	35.77
-5	4	2	17.34	13.46
-6	4	2	19.89	-14.11
-7	4	2	14.32	-14.71
-8	4	2	13.07	12.39
-11	4	2	4.53	-0.03
0	5	2	33.69	-35.67
1	5	2	35.48	-34.83
2	5	2	32.14	34.21
3	5	2	23.20	19.90
4	5	2	27.23	-29.75
-1	5	2	38.88	32.98
-2	5	2	37.09	37.36
-3	5	2	38.07	-32.70
-4	5	2	46.91	-39.03
-5	5	2	30.17	27.91
-6	5	2	32.53	37.35
-7	5	2	17.09	-14.74
-8	5	2	25.73	-24.66
-9	5	2	11.63	14.58
-10	5	2	10.65	11.24
1	6	2	26.75	-21.46
2	6	2	14.26	-22.09
3	6	2	30.23	27.80
5	6	2	15.54	-18.56
7	6	2	15.58	21.28
-1	6	2	29.78	28.60
-3	6	2	30.82	-28.94
-4	6	2	23.71	20.36
-5	6	2	16.04	15.17
-6	6	2	12.63	-9.75
-10	6	2	6.98	-2.18
0	7	2	17.14	-12.96
1	7	2	12.95	-11.21
2	7	2	28.46	24.57
4	7	2	15.53	-21.42
-1	7	2	15.38	-17.06
-2	7	2	49.62	49.52
-4	7	2	35.11	-34.93
-5	7	2	5.67	5.92
-6	7	2	19.45	19.13
-8	7	2	15.13	-15.20
-10	7	2	9.82	14.91
1	8	2	33.71	-36.92
2	8	2	20.10	21.29
3	8	2	15.59	12.05
4	8	2	8.34	1.92
5	8	2	15.20	-18.89
-1	8	2	30.10	27.73
-4	8	2	14.21	-11.63
-5	8	2	20.42	17.10
0	9	2	37.71	-29.37
1	9	2	13.20	19.55
2	9	2	16.70	15.32
4	9	2	8.00	-6.85
6	9	2	10.57	9.59
-1	9	2	5.85	7.98
-2	9	2	17.66	16.89
-3	9	2	14.46	13.66
-4	9	2	20.46	-22.99
-5	9	2	11.69	-10.82
-6	9	2	16.03	16.07
-8	9	2	12.43	-15.53
0	10	2	11.67	-12.25
3	10	2	16.42	19.28
4	10	2	7.23	-10.46
5	10	2	6.47	-10.00
-1	10	2	8.26	11.35
-3	10	2	20.05	-19.71
-4	10	2	9.82	-9.36
-7	10	2	10.21	-10.03
0	11	2	13.18	-11.42
2	11	2	7.15	8.15
4	11	2	5.96	-6.16
-1	11	2	15.32	-15.82
-2	11	2	10.75	10.89
-3	11	2	5.25	6.50
-5	11	2	11.57	-12.05
-6	11	2	11.92	14.31
0	12	2	6.38	-6.02
-1	12	2	7.90	6.78
-2	12	2	10.10	9.31
-3	12	2	6.14	-3.75
-5	12	2	5.00	4.57
0	0	3	53.71	52.04
2	0	3	19.70	-18.23
4	0	3	17.24	14.64
6	0	3	13.74	-13.10
8	0	3	16.67	23.89
-2	0	3	35.38	32.38
-4	0	3	30.04	24.92
-6	0	3	29.58	23.69
-8	0	3	8.00	-6.11
-12	0	3	9.39	-10.33
1	1	3	79.57	-75.79
2	1	3	27.50	27.03
3	1	3	63.75	62.90
4	1	3	5.42	-0.68
5	1	3	37.50	-38.84
7	1	3	17.54	19.78
-1	1	3	109.94	123.06
-2	1	3	13.05	11.52
-3	1	3	106.22	-97.68
-4	1	3	23.73	-20.86
-5	1	3	91.77	93.61
-7	1	3	55.78	-48.82
-8	1	3	17.09	-17.28
-9	1	3	33.35	33.53
-11	1	3	16.00	-19.38
0	2	3	6.57	5.82
1	2	3	13.89	-9.30
2	2	3	43.68	-46.33
3	2	3	37.52	37.06
4	2	3	21.99	19.17
5	2	3	5.21	-5.16
6	2	3	18.33	-21.46
7	2	3	9.00	10.92
-1	2	3	18.21	18.21
-2	2	3	32.32	-31.23
-3	2	3	38.69	-32.35
-4	2	3	14.24	-11.98
-5	2	3	13.47	12.13
-6	2	3	11.86	-9.46
-8	2	3	3.69	-5.88
0	3	3	11.46	-16.60
1	3	3	84.52	-83.70
2	3	3	28.11	31.00
3	3	3	30.85	29.04
4	3	3	23.00	-28.51
5	3	3	16.95	-16.36
7	3	3	14.12	15.10
-1	3	3	22.54	25.92
-2	3	3	45.64	44.44
-3	3	3	83.86	-68.30
-4	3	3	44.18	-35.23
-5	3	3	51.94	46.53
-6	3	3	46.83	39.32
-7	3	3	43.26	-41.56
-8	3	3	16.74	-16.07
-9	3	3	18.41	16.98
-10	3	3	10.57	13.51
-11	3	3	10.47	-14.01
0	4	3	26.90	29.32
1	4	3	42.28	-38.45
4	4	3	28.11	32.23
5	4	3	22.14	-26.88
6	4	3	3.88	-11.74
7	4	3	6.53	7.59
-1	4	3	27.02	29.95
-2	4	3	30.82	-27.14
-3	4	3	3.64	4.14
-4	4	3	27.32	22.34
-5	4	3	9.84	7.68
-6	4	3	4.75	-8.21
-8	4	3	2.62	-4.72
-11	4	3	5.84	8.39
0	5	3	82.06	-70.60
2	5	3	33.96	33.43
3	5	3	21.67	20.35
4	5	3	19.22	-21.85
5	5	3	15.39	-14.85
6	5	3	17.71	23.63
-1	5	3	54.02	48.32
-2	5	3	62.17	53.45
-3	5	3	17.12	-12.19
-4	5	3	72.09	-59.48
-5	5	3	32.65	25.46
-6	5	3	38.59	28.00
-7	5	3	11.13	-11.49
-8	5	3	28.42	-24.12
-9	5	3	14.96	17.89
-10	5	3	20.82	22.22
1	6	3	8.13	-4.08
2	6	3	14.82	-16.94
3	6	3	27.06	27.43
-1	6	3	13.25	11.96
-8	6	3	13.47	11.10
0	7	3	43.53	-36.19
1	7	3	10.82	-7.36
2	7	3	36.02	39.46
4	7	3	26.95	-26.11
6	7	3	12.32	15.53
-2	7	3	60.06	49.80
-3	7	3	21.99	-21.73
-4	7	3	40.15	-34.37
-5	7	3	11.19	-12.98
-6	7	3	37.13	38.59
-8	7	3	25.37	-26.65
1	8	3	13.25	-11.31
2	8	3	13.42	6.59
3	8	3	11.64	10.23
-3	8	3	19.62	-18.08
-6	8	3	9.51	-3.49
-7	8	3	14.74	14.08
0	9	3	30.89	-29.89
2	9	3	18.85	15.67
4	9	3	13.72	-14.03
6	9	3	8.07	7.92
-1	9	3	17.79	-11.14
-2	9	3	28.56	22.06
-3	9	3	19.05	18.70
-4	9	3	30.85	-22.45
-6	9	3	22.46	21.60
-8	9	3	12.35	-11.51
-1	10	3	13.20	12.11
-2	10	3	11.43	9.75
-7	10	3	7.50	-7.83
0	11	3	8.34	-8.47
1	11	3	5.07	7.57
2	11	3	10.75	10.04
-1	11	3	8.48	-10.17
-2	11	3	12.01	11.35
-3	11	3	8.34	7.72
-4	11	3	15.08	-13.14
-5	11	3	15.17	-14.39
-6	11	3	6.84	4.86
-2	12	3	6.98	1.03
0	0	4	33.73	32.27
2	0	4	13.32	11.21
4	0	4	25.29	27.10
8	0	4	5.15	8.20
-2	0	4	52.53	39.21
-4	0	4	14.59	-12.70
-6	0	4	20.89	19.32
-8	0	4	31.73	-26.25
-12	0	4	16.16	-16.14
0	1	4	20.35	-17.08
1	1	4	67.35	-65.53
3	1	4	59.42	60.39
5	1	4	30.90	-34.24
6	1	4	8.09	10.60
7	1	4	14.95	19.89
9	1	4	5.77	-9.83
-1	1	4	109.52	100.47
-2	1	4	32.17	-26.03
-3	1	4	116.86	-105.80
-4	1	4	45.51	-41.43
-5	1	4	69.53	63.82
-6	1	4	16.85	-16.07
-7	1	4	61.27	-50.18
-8	1	4	15.49	-19.03
-9	1	4	29.90	33.60
-11	1	4	14.46	-15.81
0	2	4	28.85	-31.56
1	2	4	2.54	-0.66
2	2	4	21.39	-17.35
6	2	4	10.59	-12.32
-1	2	4	41.97	-37.19
-2	2	4	23.42	-15.69
-3	2	4	15.92	-7.88
-4	2	4	31.08	-23.69
-5	2	4	17.59	-11.46
-6	2	4	29.54	22.37
-7	2	4	13.82	14.70
-8	2	4	15.64	-13.57
-9	2	4	10.18	-7.72
-10	2	4	20.32	22.39
0	3	4	29.39	-30.00
1	3	4	55.49	-58.29
2	3	4	28.25	23.96
3	3	4	27.94	25.84
4	3	4	18.68	-20.61

Table 5 (*cont.*)

5	3	4	21.87	-25.18
7	3	4	9.05	11.36
-1	3	4	41.97	41.03
-2	3	4	51.39	53.76
-3	3	4	47.20	-42.64
-4	3	4	6.89	-4.85
-5	3	4	60.73	49.96
-6	3	4	37.85	33.67
-7	3	4	32.50	-26.42
-8	3	4	3.10	-4.10
-9	3	4	21.21	19.14
-10	3	4	13.42	15.53
-11	3	4	6.96	-9.64
0	4	4	6.86	6.81
2	4	4	13.72	9.72
3	4	4	3.50	4.95
4	4	4	4.46	7.53
-2	4	4	37.22	28.67
-3	4	4	32.71	27.55
-4	4	4	16.76	-12.75
-5	4	4	7.48	-4.61
-6	4	4	15.71	14.03
-7	4	4	23.77	20.07
-8	4	4	14.05	-10.14
-9	4	4	4.31	-8.50
-11	4	4	4.88	5.62
-12	4	4	7.47	-10.17
0	5	4	52.67	-47.53
1	5	4	21.93	-14.53
2	5	4	38.89	38.05
3	5	4	20.67	17.96
4	5	4	26.07	-25.28
6	5	4	17.71	22.92
-1	5	4	30.12	27.64
-2	5	4	46.85	46.22
-3	5	4	14.87	-12.71
-4	5	4	63.46	-54.65
-5	5	4	21.28	16.18
-6	5	4	43.24	35.14
-7	5	4	16.55	-14.56
-8	5	4	28.46	-28.45
0	6	4	11.40	-4.08
2	6	4	8.81	-1.48
4	6	4	11.40	-5.77
-5	6	4	20.71	-18.79
-7	6	4	11.22	6.57
-9	6	4	12.82	-14.14
0	7	4	49.22	-44.53
2	7	4	35.71	33.96
4	7	4	24.23	-24.55
-2	7	4	50.58	42.60
-4	7	4	43.00	-36.72
-5	7	4	11.03	7.82
-6	7	4	35.75	28.85
-8	7	4	25.85	-23.36
-10	7	4	9.26	14.04
-3	8	4	15.85	13.60
-5	8	4	13.14	-10.62
0	9	4	20.74	-16.14
2	9	4	22.78	22.00
4	9	4	9.48	-12.82
-2	9	4	27.16	24.07
-3	9	4	6.57	3.60
-4	9	4	31.44	-24.42
-5	9	4	15.85	-9.35
-6	9	4	17.84	17.30
0	11	4	12.11	-11.36
1	11	4	17.04	15.42
-1	11	4	12.46	-11.53
-2	11	4	12.57	7.94
-3	11	4	7.85	6.81
-4	11	4	9.35	-9.60
0	12	4	5.89	-1.32
-1	12	4	9.82	-7.48
0	0	5	49.01	-41.96
2	0	5	12.28	8.83
8	0	5	4.13	1.08
-2	0	5	5.07	8.21
-4	0	5	11.71	-9.38
-6	0	5	53.81	49.52
-8	0	5	36.80	-28.50
-10	0	5	18.25	19.17
-12	0	5	14.24	-12.35
0	1	5	24.50	-19.93
1	1	5	60.07	-52.82
3	1	5	33.46	33.42
4	1	5	9.00	-9.75
5	1	5	21.51	-24.98
7	1	5	10.00	14.42
-1	1	5	68.72	59.43
-2	1	5	47.87	38.42
-3	1	5	36.10	-40.82
-4	1	5	11.78	9.32
-5	1	5	57.12	45.90
-7	1	5	54.64	-45.91
-8	1	5	11.76	-12.45
-9	1	5	13.92	8.87
-11	1	5	8.73	-7.86
0	2	5	21.43	-14.71
1	2	5	20.96	18.67
2	2	5	15.60	12.88
3	2	5	9.72	-11.86
4	2	5	9.84	-7.62
-1	2	5	12.82	-15.91
-2	2	5	49.91	43.14
-3	2	5	25.85	25.05
-4	2	5	57.71	-50.75
-5	2	5	62.17	-52.17
-6	2	5	30.32	22.46
-7	2	5	18.18	11.55
-8	2	5	30.81	-25.88
-9	2	5	8.10	-1.85
-10	2	5	19.92	18.51
-11	2	5	16.32	20.15
-12	2	5	11.59	-12.35
0	3	5	34.51	-27.39
1	3	5	37.82	-35.49
2	3	5	26.39	21.78
3	3	5	25.23	26.84
4	3	5	19.41	-20.91
5	3	5	14.47	-18.79
6	3	5	10.75	12.12
7	3	5	6.05	12.96
-1	3	5	47.62	45.67
-2	3	5	33.42	30.23
-3	3	5	55.61	-48.10
-4	3	5	40.53	-30.78
-5	3	5	41.22	34.85
-6	3	5	30.48	25.32
-7	3	5	7.57	-0.37
-8	3	5	8.76	-8.46
-9	3	5	25.95	25.26
-10	3	5	7.19	7.47
-11	3	5	11.36	-9.65
0	4	5	16.21	-8.50
1	4	5	26.54	26.00
2	4	5	24.38	20.47
4	4	5	14.20	-11.92
-1	4	5	14.53	-13.46
-2	4	5	37.10	35.35
-3	4	5	32.88	29.07
-4	4	5	36.73	-29.24
-5	4	5	25.85	-20.11
-6	4	5	36.07	29.04
-7	4	5	29.75	24.38
-8	4	5	26.45	-22.30
-9	4	5	27.06	-27.07
-10	4	5	13.67	15.27
-11	4	5	2.44	5.21
-12	4	5	6.46	-8.21
-13	4	5	3.73	-7.14
0	5	5	39.05	-31.65
1	5	5	13.93	-12.76
2	5	5	47.14	41.82
3	5	5	20.60	22.08
4	5	5	15.49	-12.66
-1	5	5	13.72	10.46
-2	5	5	31.84	21.45
-3	5	5	35.00	-33.39
-4	5	5	48.39	-39.60
-5	5	5	16.70	8.63
-6	5	5	26.57	19.03
-7	5	5	19.85	-16.96
-8	5	5	18.20	-17.53
0	6	5	33.82	-26.85
-1	6	5	32.77	-25.13
-3	6	5	24.35	17.53
-4	6	5	12.36	-9.94
-5	6	5	23.08	-14.53
-6	6	5	9.39	9.32
-7	6	5	25.70	20.66
-9	6	5	13.53	-11.15
-11	6	5	7.55	10.21
0	7	5	34.60	-25.71
4	7	5	20.37	-22.00
-2	7	5	47.14	36.47
-4	7	5	26.69	-18.32
-6	7	5	27.60	23.55
-5	7	5	6.77	-8.79
0	8	5	9.78	12.66
1	8	5	13.80	10.20
-3	8	5	21.82	15.74
-5	8	5	19.64	-15.90
-7	8	5	16.51	16.45
-8	5	5	6.38	3.37
-9	8	5	10.01	-11.71
0	9	5	15.08	-16.65
2	9	5	13.97	15.88
-2	9	5	23.83	17.66
-4	9	5	21.64	-16.03
-6	9	5	11.32	9.52
-8	9	5	13.89	-12.01
1	10	5	8.26	4.95
-1	10	5	12.67	-12.57
-3	10	5	11.10	10.50
-5	10	5	12.28	-11.10
-6	10	5	8.22	-9.17
-7	10	5	9.22	6.29
2	11	5	9.71	9.67
-3	11	5	12.35	9.65
-4	11	5	7.60	-7.86
0	0	6	41.07	-34.72
2	0	6	30.67	26.16
4	0	6	19.41	-13.74
6	0	6	5.21	8.10
-2	0	6	65.99	56.78
-4	0	6	71.78	-58.23
-6	0	6	56.17	43.25
-8	0	6	19.03	-13.79
-10	0	6	39.05	36.12
-12	0	6	18.63	-14.97
1	1	6	28.73	-24.08
2	1	6	15.16	10.42
3	1	6	21.33	22.78
4	1	6	6.46	-4.86
5	1	6	10.68	-12.62
6	1	6	6.71	7.17
-1	1	6	22.77	20.51
-2	1	6	14.50	12.71
-3	1	6	27.82	-23.86
-4	1	6	14.99	-13.00
-5	1	6	28.11	19.86
-6	1	6	29.50	25.52
-9	1	6	7.88	7.51
0	2	6	43.39	-32.96
1	2	6	15.83	12.45
2	2	6	28.44	6.22
4	2	6	17.21	-15.93
-1	2	6	16.04	-14.81
-2	2	6	40.99	32.43
-3	2	6	36.68	29.40
-4	2	6	54.78	-45.19
-5	2	6	13.14	-10.36
-6	2	6	49.85	39.07
-7	2	6	21.51	18.84
-8	2	6	46.30	-44.32
-9	2	6	24.89	-26.57
-10	2	6	14.00	13.53
-12	2	6	10.78	-12.78
0	3	6	33.64	-30.89
1	3	6	23.08	-23.83
2	3	6	19.99	19.67
3	3	6	18.54	18.71
4	3	6	11.40	-11.10
5	3	6	10.67	-13.92
6	3	6	4.92	6.95
-1	3	6	21.05	19.78
-2	3	6	20.43	14.35
-3	3	6	37.19	-33.07
-4	3	6	21.70	-17.99
-5	3	6	14.92	13.25
-6	3	6	15.07	12.03
-7	3	6	25.58	-23.94
-8	3	6	11.28	-9.00
0	4	6	32.85	-27.06
2	4	6	13.85	9.33
3	4	6	14.03	-16.24
4	4	6	10.00	-6.69
5	4	6	6.00	5.36
-1	4	6	38.43	-37.92
-2	4	6	39.32	33.64
-3	4	6	42.03	37.61
-4	4	6	24.31	-18.40
-5	4	6	29.33	-22.12
-6	4	6	35.75	29.37
-7	4	6	32.92	26.47
-8	4	6	22.78	-19.33
-9	4	6	15.55	-13.35
-10	4	6	15.96	15.29
-11	4	6	15.35	16.39
-12	4	6	7.01	-9.22
-13	4	6	6.00	-8.80
0	0	7	33.65	-26.92
2	0	7	45.82	39.80
4	0	7	19.57	-16.42
6	0	7	12.21	16.07
-2	0	7	61.11	52.01
-4	0	7	67.90	-57.93
-6	0	7	60.88	51.45
-8	0	7	50.33	-40.70
-10	0	7	21.05	18.49
-12	0	7	15.91	-13.79
0	1	7	16.84	-14.97
3	1	7	7.85	6.03
5	1	7	10.00	-11.42
-1	1	7	29.08	21.83
-2	1	7	18.25	-15.00
-4	1	7	11.36	-7.55
-5	1	7	5.77	-7.69
-8	1	7	10.07	-9.92
-9	1	7	9.15	-9.43
-11	1	7	7.35	8.57
0	2	7	52.39	-45.35
1	2	7	22.03	21.76
2	2	7	18.01	13.89
3	2	7	8.51	5.00
4	2	7	18.42	-18.25
-1	2	7	21.70	-16.85
-2	2	7	53.15	42.35
-3	2	7	7.67	-6.03
-4	2	7	48.29	-36.38
-5	2	7	33.19	-24.11
-6	2	7	42.80	33.85
-7	2	7	9.57	6.52
-8	2	7	34.21	-26.39
-9	2	7	9.98	-7.78
-10	2	7	24.49	24.30
-12	2	7	11.21	-11.84
1	3	7	20.37	-21.51
2	3	7	7.57	6.35
3	3	7	8.48	10.84
4	3	7	6.80	-6.03
-1	3	7	14.84	-11.71
-2	3	7	22.77	18.53
-3	3	7	15.88	-12.58
-8	3	7	10.63	6.80
0	4	7	14.34	-10.30
1	4	7	15.55	12.34
2	4	7	19.68	18.17
3	4	7	18.14	-19.26
4	4	7	4.73	-4.72
5	4	7	3.96	7.62
6	4	7	3.27	5.89
-1	4	7	22.17	-19.96
-2	4	7	21.42	17.14
-3	4	7	40.28	30.89
-4	4	7	30.42	-23.57
-5	4	7	27.53	-21.34
0	4	7	27.60	-10.30
-7	4	7	42.45	36.21
-8	4	7	21.31	-17.73
-9	4	7	6.65	-6.17
-10	4	7	9.72	7.75
-11	4	7	11.03	11.76
-12	4	7	5.51	-6.75
-13	4	7	4.27	-5.60
0	0	8	45.95	-30.33
2	0	8	36.55	33.97
-2	0	8	46.34	38.56
-4	0	8	45.34	-38.39
-6	0	8	27.98	21.35
-8	0	8	51.24	-40.14
-10	0	8	17.30	15.57
-12	0	8	16.50	-11.98
0	1	8	7.92	-7.28
1	1	8	7.90	-8.06
2	1	8	7.67	-8.37
-1	1	8	14.32	-12.29
-2	1	8	14.05	-10.85
-3	1	8	16.43	12.70
-4	1	8	13.82	-10.05
-6	1	8	24.42	-18.10
-7	1	8	17.54	14.57
-8	1	8	9.15	6.98
-9	1	8	18.80	-17.15
-11	1	8	9.10	8.23
-13	1	8	9.22	-8.04
0	2	8	30.00	-27.63
2	2	8	15.88	10.90
3	2	8	17.66	-15.05
4	2	8	19.43	-17.94
-2	2	8	31.27	25.46
-3	2	8	35.48	25.60
-4	2	8	41.96	-33.04
-5	2	8	17.42	-13.05
-6	2	8	50.39	39.23
-8	2	8	13.21	-10.50
-9	2	8	8.56	-8.60
-10	2	8	17.14	15.57
0	3	8	6.17	6.80
1	3	8	14.28	13.87
-1	3	8	6.15	6.27
-4	3	8	26.29	22.29
-5	3	8	31.17	-22.82
-7	3	8	19.99	14.39
-8	3	8	13.80	9.65
-10	3	8	11.55	-8.35
-11	3	8	10.44	10.83
-12	3	8	5.36	5.75
0	4	8	13.93	-11.14
1	4	8	22.62	20.95
2	4	8	14.21	12.78
3	4	8	4.48	-5.74
-1	4	8	29.14	-23.17
-2	4	8	28.50	22.31
-3	4	8	19.64	14.95
-4	4	8	18.84	-13.39
-5	4	8	21.82	-15.90
-6	4	8	15.50	10.67
-7	4	8	25.83	19.19
-8	4	8	18.13	-12.99
-9	4	8	17.60	-12.82
-10	4	8	8.61	5.37
-11	4	8	7.00	8.01
-12	4	8	6.73	-7.78
0	0	9	11.94	-10.42
2	0	9	11.61	10.71
4	0	9	9.77	-10.87
-2	0	9	40.11	27.25
-4	0	9	24.16	-18.35
-6	0	9	23.41	18.82
-8	0	9	8.63	-8.67
-10	0	9	9.76	7.86
-12	0	9	5.27	-4.05
0	1	9	12.55	9.85
1	1	9	12.67	9.08
-1	1	9	15.08	-11.82
-2	1	9	7.92	-6.82
-3	1	9	15.85	11.35
-5	1	9	31.73	-22.25
-6	1	9	12.13	-5.76
-7	1	9	27.11	20.47
-8	1	9	9.06	2.94
-9	1	9	14.66	-12.72
-10	1	9	10.25	-7.71
-11	1	9	13.11	12.86
-13	1	9	9.09	-8.41
0	2	9	22.53	-19.94
1	2	9	7.85	6.75
2	2	9	16.42	13.25
4	2	9	6.69	-6.82
-1	2	9	19.10	-13.49
-2	2	9	15.78	13.27
-3	2	9	11.15	8.25
-4	2	9	25.48	-19.73
-5	2	9	8.64	-2.69
-6	2	9	15.78	10.56
-7	2	9	20.55	14.22
-8	2	9	19.70	-15.18
-9	2	9	6.73	-4.66
-10	2	9	8.97	9.17
1	3	9	9.46	7.35
-1	3	9	15.42	-10.41
-2	3	9	11.47	-10.28
-3	3	9	27.28	20.35
-4	3	9	13.82	11.83
-5	3	9	18.03	-12.76
-6	3	9	19.53	-13.62
-7	3	9	17.34	13.33
-8	3	9	19.05	18.18
-9	3	9	23.23	-18.76
-10	3	9	7.64	-6.01
-11	3	9	10.18	10.08
-12	3	9	9.11	7.57
0	4	9	10.10	-5.41
1	4	9	11.89	9.76
2	4	9	8.15	8.63
3	4	9	5.06	-4.56
-1	4	9	17.49	-13.45
-2	4	9	18.71	14.53
-3	4	9	21.82	12.79
-4	4	9	16.43	-10.82
-5	4	9	26.85	-16.87
-6	4	9	21.12	15.77
-7	4	9	10.75	6.10
-8	4	9	7.42	-5.89
-9	4	9	7.90	-6.13
-11	4	9	4.00	4.15
2	0	10	10.40	7.91
-2	0	10	16.49	11.55
-6	0	10	12.03	6.92
-10	0	10	5.13	-0.85
1	1	10	15.71	10.67
3	1	10	20.32	3.22
-3	1	10	31.98	20.32
-5	1	10	25.82	-19.73
-6	1	10	11.82	-8.32
-7	1	10	28.32	21.87
-8	1	10	9.63	1.01
-9	1	10	21.39	-15.78
-10	1	10	8.51	-5.69
-11	1	10	15.10	11.48
0	2	10	16.46	-10.35
1	2	10	7.25	5.39
-1	2	10	7.68	-5.26
-3	2	10	8.27	5.27
-4	2	10	16.04	-10.85
-5	2	10	9.71	-5.45
-9	2	10	7.61	-6.37
0	3	10	6.00	6.26
1	3	10	5.21	4.88
-1	3	10	19.29	-12.54
-2	3	10	11.28	-9.25
-3	3	10	16.95	12.34
-4	3	10	13.84	11.97
-5	3	10	21.39	-17.45
-6	3	10	11.03	-8.68
-7	3	10	14.20	10.83
-8	3	10	13.14	9.28
-9	3	10	19.83	-14.74
-10	3	10	7.61	-7.28
-11	3	10	13.74	10.80
-12	3	10	10.18	8.75
0	4	10	7.11	-7.25
1	4	10	9.11	5.95
-1	4	10	5.55	-3.60
-2	4	10	10.26	6.69
-3	4	10	12.28	6.90
-5	4	10	8.88	-4.75
-6	4	10	7.19	5.67
-7	4	10	9.35	5.38
-11	4	10	4.09	4.47
-6	0	11	6.65	-5.16
-10	0	11	12.78	-8.71
1	1	11	7.85	9.80
-1	1	11	18.95	-12.94
-3	1	11	26.73	15.88
-5	1	11	28.94	-18.12
-6	1	11	8.07	-5.37
-7	1	11	25.77	15.32
-9	1	11	23.29	-14.92
-11	1	11	16.87	10.71
-8	2	11	9.11	6.63
0	3	11	6.84	5.67
-1	3	11	13.13	-8.88
-2	3	11	6.44	-4.11
-3	3	11	16.26	10.42
-4	3	11	16.53	9.90
-5	3	11	18.01	-10.54
-6	3	11	7.31	-5.40
-7	3	11	21.26	12.71
-8	3	11	14.99	9.73
-9	3	11	8.42	-6.66
-10	3	11	5.57	-5.23
-11	3	11	8.61	6.16
-5	4	11	5.21	2.92
-6	4	11	4.36	-2.17
-10	4	11	6.27	-4.76
-4	0	12	12.90	7.87
-6	0	12	11.28	-6.60
-10	0	12	13.57	-9.14
-3	1	12	15.25	9.55
-5	1	12	17.37	-10.21
-6	1	12	13.47	-7.83
-7	1	12	17.29	10.41
-9	1	12	16.42	-7.99
-2	2	12	4.13	-2.70
-5	2	12	7.59	4.47
-6	2	12	11.92	-4.21
-7	2	12	5.84	-3.14
-8	2	12	16.93	9.40
-9	2	12	6.42	4.19
-10	2	12	6.38	-4.36
-3	3	12	12.53	8.20
-4	3	12	11.76	6.42
-5	3	12	14.20	-7.72
-6	3	12	9.78	-3.72
-7	3	12	12.39	7.24
-8	3	12	10.36	4.72
-9	3	12	9.28	-6.67
-10	3	12	3.96	-3.00
-3	4	12	5.61	-4.13
-4	4	12	6.07	2.67
-5	4	12	3.79	2.88
-6	4	12	11.03	-4.92
-7	4	12	10.01	-6.25
-8	4	12	8.19	4.04
-9	4	12	2.98	1.91
-6	0	13	3.38	-2.50
-7	1	13	5.15	3.80

Table 6. *Observed and calculated structure factors for cis*-AMCHA . HCl

H	K	L	$\|F_o\|$	F_c
2	0	0	3.20	0.40
4	0	0	0.00	4.28
6	0	0	48.62	-54.55
8	0	0	18.78	23.62
10	0	0	22.85	-37.64
12	0	0	5.52	-5.24
14	0	0	9.28	13.49
16	0	0	0.00	0.51
18	0	0	4.89	-4.34
0	1	0	0.00	0.00
1	1	0	23.00	20.87
2	1	0	77.81	-71.00
3	1	0	29.82	-24.59
4	1	0	37.09	37.17
5	1	0	35.34	37.60
6	1	0	9.33	-10.53
7	1	0	14.62	16.49
8	1	0	8.17	9.43
9	1	0	15.63	18.47
10	1	0	21.12	-23.12
11	1	0	23.31	-26.18
12	1	0	31.42	42.22
15	1	0	6.46	-10.14
16	1	0	0.00	2.01
18	1	0	5.48	-9.85
0	2	0	44.25	-51.75
1	2	0	62.17	-75.55
2	2	0	40.75	38.95
3	2	0	44.48	51.00
4	2	0	1.85	3.57
5	2	0	6.58	-4.14
6	2	0	16.94	18.34
7	2	0	33.96	34.58
8	2	0	20.46	-25.39
9	2	0	19.86	-21.22
12	2	0	4.57	-5.67
13	2	0	0.00	0.55
14	2	0	0.00	-1.54
15	2	0	0.00	-3.03
16	2	0	0.00	1.11
17	2	0	0.00	2.99
18	2	0	0.00	1.73
0	3	0	0.00	0.00
1	3	0	6.71	1.80
2	3	0	18.45	-18.77
3	3	0	15.55	16.00
4	3	0	16.17	-14.30
5	3	0	24.31	-26.71
6	3	0	5.68	-8.42
7	3	0	16.00	18.84
8	3	0	4.60	1.24
9	3	0	17.61	-21.95
11	3	0	12.88	17.35
13	3	0	10.94	-16.92
17	3	0	0.00	-7.18
0	4	0	10.31	9.22
1	4	0	26.93	26.54
2	4	0	30.08	32.31
3	4	0	22.35	-23.36
4	4	0	18.67	-20.28
5	4	0	20.02	27.93
6	4	0	2.36	2.21
7	4	0	18.65	-23.93
8	4	0	8.96	-8.77
9	4	0	8.47	-5.78
10	4	0	0.00	-0.10
11	4	0	8.25	-9.75
12	4	0	0.00	-2.01
13	4	0	0.00	2.82
14	4	0	0.00	0.58
15	4	0	0.00	-2.71
0	5	0	0.00	0.00
1	5	0	1.22	0.46
2	5	0	10.85	-12.98
3	5	0	9.66	12.35
4	5	0	16.01	-18.60
5	5	0	13.83	15.36
6	5	0	8.33	10.09
7	5	0	9.59	-7.73
8	5	0	14.41	-18.99
11	5	0	6.15	-6.85
14	5	0	6.57	10.73
0	6	0	10.97	8.49
1	6	0	0.00	2.25
2	6	0	11.90	-14.62
4	6	0	23.74	27.82
0	7	0	0.00	0.00
1	7	0	5.92	5.93
0	8	0	4.46	-3.29
1	8	0	5.92	-7.18
2	8	0	0.00	3.02
3	8	0	5.07	6.46
1	0	1	29.03	-44.79
3	0	1	27.90	28.13
5	0	1	45.32	-58.70
7	0	1	39.74	42.76
9	0	1	15.09	-21.18
11	0	1	17.25	-18.90
13	0	1	16.46	-23.94
15	0	1	12.87	20.28
17	0	1	6.64	3.42
-1	0	1	20.42	-20.69
-3	0	1	111.67	-125.61
-5	0	1	46.82	43.47
-7	0	1	17.57	24.55
-9	0	1	5.74	4.63
-11	0	1	10.57	16.85
-13	0	1	12.10	11.65
-15	0	1	10.64	16.32
-17	0	1	8.91	-15.61
0	1	1	33.89	-32.28
1	1	1	41.64	44.42
2	1	1	26.70	-23.68
3	1	1	43.96	-51.96
4	1	1	53.60	-65.78
5	1	1	5.32	4.86
6	1	1	45.21	-43.07
7	1	1	8.56	7.83
8	1	1	4.10	7.09
9	1	1	17.10	-18.71
10	1	1	10.17	11.85
11	1	1	6.87	-7.22
12	1	1	3.72	5.23
17	1	1	3.97	-7.16
-1	1	1	83.43	67.28
-2	1	1	0.00	2.46
-3	1	1	65.98	69.03
-4	1	1	13.78	9.17
-5	1	1	62.19	-73.57
-6	1	1	52.35	58.00
-7	1	1	15.04	22.46
-8	1	1	9.58	-9.48
-9	1	1	15.41	-20.85
-10	1	1	11.10	13.89
-11	1	1	17.93	24.05
-13	1	1	5.75	-10.56
-14	1	1	6.45	8.61
-15	1	1	10.33	16.74
-16	1	1	3.25	-6.20
-17	1	1	3.99	-5.80
-18	1	1	0.00	3.92
0	2	1	38.06	-35.19
1	2	1	37.56	35.34
2	2	1	27.50	20.51
3	2	1	7.76	4.96
4	2	1	34.98	-21.70
5	2	1	3.42	1.25
6	2	1	36.52	39.18
7	2	1	44.23	-41.36
8	2	1	2.62	-3.90
9	2	1	6.65	1.42
11	2	1	5.93	2.92
12	2	1	11.05	-14.25
13	2	1	6.07	0.60
14	2	1	5.41	6.59
-1	2	1	28.79	-24.42
-2	2	1	10.43	9.36
-3	2	1	8.34	13.11
-4	2	1	32.50	-37.14
-5	2	1	9.29	-1.41
-6	2	1	36.35	34.15
-7	2	1	10.55	-6.11
-8	2	1	16.71	16.49
-9	2	1	8.94	7.60
-10	2	1	0.00	-0.38
-11	2	1	9.37	1.23
-13	2	1	6.51	7.03
-15	2	1	6.34	-0.95
-16	2	1	0.00	6.13
-17	2	1	0.00	3.33
-18	2	1	3.14	-1.26
0	3	1	13.39	12.07
1	3	1	8.26	11.21
2	3	1	30.19	-20.42
3	3	1	3.05	2.81
4	3	1	0.00	-2.53
5	3	1	17.42	-21.43
6	3	1	5.16	1.76
7	3	1	0.00	4.02
8	3	1	2.71	4.67
9	3	1	2.89	5.02
11	3	1	0.00	-0.18
13	3	1	3.05	3.64
15	3	1	3.60	6.09
-1	3	1	6.64	-4.54
-2	3	1	22.19	-22.19
-3	3	1	23.14	-25.96
-4	3	1	43.58	43.32
-5	3	1	11.83	12.10
-6	3	1	12.17	-14.65
-7	3	1	11.04	12.03
-8	3	1	22.92	21.07
-9	3	1	12.21	-12.25
-10	3	1	20.14	-27.08
-11	3	1	9.08	-12.00
-12	3	1	8.35	15.10
-13	3	1	0.00	0.87
-14	3	1	5.10	-10.34
-15	3	1	0.00	3.18
-16	3	1	0.00	5.85
-17	3	1	0.00	-0.10
0	4	1	17.90	17.39
1	4	1	1.25	-1.10
2	4	1	29.75	-33.29
3	4	1	23.39	-27.00
4	4	1	11.56	1.26
5	4	1	10.49	11.37
6	4	1	2.44	-1.67
7	4	1	6.74	0.27
8	4	1	24.38	21.10
9	4	1	0.00	-0.25
10	4	1	7.05	-10.41
11	4	1	8.50	-11.11
12	4	1	5.82	0.53
13	4	1	0.00	2.35
-1	4	1	18.21	-15.04
-2	4	1	23.07	-24.10
-3	4	1	0.00	-1.82
-4	4	1	12.05	-13.60
-5	4	1	10.85	-1.75
-6	4	1	10.72	-12.58
-7	4	1	26.93	22.55
-8	4	1	0.00	3.83
-9	4	1	7.09	10.56
-10	4	1	0.00	2.27
-11	4	1	0.00	-2.20
-12	4	1	4.67	-6.02
-13	4	1	0.00	3.26
-14	4	1	6.54	10.08
-15	4	1	0.00	-1.14
0	5	1	8.05	-7.71
1	5	1	7.23	-6.87
2	5	1	0.00	-2.64
3	5	1	0.00	-2.71
4	5	1	12.34	-15.21
6	5	1	5.51	-3.36
8	5	1	10.09	-12.98
9	5	1	6.40	-6.59
12	5	1	5.62	6.76
13	5	1	5.17	1.14
-1	5	1	21.66	24.37
-2	5	1	16.28	21.15
-3	5	1	12.28	-12.59
-4	5	1	14.98	-16.78
-5	5	1	6.99	-4.73
-7	5	1	18.07	-25.07
-9	5	1	11.40	14.80
-10	5	1	10.89	13.58
-11	5	1	7.23	-11.32
-13	5	1	6.14	0.60
0	6	1	8.79	-1.76
1	6	1	22.79	-24.47
2	6	1	0.00	-3.20
4	6	1	2.92	3.08
-1	6	1	7.32	7.92
-2	6	1	6.64	-4.24
-4	6	1	5.09	6.69
0	7	1	4.49	-4.10
1	7	1	6.45	7.50
2	7	1	0.00	-0.19
-1	7	1	10.57	-11.27
-2	7	1	0.00	0.14
-3	7	1	7.60	10.37
0	8	1	4.05	-3.82
1	8	1	0.00	2.88
2	8	1	2.75	4.03
3	8	1	3.27	-3.67
-1	8	1	0.00	-2.13
-2	8	1	4.88	5.19
-3	8	1	0.00	0.42
0	0	2	2.17	7.03
2	0	2	11.03	11.32
4	0	2	27.71	34.14
6	0	2	9.95	11.17
8	0	2	22.61	24.53
10	0	2	21.28	20.07
12	0	2	0.00	-4.94
14	0	2	0.00	6.64
16	0	2	5.73	-11.26
-2	0	2	79.03	-82.78
-4	0	2	15.58	-17.65
-6	0	2	27.28	-30.39
-8	0	2	9.84	13.08
-10	0	2	12.37	-20.45
-12	0	2	0.00	5.36
-14	0	2	11.92	-10.50
-16	0	2	0.00	0.32
-18	0	2	0.00	-3.60
0	1	2	13.85	-11.71
1	1	2	19.68	17.83
2	1	2	45.01	-40.24
3	1	2	18.00	11.72
4	1	2	43.92	46.26
5	1	2	19.77	24.46
6	1	2	5.13	-7.12
7	1	2	9.42	-15.78
8	1	2	17.72	10.17
9	1	2	16.89	10.07
10	1	2	24.66	-21.82
11	1	2	0.00	-1.85
12	1	2	6.14	10.71
13	1	2	7.20	1.21
17	1	2	0.00	4.78
-1	1	2	14.10	-14.14
-2	1	2	61.45	-61.28
-3	1	2	14.28	14.63
-4	1	2	12.46	5.40
-5	1	2	20.83	-23.97
-6	1	2	0.00	-4.85
-7	1	2	25.10	-27.45
-8	1	2	18.55	10.89
-9	1	2	22.27	-20.99
-10	1	2	5.75	-7.98
-11	1	2	0.00	1.55
-13	1	2	0.00	-1.31
0	2	2	63.04	-56.01
1	2	2	14.52	-16.74
2	2	2	0.00	1.03
3	2	2	0.00	2.50
4	2	2	38.81	32.41
5	2	2	29.87	-26.90
6	2	2	19.23	17.28
7	2	2	0.00	-0.93
8	2	2	6.97	7.25
9	2	2	12.09	15.67
11	2	2	0.00	-1.21
12	2	2	0.00	0.65
13	2	2	0.00	4.28
14	2	2	11.19	-15.98
-1	2	2	3.00	1.29
-2	2	2	9.97	-4.03
-3	2	2	15.19	-15.39
-4	2	2	4.39	-2.83
-5	2	2	15.04	20.00
-6	2	2	2.16	-0.54
-7	2	2	13.85	-17.88
-8	2	2	21.52	-24.25
-9	2	2	0.00	5.00
-10	2	2	14.56	14.96
-11	2	2	4.42	-6.49
-13	2	2	8.32	10.89
-14	2	2	3.18	1.09
-15	2	2	5.18	-10.82
-18	2	2	0.00	3.90
0	3	2	28.52	27.10
1	3	2	3.38	-0.35
2	3	2	45.16	47.14
3	3	2	29.42	35.35
4	3	2	9.75	-11.25
5	3	2	25.91	-32.44
6	3	2	18.97	-11.96
7	3	2	13.31	14.82
8	3	2	0.00	0.28
9	3	2	12.29	-15.28
11	3	2	13.21	13.92
12	3	2	6.24	-0.62
13	3	2	4.23	-10.64
14	3	2	3.89	-2.99
15	3	2	3.40	7.05
16	3	2	4.92	7.54
-1	3	2	13.60	12.45
-2	3	2	8.74	1.22
-3	3	2	33.85	-35.31
-4	3	2	1.14	-3.31
-5	3	2	9.41	1.42
-6	3	2	0.00	-1.81
-7	3	2	11.23	-12.05
-8	3	2	13.51	-11.69
-9	3	2	3.50	1.55
-10	3	2	7.06	-6.87
-11	3	2	3.11	-1.28
-12	3	2	8.64	0.32
-13	3	2	6.58	1.52
-14	3	2	0.00	3.53
-15	3	2	0.00	1.40
-16	3	2	2.32	-0.39
0	4	2	3.96	4.53
1	4	2	14.85	16.59
2	4	2	5.95	4.03
3	4	2	0.00	-2.47
4	4	2	17.05	-11.70
5	4	2	0.00	1.62
6	4	2	7.27	5.75
7	4	2	13.43	13.53
8	4	2	9.57	13.83
10	4	2	4.75	3.01
11	4	2	0.00	1.81
12	4	2	0.00	1.31
13	4	2	6.70	-1.46
-1	4	2	7.46	-0.79
-2	4	2	9.27	-6.89
-3	4	2	10.50	0.48
-4	4	2	11.14	-11.85
-5	4	2	5.21	3.35
-6	4	2	9.99	11.60
-7	4	2	22.60	30.86
-8	4	2	4.80	1.02
-9	4	2	11.45	-13.47
-10	4	2	7.34	-7.76
-11	4	2	0.00	0.61
-12	4	2	5.91	-0.39
-13	4	2	7.42	-11.37
-14	4	2	0.00	2.54
-15	4	2	0.00	6.15
0	5	2	0.00	-2.66
1	5	2	11.03	14.58
2	5	2	12.67	11.68
3	5	2	9.02	-1.32
4	5	2	2.50	-4.41
5	5	2	19.07	23.78
6	5	2	16.67	23.22
7	5	2	6.78	5.08
8	5	2	7.93	-1.10
9	5	2	5.10	6.60
12	5	2	6.89	-10.55
-1	5	2	7.90	-0.64
-2	5	2	8.32	7.85
-3	5	2	0.00	-0.10
-4	5	2	13.79	-12.85
-5	5	2	18.03	-23.95
-6	5	2	7.12	0.03
-12	5	2	6.05	-5.92
-13	5	2	3.53	2.25
0	6	2	0.00	3.96
1	6	2	0.00	2.11
2	6	2	4.17	-4.88
3	6	2	0.00	-6.57
4	6	2	5.02	5.22
-1	6	2	10.33	10.07
-2	6	2	0.00	-5.82
-3	6	2	0.00	3.06
0	7	2	6.72	10.11
1	7	2	0.00	2.63
2	7	2	7.16	-0.78
4	7	2	8.62	0.31
-1	7	2	0.00	-2.00
-2	7	2	9.93	-10.95
-3	7	2	0.00	-3.30
-4	7	2	4.25	2.64
0	8	2	0.00	-0.96
1	8	2	0.00	0.03
2	8	2	0.00	-4.07
3	8	2	0.00	-0.13
-1	8	2	4.47	5.22
-2	8	2	4.83	6.26
1	0	3	43.23	-47.67
3	0	3	33.89	39.00
5	0	3	42.99	-46.83
7	0	3	25.82	23.46
9	0	3	19.39	-20.26
11	0	3	7.34	-6.92
13	0	3	7.10	-5.18
15	0	3	4.17	-5.57
17	0	3	0.00	2.43
-1	0	3	127.65	131.96
-3	0	3	8.17	-1.35
-5	0	3	46.35	61.03
-7	0	3	23.47	-31.86
-9	0	3	13.39	13.00
-11	0	3	4.93	-5.82
-13	0	3	5.27	9.52
-15	0	3	0.00	-1.54
-17	0	3	3.03	-2.92
0	1	3	25.02	23.68
1	1	3	11.11	11.17
2	1	3	8.17	6.64
3	1	3	17.39	17.27
4	1	3	24.83	26.91
5	1	3	24.24	-30.81
6	1	3	18.05	-17.45
7	1	3	17.21	22.97
8	1	3	0.00	-3.35
9	1	3	14.75	-19.87
10	1	3	21.80	-25.39
11	1	3	20.67	27.15
12	1	3	0.00	6.63
13	1	3	4.78	-9.42
14	1	3	5.72	-9.41
17	1	3	6.75	-10.46
-1	1	3	37.04	42.04
-2	1	3	37.21	35.35
-3	1	3	29.89	29.52
-4	1	3	5.26	4.38
-5	1	3	27.91	-33.88
-6	1	3	17.80	21.00
-7	1	3	4.15	5.60
-8	1	3	5.87	-3.28
-9	1	3	14.25	-18.07
-10	1	3	9.75	11.21
-11	1	3	9.88	14.09
-12	1	3	8.82	-12.98
-13	1	3	10.59	-14.63
0	2	3	76.99	-62.70
1	2	3	17.65	17.21
2	2	3	36.98	39.09
3	2	3	9.50	-8.42
4	2	3	21.34	-19.36
5	2	3	18.50	17.38
6	2	3	20.89	24.74
7	2	3	17.35	-21.97
8	2	3	13.50	-16.69
9	2	3	0.00	2.43
10	2	3	8.42	10.75
11	2	3	6.51	7.37
12	2	3	3.24	3.10
13	2	3	0.00	2.21
-1	2	3	32.72	-32.34
-2	2	3	52.89	50.33
-3	2	3	38.01	34.12
-4	2	3	15.75	-15.65
-5	2	3	4.48	-3.70
-6	2	3	24.44	28.33
-7	2	3	18.82	21.52
-8	2	3	15.95	-15.64
-9	2	3	2.84	-8.36
-10	2	3	5.64	10.06
-11	2	3	0.00	-1.27
-12	2	3	6.07	-8.45
-13	2	3	9.21	-13.73
-14	2	3	3.16	-3.16
-15	2	3	4.18	-3.61
0	3	3	13.22	-8.02
1	3	3	9.85	-8.05
2	3	3	24.71	23.44
3	3	3	14.04	12.70
4	3	3	13.53	-11.60
5	3	3	10.43	8.45
6	3	3	17.39	17.00
7	3	3	0.00	-1.70
8	3	3	16.75	-21.85

Table 6 (*cont.*)

9	3	3	0.00	-1.84
10	3	3	12.96	20.69
12	3	3	12.64	-20.42
13	3	3	6.44	-8.75
14	3	3	3.17	8.55
15	3	3	0.00	-1.03
-1	3	3	32.52	-30.24
-2	3	3	9.03	-5.57
-3	3	3	7.02	-5.57
-4	3	3	19.36	23.00
-5	3	3	8.32	3.17
-6	3	3	15.89	-17.70
-7	3	3	3.63	7.13
-8	3	3	0.00	2.38
-9	3	3	0.00	2.72
-10	3	3	12.56	-16.10
-11	3	3	0.00	4.50
-12	3	3	12.63	16.45
-13	3	3	4.88	3.74
-14	3	3	5.46	-12.80
-16	3	3	0.00	2.67
0	4	3	33.10	32.07
1	4	3	28.38	28.56
2	4	3	24.17	-25.97
3	4	3	10.76	-12.50
4	4	3	1.46	-4.10
5	4	3	0.00	-0.00
6	4	3	25.28	-31.39
7	4	3	13.39	-15.10
8	4	3	5.53	8.10
10	4	3	0.00	-1.26
11	4	3	7.13	-4.84
13	4	3	0.00	-2.37
-1	4	3	0.00	0.94
-2	4	3	24.94	-27.66
-3	4	3	24.73	30.17
-4	4	3	19.46	19.28
-5	4	3	0.00	-3.30
-6	4	3	12.40	-11.25
-7	4	3	0.00	-4.47
-8	4	3	12.82	16.65
-9	4	3	11.77	-12.84
-10	4	3	5.62	-9.94
-12	4	3	8.03	9.26
-13	4	3	0.00	1.09
0	5	3	5.17	3.82
1	5	3	0.00	3.85
2	5	3	0.00	-3.09
3	5	3	14.05	-15.55
4	5	3	12.18	11.56
7	5	3	10.85	-13.55
9	5	3	9.89	13.59
10	5	3	8.35	-9.92
11	5	3	6.11	-9.99
13	5	3	3.85	5.64
-1	5	3	4.10	0.06
-2	5	3	0.00	-1.10
-3	5	3	5.79	-5.18
-4	5	3	0.00	1.19
-5	5	3	9.75	13.02
-6	5	3	11.85	9.52
-8	5	3	6.89	9.26
-9	5	3	6.10	6.00
-10	5	3	7.64	11.13
-12	5	3	6.67	-7.54
-13	5	3	6.57	9.28
0	6	3	0.00	-3.51
1	6	3	10.66	-12.01
2	6	3	0.00	4.58
3	6	3	9.92	13.23
4	6	3	4.93	6.67
-1	6	3	22.57	22.49
-3	6	3	7.65	-7.34
0	7	3	0.00	1.48
2	7	3	0.00	1.91
-2	7	3	0.00	-0.93
-4	7	3	3.36	-3.64
1	8	3	4.90	6.59
-2	8	3	4.38	5.92
0	0	4	130.94	-117.34
2	0	4	28.03	29.18
4	0	4	35.06	-35.72
6	0	4	29.00	28.76
8	0	4	19.97	-23.35
10	0	4	13.50	15.51
14	0	4	7.55	10.18
16	0	4	0.00	-0.06
-2	0	4	10.56	-14.67
-4	0	4	41.35	-50.36
-6	0	4	22.35	27.83
-8	0	4	6.41	8.72
-10	0	4	12.96	19.42
-12	0	4	8.13	12.52
-14	0	4	7.60	-13.51
-16	0	4	4.17	6.84
0	1	4	7.76	5.70
1	1	4	24.01	-20.55
2	1	4	13.03	-8.95
3	1	4	21.10	-22.89
4	1	4	7.62	7.11
5	1	4	15.19	-13.92
6	1	4	14.85	14.18
7	1	4	0.00	3.57
8	1	4	11.41	-11.10
10	1	4	3.69	-4.60
11	1	4	7.53	8.29
12	1	4	13.67	-15.45
-1	1	4	24.55	-24.48
-2	1	4	47.25	-40.53
-3	1	4	24.91	17.92
-4	1	4	40.06	38.20
-5	1	4	15.64	-21.13
-6	1	4	19.85	-24.52
-7	1	4	11.04	14.96
-8	1	4	20.03	25.10
-9	1	4	11.51	-13.49
-10	1	4	16.52	-24.16
-11	1	4	14.53	18.07
-12	1	4	17.30	31.10
-15	1	4	5.33	8.67
0	2	4	27.54	28.34
1	2	4	34.58	35.14
2	2	4	30.64	-30.27
3	2	4	36.03	-38.02
4	2	4	6.68	2.03
5	2	4	21.11	16.87
6	2	4	22.56	-21.22
7	2	4	25.85	-25.43
8	2	4	8.29	7.89
9	2	4	8.65	10.46
10	2	4	3.97	-5.11
11	2	4	3.95	-6.01
12	2	4	7.80	10.91
13	2	4	4.75	7.08
-1	2	4	28.15	-30.79
-2	2	4	1.12	1.66
-3	2	4	33.89	31.78
-4	2	4	15.00	13.44
-5	2	4	17.55	-16.40
-6	2	4	10.53	-15.54
-7	2	4	13.56	14.55
-8	2	4	0.00	0.10
-9	2	4	2.93	-0.24
-10	2	4	0.00	5.19
-11	2	4	3.19	-1.93
-13	2	4	0.00	5.59
-14	2	4	5.85	9.92
-15	2	4	4.58	-7.17
0	3	4	0.00	2.32
1	3	4	32.02	-24.95
2	3	4	2.79	6.24
3	3	4	5.82	4.50
4	3	4	1.86	-5.04
5	3	4	4.93	6.67
6	3	4	0.00	2.46
7	3	4	7.17	-7.08
8	3	4	0.00	3.90
9	3	4	5.85	9.14
10	3	4	8.04	8.70
12	3	4	4.17	3.07
15	3	4	2.32	-8.14
-1	3	4	1.03	2.73
-2	3	4	1.77	-3.01
-3	3	4	19.85	-21.79
-4	3	4	8.60	-11.92
-5	3	4	40.01	39.82
-6	3	4	0.00	-5.42
-7	3	4	13.25	-14.80
-8	3	4	0.00	2.00
-9	3	4	23.72	32.68
-10	3	4	0.00	-1.10
-11	3	4	12.21	-17.17
-12	3	4	0.00	-2.02
-13	3	4	5.70	11.43
-14	3	4	0.00	-0.59
-15	3	4	6.32	-12.40
0	4	4	5.07	2.87
1	4	4	19.93	-17.82
2	4	4	13.93	-16.25
3	4	4	23.35	25.08
4	4	4	14.60	17.49
5	4	4	12.43	-13.47
6	4	4	7.83	-4.82
7	4	4	20.69	21.91
8	4	4	0.00	-0.25
9	4	4	5.63	-6.04
10	4	4	5.50	-6.33
11	4	4	5.59	7.65
13	4	4	4.20	-5.68
-1	4	4	13.52	11.22
-2	4	4	19.22	-18.51
-3	4	4	17.79	-21.71
-4	4	4	4.46	2.86
-5	4	4	10.95	13.14
-6	4	4	9.82	-10.91
-7	4	4	8.15	-8.03
-8	4	4	7.95	9.95
-9	4	4	9.43	-8.82
-10	4	4	3.68	9.66
-12	4	4	0.00	-0.60
0	5	4	12.32	-11.75
1	5	4	8.19	-9.26
2	5	4	10.21	10.03
3	5	4	16.57	-23.10
4	5	4	7.05	8.96
-1	5	4	6.99	-4.90
-2	5	4	6.10	5.32
-3	5	4	9.14	9.32
-4	5	4	12.74	-12.09
-5	5	4	12.68	-14.91
-6	5	4	7.41	9.20
-7	5	4	7.84	9.36
-8	5	4	16.71	-24.55
-10	5	4	7.05	11.50
-11	5	4	5.10	5.08
0	6	4	11.42	-9.85
1	6	4	0.00	-6.70
2	6	4	11.10	14.10
3	6	4	0.00	5.33
4	6	4	13.27	-16.76
-2	6	4	7.66	9.78
-3	6	4	0.00	2.56
-4	6	4	10.64	-14.05
2	7	4	6.03	-5.35
3	7	4	0.00	3.08
-1	7	4	11.64	-11.50
-4	7	4	9.82	12.62
1	0	5	16.85	-7.10
3	0	5	1.08	-3.93
5	0	5	18.92	22.22
7	0	5	0.00	0.53
9	0	5	13.89	17.96
11	0	5	5.25	4.10
13	0	5	6.03	9.86
15	0	5	8.82	-12.74
-1	0	5	18.84	24.21
-3	0	5	40.57	37.92
-5	0	5	8.44	-9.42
-7	0	5	29.10	-35.34
-9	0	5	6.92	12.53
-11	0	5	12.00	-13.39
-13	0	5	5.25	-5.01
-15	0	5	11.62	-19.32
-17	0	5	8.32	14.50
0	1	5	26.43	22.23
1	1	5	21.85	-18.54
2	1	5	2.38	5.03
3	1	5	29.51	34.52
4	1	5	30.28	29.43
5	1	5	17.23	-18.34
6	1	5	9.17	7.27
7	1	5	8.36	9.29
8	1	5	5.46	4.01
10	1	5	4.85	-6.94
11	1	5	12.83	14.14
12	1	5	4.68	4.77
-1	1	5	18.30	-14.04
-2	1	5	11.39	2.07
-3	1	5	42.65	-42.83
-4	1	5	0.00	-1.18
-5	1	5	26.12	28.58
-6	1	5	33.01	-36.31
-7	1	5	18.15	-17.77
-8	1	5	0.00	-2.60
-9	1	5	10.82	12.50
-10	1	5	8.52	-10.52
-11	1	5	0.00	-4.42
-12	1	5	0.00	0.85
-15	1	5	7.57	-14.54
0	2	5	0.00	-2.46
1	2	5	4.75	-3.00
2	2	5	2.34	-1.60
3	2	5	12.73	13.03
4	2	5	8.49	6.92
5	2	5	11.43	12.78
6	2	5	7.70	-10.10
7	2	5	14.94	16.75
8	2	5	3.15	2.50
9	2	5	7.25	-8.29
10	2	5	0.00	-3.21
11	2	5	3.91	-2.23
12	2	5	3.05	7.71
13	2	5	4.43	-6.96
-1	2	5	18.96	-21.09
-2	2	5	6.25	5.58
-3	2	5	23.03	-25.97
-4	2	5	11.75	13.17
-5	2	5	13.35	-10.42
-6	2	5	0.00	-2.82
-7	2	5	18.33	19.34
-8	2	5	20.12	-24.88
-9	2	5	3.73	-4.18
-10	2	5	0.00	2.47
-11	2	5	0.00	0.85
-13	2	5	0.00	-6.53
-14	2	5	3.03	7.23
0	3	5	12.46	-8.84
1	3	5	0.00	3.37
2	3	5	18.44	16.29
3	3	5	1.10	-1.71
4	3	5	23.85	-23.02
5	3	5	9.66	8.90
6	3	5	6.53	7.02
7	3	5	0.00	-1.90
8	3	5	7.65	-8.55
9	3	5	3.15	-2.57
10	3	5	10.31	10.42
-1	3	5	0.00	0.16
-2	3	5	26.71	23.80
-3	3	5	11.22	11.92
-4	3	5	23.92	-23.23
-5	3	5	0.00	-3.73
-6	3	5	10.94	7.52
-7	3	5	0.00	-3.94
-8	3	5	18.67	-24.52
-9	3	5	0.00	2.54
-10	3	5	7.01	6.26
-11	3	5	0.00	4.20
-13	3	5	0.00	2.49
-14	3	5	4.77	8.78
0	4	5	7.04	5.78
1	4	5	0.00	0.67
2	4	5	8.90	9.49
3	4	5	0.00	0.87
4	4	5	7.24	-6.42
5	4	5	4.58	3.28
6	4	5	0.00	-1.69
7	4	5	5.63	6.02
8	4	5	10.20	-9.86
9	4	5	4.65	1.01
10	4	5	4.87	6.21
11	4	5	0.00	1.14
12	4	5	4.64	-7.78
-1	4	5	7.71	7.32
-2	4	5	2.13	3.74
-3	4	5	0.00	-1.50
-4	4	5	12.11	14.23
-5	4	5	2.71	-6.50
-6	4	5	0.00	1.55
-7	4	5	7.11	-6.94
-8	4	5	11.14	10.47
-9	4	5	0.00	-3.53
-10	4	5	6.01	-8.47
-12	4	5	3.42	7.00
-14	4	5	5.42	-10.92
0	5	5	15.25	17.00
1	5	5	7.92	6.50
2	5	5	7.51	-6.80
3	5	5	0.00	-0.69
4	5	5	9.38	10.88
5	5	5	9.45	10.24
7	5	5	7.35	-8.71
8	5	5	7.79	9.10
-1	5	5	10.02	-12.80
-2	5	5	8.17	-9.94
-3	5	5	13.22	12.46
-4	5	5	6.28	5.42
-5	5	5	5.30	-5.00
-6	5	5	4.26	-4.16
-7	5	5	8.85	9.07
-10	5	5	6.36	-10.54
-11	5	5	7.14	10.51
-13	5	5	5.29	-5.01
0	6	5	3.90	-4.68
1	6	5	6.85	9.58
2	6	5	6.15	-6.92
3	6	5	5.96	6.40
4	6	5	3.70	5.53
-2	6	5	8.42	11.10
-3	6	5	8.26	-11.28
2	7	5	0.00	1.54
3	7	5	7.01	8.00
-1	7	5	12.93	13.76
-3	7	5	6.30	-7.71
-4	7	5	6.53	7.64
0	0	6	31.67	-30.70
2	0	6	0.90	3.82
4	0	6	26.88	-26.44
6	0	6	12.66	15.45
8	0	6	24.00	-27.82
10	0	6	11.08	-11.80
14	0	6	0.00	0.44
-2	0	6	66.78	65.40
-4	0	6	9.75	-4.04
-6	0	6	26.63	29.57
-8	0	6	1.78	-3.22
-10	0	6	13.43	14.00
-12	0	6	10.93	-17.99
-14	0	6	0.00	5.28
-16	0	6	5.07	3.46
0	1	6	20.32	-14.67
1	1	6	3.92	4.26
2	1	6	14.61	10.49
3	1	6	0.00	0.37
4	1	6	12.02	-13.76
5	1	6	10.42	-8.20
6	1	6	9.88	10.35
7	1	6	8.09	10.54
8	1	6	15.35	-17.67
9	1	6	15.87	-19.42
10	1	6	16.79	22.63
11	1	6	0.00	-1.34
12	1	6	7.11	-10.51
13	1	6	3.57	-7.10
-1	1	6	19.50	17.11
-2	1	6	19.22	21.64
-3	1	6	9.24	-3.78
-4	1	6	35.68	35.64
-5	1	6	13.67	-11.99
-7	1	6	17.55	17.83
-8	1	6	7.15	-9.32
-9	1	6	8.25	10.30
-10	1	6	7.37	-6.35
-11	1	6	3.06	5.79
-12	1	6	6.52	12.54
-14	1	6	4.95	-8.45
-15	1	6	0.00	4.70
0	2	6	36.66	36.27
1	2	6	20.73	21.33
2	2	6	15.64	-14.76
3	2	6	7.22	-8.25
4	2	6	17.83	-18.33
5	2	6	25.03	24.82
6	2	6	13.53	-14.11
7	2	6	17.95	-17.45
8	2	6	14.00	13.48
9	2	6	0.00	-3.66
10	2	6	4.52	4.26
12	2	6	0.00	-0.53
15	2	6	1.31	0.35
-1	2	6	17.45	-15.30
-2	2	6	7.33	-3.53
-3	2	6	33.75	30.54
-4	2	6	20.43	18.11
-5	2	6	22.98	-24.52
-6	2	6	4.50	7.82
-7	2	6	6.27	6.71
-8	2	6	12.08	16.14
-9	2	6	0.00	-2.21
-10	2	6	14.66	-21.47
-11	2	6	9.79	11.29
-13	2	6	6.24	-8.70
-14	2	6	2.92	-4.52
0	3	6	11.08	-10.53
1	3	6	18.74	16.35
2	3	6	19.75	-20.81
3	3	6	0.00	-1.70
4	3	6	5.31	5.92
5	3	6	15.32	17.80
6	3	6	12.22	10.55
7	3	6	14.25	-18.39
8	3	6	0.00	-0.16
9	3	6	10.27	12.54
10	3	6	0.00	-1.87
11	3	6	11.44	-15.60
13	3	6	3.94	8.53
-1	3	6	6.53	-5.71
-2	3	6	5.97	-6.38
-3	3	6	0.00	0.61
-4	3	6	9.60	-8.55
-5	3	6	6.34	7.75
-6	3	6	0.00	-3.42
-7	3	6	6.71	-5.93
-8	3	6	16.01	22.48
-10	3	6	9.47	12.64
-11	3	6	3.11	-6.77
-12	3	6	7.41	-9.80
-14	3	6	0.00	-5.76
0	4	6	0.00	1.01
1	4	6	19.06	-18.94
2	4	6	6.63	-7.54
3	4	6	5.67	5.06
4	4	6	12.96	14.89
5	4	6	13.60	-13.14
6	4	6	8.53	-7.10
7	4	6	0.00	2.12
8	4	6	0.00	-1.64
9	4	6	5.59	-5.12
10	4	6	4.10	-3.52
11	4	6	0.00	0.82
-1	4	6	18.51	20.78
-2	4	6	5.30	-4.18
-3	4	6	15.26	-11.94
-4	4	6	12.75	16.89
-5	4	6	7.37	6.14
-6	4	6	6.58	-4.53
-7	4	6	19.28	-23.67
-8	4	6	0.00	0.44
-9	4	6	6.01	6.71
-10	4	6	0.00	3.48
-12	4	6	3.27	3.32
-13	4	6	4.21	8.25
-14	4	6	2.57	-4.76
0	5	6	0.00	-4.45
1	5	6	0.00	-2.80
2	5	6	9.67	-10.39
4	5	6	6.10	4.83
5	5	6	14.08	-15.63
6	5	6	7.50	-10.57
8	5	6	7.05	8.84
9	5	6	5.19	-6.80
-1	5	6	8.75	8.96
-2	5	6	2.23	-2.00
-3	5	6	2.91	3.29
-5	5	6	6.09	7.35
0	6	6	13.05	-12.57
1	6	6	0.00	0.26
2	6	6	6.30	9.60
3	6	6	0.00	0.44
4	6	6	7.22	-10.69
-2	6	6	5.51	7.25
-3	6	6	0.00	0.96
3	7	6	0.00	5.27
4	7	6	3.14	-5.71
-1	7	6	0.00	-1.78
-3	7	6	0.00	4.94
1	0	7	35.26	34.47
3	0	7	32.44	-35.00
5	0	7	21.27	18.07
7	0	7	16.56	-20.39
9	0	7	13.74	16.09
11	0	7	0.00	-1.92
13	0	7	10.22	10.36
-1	0	7	32.46	-33.75
-3	0	7	15.49	12.13
-5	0	7	33.39	-37.35
-7	0	7	0.00	1.40
-9	0	7	6.45	-6.41
-11	0	7	0.00	1.53
-13	0	7	0.00	4.56

Table 6 (*cont.*)

-15	0	7	2.27	-3.97
-17	0	7	2.79	7.53
0	1	7	9.16	-9.77
1	1	7	5.33	-10.13
2	1	7	7.35	-8.61
3	1	7	6.67	9.00
4	1	7	10.50	-10.23
5	1	7	0.00	6.25
6	1	7	11.07	10.97
7	1	7	15.49	-16.39
8	1	7	8.71	9.37
9	1	7	0.00	4.82
10	1	7	8.83	9.78
11	1	7	5.53	-8.12
12	1	7	4.69	-7.19
13	1	7	4.34	6.89
-1	1	7	5.45	-7.32
-2	1	7	35.17	-37.46
-3	1	7	25.05	-27.48
-4	1	7	0.00	0.63
-5	1	7	20.72	24.74
-7	1	7	19.08	-17.07
-8	1	7	13.86	18.64
-9	1	7	16.59	20.71
-10	1	7	10.64	-11.63
-11	1	7	5.33	-12.02
-12	1	7	5.66	11.85
-13	1	7	8.22	14.00
-15	1	7	4.55	-9.53
0	2	7	33.28	30.91
1	2	7	2.17	2.07
2	2	7	30.38	-32.42
3	2	7	10.63	8.74
4	2	7	20.84	18.18
5	2	7	26.53	-26.72
6	2	7	8.86	-9.04
7	2	7	3.25	6.96
8	2	7	11.48	11.81
9	2	7	3.16	-4.31
10	2	7	12.29	-14.41
12	2	7	2.49	3.71
-1	2	7	16.82	14.20
-2	2	7	22.74	-20.33
-3	2	7	23.08	-20.64
-4	2	7	0.00	1.41
-5	2	7	12.82	15.12
-6	2	7	16.16	-20.39
-7	2	7	0.00	-2.50
-8	2	7	11.07	11.18
-9	2	7	11.01	-11.67
-10	2	7	0.00	0.35
-11	2	7	6.04	-4.10
-13	2	7	6.65	13.67
-14	2	7	5.46	9.69
-15	2	7	5.89	11.12
0	3	7	14.43	-15.32
1	3	7	0.00	-2.92
2	3	7	0.00	-1.76
3	3	7	25.57	-27.00
4	3	7	3.30	2.53
5	3	7	0.00	-1.38
6	3	7	7.39	-6.37
7	3	7	10.39	10.90
8	3	7	6.84	9.14
9	3	7	0.00	1.30
10	3	7	3.33	-5.98
12	3	7	4.17	7.35
13	3	7	4.17	7.40
-1	3	7	21.70	26.98
-2	3	7	9.99	7.65
-3	3	7	7.78	7.53
-4	3	7	17.77	-19.65
-5	3	7	6.03	-6.34
-6	3	7	19.43	22.21
-7	3	7	7.30	6.10
-8	3	7	8.03	-8.56
-10	3	7	16.22	24.70
-11	3	7	10.52	-15.65
-12	3	7	7.90	-11.25
-13	3	7	6.26	-7.53
-14	3	7	2.90	8.77
0	4	7	10.38	-9.84
1	4	7	23.26	-25.18
2	4	7	22.32	25.26
3	4	7	6.02	7.96
4	4	7	5.64	-4.08
5	4	7	0.00	-1.23
6	4	7	17.25	22.01
8	4	7	6.10	-8.22
9	4	7	3.58	-4.89
10	4	7	0.00	1.42
11	4	7	7.87	8.52
-1	4	7	7.37	6.39
-2	4	7	12.21	10.54
-3	4	7	0.00	-3.11
-4	4	7	19.03	-24.51
-5	4	7	0.00	-1.03
-6	4	7	0.00	3.48
-7	4	7	7.97	-8.10
-9	4	7	9.06	11.14
-12	4	7	0.00	-1.03
-13	4	7	3.10	-6.75
0	5	7	0.00	-2.82
1	5	7	6.09	3.59
2	5	7	5.11	-5.39
-1	5	7	6.71	-9.86
-2	5	7	6.10	-3.32
-3	5	7	9.39	9.51
-6	5	7	9.11	-12.50
-9	5	7	6.70	-12.74
-11	5	7	4.61	8.41
0	6	7	3.36	-0.28
1	6	7	6.32	9.75
2	6	7	0.00	-0.53
3	6	7	6.96	-11.75
-1	6	7	12.01	-13.70
-2	6	7	0.00	0.58
-3	6	7	5.85	6.11
-1	7	7	2.98	3.52
0	0	8	12.73	13.55
2	0	8	0.00	1.42
4	0	8	30.52	32.13
6	0	8	7.97	-8.35
8	0	8	0.00	2.08
10	0	8	8.32	-10.02
-2	0	8	4.75	8.41
-4	0	8	18.85	19.42
-6	0	8	7.64	-12.72
-8	0	8	16.75	-23.10
-10	0	8	7.96	8.07
-12	0	8	5.02	-5.60
-14	0	8	0.00	8.24
-16	0	8	2.02	-8.00
0	1	8	17.45	-13.85
1	1	8	0.00	-2.02
2	1	8	17.57	17.22
3	1	8	9.32	11.84
4	1	8	9.90	-12.20
5	1	8	4.83	-6.04
7	1	8	0.00	0.21
8	1	8	0.00	2.04
9	1	8	5.39	6.47
10	1	8	9.54	12.13
11	1	8	4.22	4.67
-1	1	8	3.69	5.24
-2	1	8	14.78	18.21
-3	1	8	0.00	-0.42
-4	1	8	7.12	-7.59
-5	1	8	23.12	23.96
-6	1	8	19.94	19.67
-7	1	8	10.89	-11.81
-8	1	8	24.59	-27.92
-11	1	8	5.64	-9.39
-15	1	8	4.33	-8.40
-16	1	8	3.65	-8.18
0	2	8	0.00	1.42
1	2	8	1.64	-1.82
2	2	8	22.69	27.76
3	2	8	9.38	12.17
4	2	8	0.00	0.76
5	2	8	7.30	-7.61
6	2	8	3.25	3.35
7	2	8	13.23	15.64
8	2	8	0.00	-0.99
9	2	8	0.00	-2.17
10	2	8	5.07	4.35
12	2	8	8.28	-11.14
-1	2	8	0.00	1.35
-2	2	8	22.46	-20.50
-3	2	8	18.35	-18.37
-4	2	8	14.11	-15.96
-5	2	8	5.92	5.04
-6	2	8	0.00	-1.32
-7	2	8	8.26	9.70
-8	2	8	0.00	1.00
-9	2	8	6.91	-7.87
-10	2	8	5.08	-6.27
-11	2	8	3.82	3.53
-12	2	8	7.28	9.64
-15	2	8	2.07	5.89
0	3	8	22.24	19.81
1	3	8	10.80	10.38
3	3	8	14.46	-14.29
4	3	8	7.67	-6.99
5	3	8	7.00	5.82
6	3	8	3.77	-3.78
7	3	8	0.00	-1.66
8	3	8	0.00	0.07
9	3	8	4.55	4.10
10	3	8	7.82	-10.01
-1	3	8	11.65	-10.98
-2	3	8	0.00	-0.35
-3	3	8	15.18	18.40
-4	3	8	9.91	-6.60
-5	3	8	15.38	-18.14
-7	3	8	13.76	12.03
-8	3	8	0.00	2.92
-9	3	8	13.30	-21.18
-10	3	8	4.75	-7.46
-11	3	8	0.00	3.27
-13	3	8	2.94	-8.13
-14	3	8	5.04	7.25
0	4	8	1.89	-1.65
1	4	8	0.00	3.96
2	4	8	0.00	-1.35
3	4	8	11.32	-12.65
4	4	8	0.00	-0.67
6	4	8	7.82	8.42
8	4	8	4.82	-4.77
9	4	8	7.11	8.21
-1	4	8	6.33	-5.32
-2	4	8	13.04	13.84
-4	4	8	3.01	-2.46
-5	4	8	3.67	3.79
-6	4	8	0.00	-4.87
-7	4	8	3.60	4.25
-9	4	8	7.57	10.25
-13	4	8	2.25	6.83
0	5	8	7.01	7.53
2	5	8	5.67	-4.45
3	5	8	6.37	9.34
6	5	8	7.20	-8.26
-1	5	8	10.52	12.45
-2	5	8	6.02	-5.07
-3	5	8	6.39	-8.21
-4	5	8	13.30	15.04
-6	5	8	5.67	-6.75
-8	5	8	5.25	6.31
-10	5	8	4.87	-8.45
0	6	8	6.51	6.71
1	6	8	0.00	1.50
3	6	8	0.00	1.64
-1	6	8	0.00	-1.40
-3	6	8	0.00	-0.18
1	0	9	0.00	-3.82
3	0	9	6.94	-4.76
5	0	9	18.01	17.23
7	0	9	9.72	-10.64
9	0	9	6.35	-10.03
11	0	9	0.00	0.93
-1	0	9	20.18	-21.28
-3	0	9	13.37	10.30
-5	0	9	22.24	-19.31
-7	0	9	7.72	13.57
-9	0	9	5.92	7.36
-11	0	9	15.89	19.28
-13	0	9	6.51	-9.58
-15	0	9	0.00	4.64
0	1	9	6.57	-5.51
1	1	9	10.28	9.87
2	1	9	0.00	-1.25
3	1	9	0.00	1.81
4	1	9	7.24	-8.85
5	1	9	6.84	8.99
7	1	9	19.02	-21.31
8	1	9	12.41	-13.67
11	1	9	3.68	-6.39
-1	1	9	10.89	-12.07
-2	1	9	10.50	13.12
-3	1	9	13.76	14.42
-4	1	9	7.35	9.32
-5	1	9	5.71	6.27
-6	1	9	0.00	0.63
-7	1	9	0.00	-3.38
-8	1	9	0.00	-2.74
-11	1	9	4.03	3.43
0	2	9	1.53	3.94
1	2	9	6.81	-7.38
2	2	9	6.36	-6.83
3	2	9	0.00	0.46
4	2	9	3.96	3.53
5	2	9	3.91	-7.14
6	2	9	8.24	-8.87
7	2	9	2.98	2.97
8	2	9	3.96	4.75
9	2	9	4.80	6.66
10	2	9	2.25	4.22
11	2	9	1.82	-0.42
-1	2	9	0.00	4.21
-2	2	9	16.46	-12.95
-3	2	9	0.00	0.88
-4	2	9	14.60	15.10
-5	2	9	22.50	20.46
-6	2	9	0.00	-1.30
-7	2	9	0.00	-1.86
-8	2	9	6.03	9.57
-10	2	9	3.74	-3.90
-11	2	9	5.03	-5.89
-12	2	9	5.73	9.43
-15	2	9	1.53	-6.34
0	3	9	14.29	13.78
3	3	9	0.00	2.53
4	3	9	9.31	10.39
6	3	9	9.65	-12.00
7	3	9	3.79	3.34
8	3	9	4.60	6.61
10	3	9	6.58	-9.41
-1	3	9	0.00	1.03
-2	3	9	6.14	-4.13
-3	3	9	8.70	-8.72
-4	3	9	0.00	4.35
-5	3	9	0.00	-2.93
-7	3	9	0.00	-1.11
-9	3	9	0.00	0.43
-10	3	9	0.00	0.35
0	4	9	11.35	-13.47
1	4	9	2.39	-4.42
3	4	9	2.50	3.60
4	4	9	5.06	-4.42
6	4	9	0.00	1.79
8	4	9	0.00	1.65
9	4	9	3.25	-3.91
-1	4	9	1.46	1.36
-2	4	9	4.45	4.70
-4	4	9	6.61	-6.67
-5	4	9	0.00	4.33
-6	4	9	7.76	8.55
-7	4	9	0.00	1.50
-8	4	9	8.41	-10.83
-9	4	9	4.35	5.16
0	5	9	4.52	-6.56
2	5	9	0.00	4.85
3	5	9	6.85	8.59
4	5	9	6.47	-9.00
-2	5	9	1.60	1.97
-3	5	9	5.08	-4.85
-6	5	9	3.59	3.67
-7	5	9	3.42	-3.89
0	6	9	0.00	2.90
1	6	9	3.03	4.34
-1	6	9	4.40	-5.02
0	0	10	13.17	13.42
2	0	10	24.73	-30.46
4	0	10	14.29	14.98
6	0	10	0.00	-2.76
8	0	10	17.21	16.81
10	0	10	0.00	-1.54
-2	0	10	15.67	-14.84
-4	0	10	14.20	12.25
-6	0	10	12.69	-14.32
-8	0	10	6.68	5.71
-10	0	10	0.00	-4.59
-12	0	10	3.50	-1.61
-14	0	10	0.00	-0.52
0	1	10	7.65	-7.51
1	1	10	0.00	-1.40
4	1	10	8.93	9.00
5	1	10	5.75	6.96
8	1	10	3.75	4.27
-1	1	10	0.00	1.36
-2	1	10	0.00	0.23
-3	1	10	5.39	-9.62
-4	1	10	14.35	-17.50
-5	1	10	0.00	-0.24
-6	1	10	5.27	3.54
-7	1	10	7.97	-10.41
-8	1	10	9.35	-9.49
-9	1	10	3.51	5.49
-10	1	10	10.29	14.57
-11	1	10	2.57	-4.35
0	2	10	8.60	-10.91
1	2	10	15.78	-18.42
2	2	10	7.08	9.24
3	2	10	11.23	11.11
4	2	10	6.78	-6.92
5	2	10	11.37	-12.82
6	2	10	0.00	2.96
7	2	10	5.79	7.70
8	2	10	4.04	-5.64
9	2	10	4.90	-5.10
10	2	10	2.33	3.08
-1	2	10	10.89	12.31
-2	2	10	6.22	3.14
-3	2	10	10.80	-10.89
-4	2	10	8.42	-10.24
-5	2	10	8.17	10.63
-6	2	10	3.16	3.35
-7	2	10	6.61	-7.42
-8	2	10	3.72	-4.00
-10	2	10	2.76	4.36
-11	2	10	0.00	-3.72
0	3	10	0.00	0.71
7	3	10	4.41	7.17
-1	3	10	7.35	-7.14
-2	3	10	0.00	4.60
-3	3	10	5.92	5.17
-4	3	10	0.00	1.66
-5	3	10	12.67	-12.79
-7	3	10	7.56	10.26
-9	3	10	3.19	-5.03
-10	3	10	0.00	-2.81
-11	3	10	6.94	11.90
0	4	10	9.46	-10.17
1	4	10	10.86	11.54
3	4	10	2.95	-6.47
4	4	10	5.53	-6.19
5	4	10	8.39	10.16
6	4	10	4.21	4.72
7	4	10	5.65	-8.21
-1	4	10	8.49	-7.64
-2	4	10	9.12	8.53
-3	4	10	12.78	13.60
-4	4	10	0.00	-0.60
-5	4	10	5.54	-7.69
0	5	10	0.00	-0.39
3	5	10	3.57	5.78
4	5	10	0.00	2.73
-2	5	10	6.05	-7.20
-3	5	10	0.00	-4.20
-4	5	10	5.89	6.39
1	0	11	5.49	-5.99
3	0	11	12.50	14.09
5	0	11	11.81	-10.62
7	0	11	3.40	5.08
9	0	11	8.79	-10.46
-1	0	11	12.51	13.24
-3	0	11	0.00	-2.43
-5	0	11	6.28	8.09
-7	0	11	0.00	1.16
-9	0	11	0.00	-4.80
-11	0	11	0.00	4.52
0	1	11	1.78	-2.39
1	1	11	5.48	6.64
2	1	11	4.73	5.14
3	1	11	5.14	-6.82
-1	1	11	7.67	-7.62
-2	1	11	8.17	10.62
-3	1	11	12.63	15.96
-4	1	11	2.92	-3.37
-5	1	11	6.48	-7.99
-6	1	11	6.04	6.85
-7	1	11	11.80	14.56
-8	1	11	5.36	-8.26
-9	1	11	8.65	-13.48
-10	1	11	4.46	5.38
-13	1	11	3.63	-7.06
0	2	11	1.41	-4.57
1	2	11	2.93	4.82
2	2	11	11.79	12.92
3	2	11	2.35	-4.16
4	2	11	7.95	-8.72
5	2	11	7.24	7.35
6	2	11	4.53	5.72
7	2	11	3.80	-5.43
-1	2	11	0.00	-1.14
-2	2	11	6.80	6.39
-3	2	11	0.00	2.52
-4	2	11	2.99	-2.62
-5	2	11	0.00	-6.20
-6	2	11	2.89	4.82
-7	2	11	0.00	-3.14
-11	2	11	2.94	-2.12
0	3	11	9.11	10.78
2	3	11	6.75	-7.41
-1	3	11	0.00	-1.64
-2	3	11	9.11	-8.89
-3	3	11	2.20	-3.98
-4	3	11	7.40	8.89
-5	3	11	0.00	-2.50
-6	3	11	7.96	-12.21
-8	3	11	7.57	11.75
-10	3	11	6.18	-13.54
0	4	11	0.00	1.32
1	4	11	5.64	8.37
2	4	11	7.53	-12.04
4	4	11	4.17	4.84
-2	4	11	0.00	-0.96
-3	4	11	4.39	3.71
-4	4	11	4.14	5.70
-5	4	11	6.88	-4.15
0	0	12	0.00	-0.93
2	0	12	0.96	-4.72
4	0	12	0.00	-1.91
6	0	12	0.00	0.07
-2	0	12	7.82	-9.10
-4	0	12	0.00	-0.09
-6	0	12	4.89	-4.24
-8	0	12	6.32	10.99
0	1	12	7.04	8.25
2	1	12	2.64	-4.36
3	1	12	3.88	-5.37
6	1	12	7.29	-7.32
-1	1	12	0.00	-1.26
-2	1	12	5.80	-8.35
-3	1	12	0.00	3.96
-4	1	12	0.00	1.46
-5	1	12	2.53	-5.42
-6	1	12	4.61	-5.51
-7	1	12	0.00	1.80
-8	1	12	2.23	7.13
0	2	12	0.00	-2.25
1	2	12	0.00	-3.28
2	2	12	0.00	-4.34
-2	2	12	5.82	6.96
-4	2	12	0.00	0.06
-5	2	12	4.72	6.31
-6	2	12	4.23	6.35
-7	2	12	4.03	-6.19
0	3	12	7.92	-8.35
1	3	12	2.91	-2.33
2	3	12	0.00	-0.92
-1	3	12	7.57	9.70
-2	3	12	0.00	0.23
-3	3	12	5.57	-5.78
-5	3	12	5.22	6.60
0	4	12	1.39	-0.17
-2	4	12	3.69	-5.62
-3	4	12	4.39	5.24
-5	4	12	4.86	-7.21
1	0	13	6.17	-6.48
3	0	13	6.93	5.57
-1	0	13	7.47	8.46
-3	0	13	7.82	-8.09
-5	0	13	10.10	15.03
0	1	13	1.85	2.42
-2	1	13	0.00	-2.45
-4	1	13	4.85	-8.53
-5	1	13	4.18	-7.04
-7	1	13	4.27	7.19
0	2	13	4.01	-5.00
1	2	13	2.05	3.46
2	2	13	5.83	7.00
-2	2	13	7.39	8.96
-3	2	13	3.64	1.95
-4	2	13	5.92	-8.01
-5	2	13	5.66	-9.42

Description and discussion of the structure of *trans*-AMCHA.HBr

The molecular structure

The bond lengths and angles of *trans*-AMCHA found in the hydrobromide are shown in Fig. 3. The standard deviations in bond lengths and angles are;

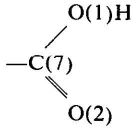
$\sigma(\text{C–C}) = 0{\cdot}030$ Å　　$\sigma(\text{C–C–C}) = 1{\cdot}7°$
$\sigma(\text{C–N}) = 0{\cdot}026$　　$\sigma(\text{C–C–N}) = 1{\cdot}6$
$\sigma(\text{C–O}) = 0{\cdot}026$　　$\sigma(\text{C–C–O}) = 1{\cdot}8$
$\sigma(\text{Br–N}) = 0{\cdot}018$

A view of the molecule along the axis C(7)–C(1) is shown in Fig. 4. It is seen that the cyclohexane ring exists in the chair form with the aminomethyl and carboxyl groups attached equatorially to the ring at the 4 and 1 positions. Bond lengths and angles within the ring have almost the normal values. The mean C–C bond length is 1·551 Å and the mean C–C–C angle is 110·4°. There is only a slight distortion from the perfect chair conformations.

Table 7. *trans*-AMCHA . HBr. *Perpendicular distances from the least-squares plane through atoms* O(1), O(2), C(1) *and* C(7)

O(1)	0·006 Å
O(2)	0·007
C(1)	0·005
C(7)	−0·017

The carboxyl group is almost planar. The deviations of the atoms from the least-squares plane through C(1), C(7), O(1) and O(2) are given in Table 7. As shown in Fig. 4, this plane is tilted at an angle of about 27° to the plane containing the atoms C(1), C(7) and the bisector of the angle C(2)–C(1)–C(6). Such rotation of the carboxyl group about the axis C(1)–C(7) would easily result from the forces involved in the hydrogen bonding. As can be seen in Figs. 4 and 6, there are two strong hydrogen bonds, O(1)H · · · Br and O(2) · · · NH_3^+, and they are connected to the carboxyl group in a direction which may result in an increase of the angle of rotation. A significant difference between the two C–O distances, C(7)–O(1) = 1·30 Å, C(7)–O(2) = 1·20 Å, indicates that the carboxyl group exists in the un-ionized form,



$$—\text{C(7)}\begin{smallmatrix}\diagup \text{O(1)H}\\ \diagdown\!\!\diagdown \text{O(2)}\end{smallmatrix}$$

The amino nitrogen atom is situated almost exactly at the *trans* position to the C(5) atom. The angle of internal rotation around the bond C(4)–C(8) is 178°. As will be shown later, the nitrogen atom exists in a protonated form ($-NH_3^+$). The C–N bond length, 1·46 Å, is somewhat shorter than the standard value, 1·49 Å, found in the terminal C–NH_3^+ bond (Hahn, 1957).

The crystal structure

Two projections of the structure along the *b* and *c* axes are shown in Figs. 5 and 6. The structure consists of alternate layers of bromine atoms and the AMCHA molecules stacked parallel to the (001) plane. Within the latter layer the molecules are piled up one another in the **a** direction, with their amino group protruding out into the layer of negatively charged bromine atoms.

The distribution of oxygen and bromine atoms around the nitrogen atom is shown by the stereographic projection (Fig. 7) in which the direction of the C–N bond is taken as the polar axis and the suggested N–H directions are indicated. The atom O(2) and the two bromine atoms are arranged approximately in the tetrahedral directions with the maximum deviation of about 28°, and this fact suggests the existence of hydrogen bonds between the nitrogen and these atoms. These hydrogen bonds hold the molecules firmly against the bromine layer, while the bromine atoms are bound together to form a layer through these links. There is another hydrogen bond (3·18 Å) between the carboxyl oxygen atom O(1) and Br uniting the tail of the molecule to the adjacent bromine layer. These

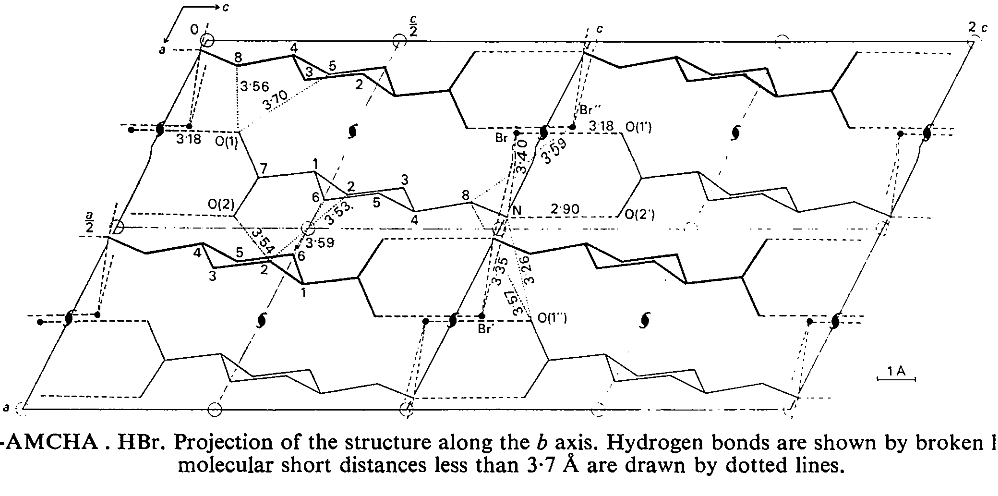


Fig. 5. *trans*-AMCHA . HBr. Projection of the structure along the *b* axis. Hydrogen bonds are shown by broken lines and intermolecular short distances less than 3·7 Å are drawn by dotted lines.

hydrogen bonds are shown by broken lines in Figs. 5 and 6, in which the intermolecular short contacts less than 3·7 Å are also shown by dotted lines.

Description and discussion of the structure of *cis*-AMCHA.HCl

The molecular structure

The bond lengths and angles of *cis*-AMCHA found in the hydrochloride are shown in Fig. 8. The average standard deviations in bond lengths and angles are:

$\sigma(\mathrm{C{-}C}) = 0{\cdot}018$ Å $\sigma(\mathrm{C{-}C{-}C}) = 1{\cdot}0^\circ$
$\sigma(\mathrm{C{-}N}) = 0{\cdot}015$ $\sigma(\mathrm{C{-}C{-}N}) = 0{\cdot}9$
$\sigma(\mathrm{C{-}O}) = 0{\cdot}017$ $\sigma(\mathrm{C{-}C{-}O}) = 1{\cdot}2$
$\sigma(\mathrm{Cl{-}N}) = 0{\cdot}011$

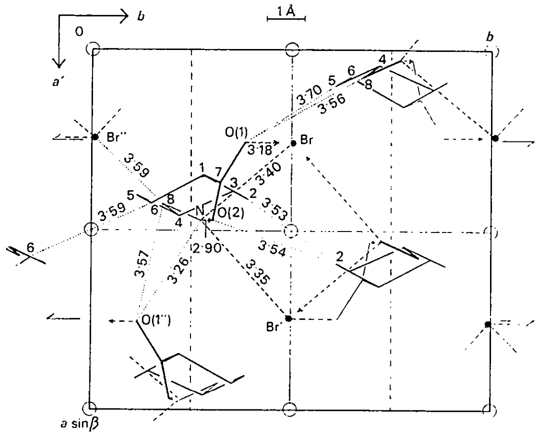


Fig. 6. *trans*-AMCHA . HBr. Projection of the structure along the *c* axis.

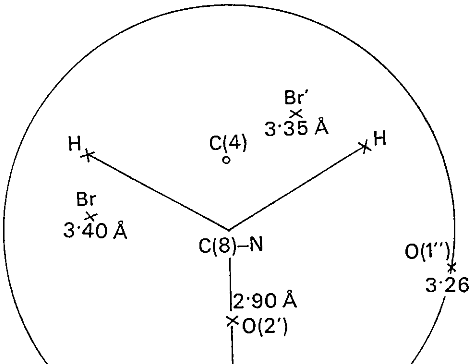


Fig. 7. *trans*-AMCHA . HBr. Stereographic projection showing the distribution of oxygen and bromine atoms around the amino nitrogen atom. Distances from the nitrogen atom are indicated. The direction of the C–N bond is taken as the polar axis. The suggested N–H directions are also indicated.

As in the case of *trans*-AMCHA, the cyclohexane ring also exists in the chair form. However, in *cis*-AMCHA, the carboxyl group is axially oriented from the ring while the aminomethyl group takes equatorial conformation. The alternative conformation of equatorial carboxyl group and axial aminomethyl group, which may result from the purely conformational inversion (the chair inversion), is not found in the present case*. The cyclohexane ring is quite regular, with the mean value of the C–C bond lengths, 1·540 Å, and that of the C–C–C angles, 110·8°.

Table 8. *cis*-AMCHA . HCl. *Perpendicular distances from the least-squares plane through atoms* O(1), O(2), C(1) *and* C(7)

O(1)	−0·002 Å
O(2)	−0·003
C(1)	−0·002
C(7)	0·007

The carboxyl group is perfectly planar within the limit of experimental error. The deviations of the atoms from the least-squares plane through atoms C(1), C(7), O(1) and O(2) are given in Table 8. As is shown in Fig. 9(*a*), this plane is tilted at an angle of about 22° to the plane containing C(1)–C(7) and the bisector of the external angle of C(2)–C(1)–C(6). The rotation of the carboxyl group about the axis C(1)–C(7) in this

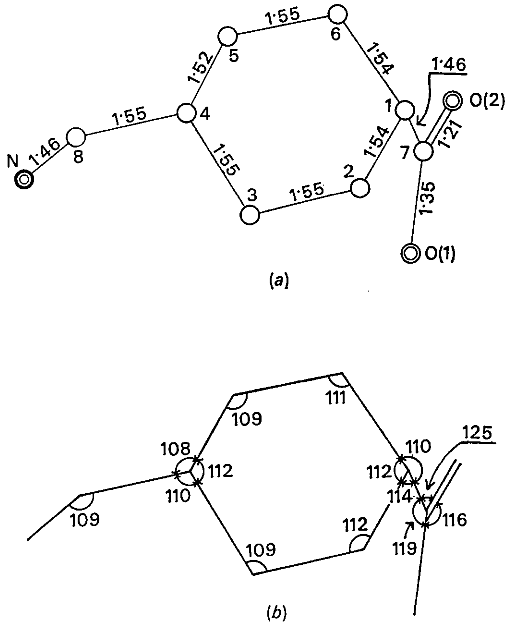


Fig. 8. *cis*-AMCHA . HCl. (*a*) Bond lengths (Å) and (*b*) angles (°) of the *cis*-AMCHA molecule found in the hydrochloride.

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* Recently, the crystal structure of *cis*-AMCHA . HBr (a= 6·006, b=33·13, c=5·520 Å, β=94·0°, space group $P2_1/n$, Z=4) has been determined from two-dimensional intensity data (Kadoya, to be published). It is shown that the molecular structure of *cis*-AMCHA in the hydrobromide is essentially the same as that found in the hydrochloride.

case is such that the C(2) atom is almost eclipsed by O(1). It seems to be that the rotation results from a steric effect between the atom O(1) and the carboxyl group of the neighbouring molecule as shown in Fig. 10. The fact that the carboxyl oxygen atom does not lie at the intermediate position between the C(6) and C(2) atoms may also be interpreted in terms of a steric effect between the carboxyl oxygen and C(5)H_2 or C(3)H_2 of the same molecule, similar to the effect known as the 1,3 interaction. The dimensions of the carboxyl group are rather unusual, for not only is the bond length, 1·46 Å found for C(7)–C(1), significantly shorter than the average C–C single bond length, but also the angle O(1)–C(7)–C(1), 119°, is somewhat larger and O(1)–C(7)–O(2), 116°, is smaller than the corresponding angles found in *trans*-AMCHA . HBr and other compounds containing un-ionized carboxyl groups.

The amino nitrogen atom is situated nearly but not exactly at the *trans* position to the C(5) atom. Fig. 9(*b*) shows the projection of the aminomethyl group viewed along the C(8)–C(4) bond. The angle of the internal rotation around the C(8)–C(4) bond is 163°. The nitrogen atom is also protonated and the C–NH_3^+ distance is again 1·46 Å.

The crystal structure

Two projections of the structure along the *b* and *c* axes are shown in Figs. 10 and 11. The structure contains chains of chlorine atoms arranged along the two-fold screw axes. The distribution of oxygen and chlorine

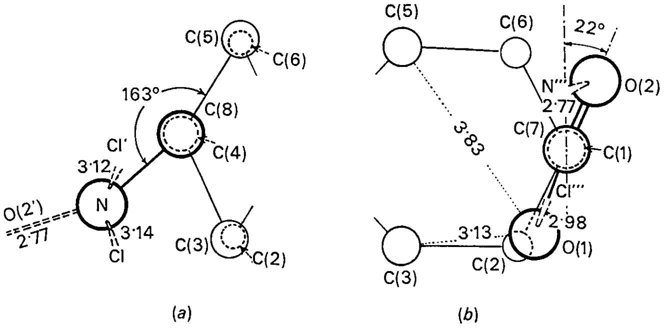

Fig. 9. *cis*-AMCHA . HCl. (*a*) Projection of the carboxyl group along the C(7)–C(1), bond showing the orientation of the carboxyl group. (*b*) Projection of the aminomethyl group along the C(8)–C(4) bond showing the orientation of the aminomethyl group.

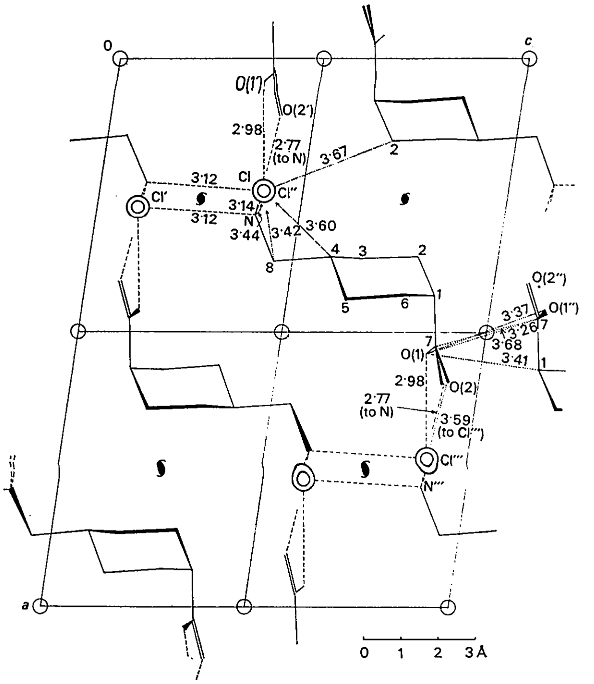

Fig. 10. *cis*-AMCHA . HCl. Projection of the structure along the *b* axis. Hydrogen bonds are shown by broken lines and intermolecular short distances less than 3·7 Å are drawn by dotted lines.

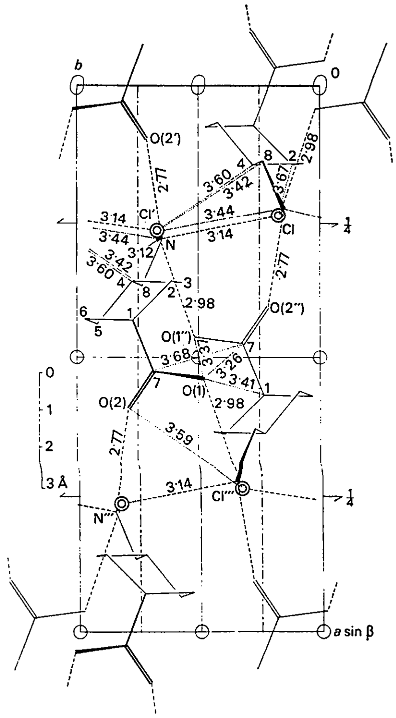

Fig. 11. *cis*-AMCHA . HCl. Projection of the structure along the *c* axis.

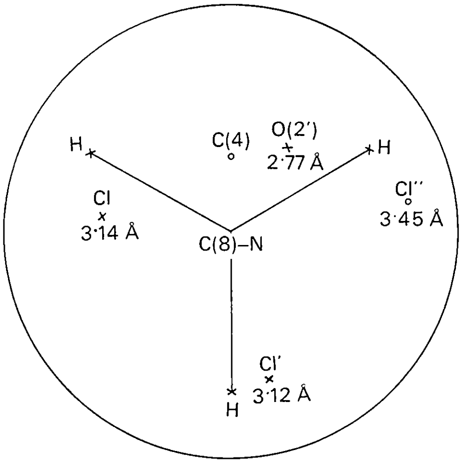

Fig. 12. *cis*-AMCHA . HCl. Stereographic projection showing the distribution of oxygen and chlorine atoms around the amino nitrogen atom. Distances from the nitrogen atom are also given. The direction of the C–N bond is taken as the polar axis. The suggested N–H directions are indicated.

atoms around the nitrogen atom is shown in Fig. 12. It is seen that the three hydrogen bonds (NH · · · Cl, 3·12 Å; NH · · · Cl, 3·14 Å and NH · · · O(2), 2·77 Å) are arranged approximately in tetrahedral directions around the nitrogen atom. In Figs. 10 and 11, the presumed hydrogen bonds are indicated by broken lines. The figures also show the intermolecular short contacts less than 3·7 Å by dotted lines. The molecules are bound to the chain of chlorine atoms through the hydrogen bonds, NH · · · Cl (3·12 Å) and NH · · · Cl (3·14 Å). There is another hydrogen bond (2·98 Å) between the carboxyl oxygen atom O(1) and Cl. This bond and the O(2) · · · HN (2·77 Å) bond hold the carboxyl group firmly within the crystal.

The authors would like to express their sincere thanks to Professor M. Tsuboi for his valuable discussions. They also wish to express their thanks to Dr M. Shimizu, Dr T. Naito and Dr A. Okano of the Central Research Laboratory, Daiichi Seiyaku Co. Ltd for their kindness in supplying the specimens and continued interest throughout the work. Special thanks are also due to the staffs, especially Mr M. Furuhara, Mr G. Ikegami and Miss T. Hiki, of the computation center of the C. Itoh Electronic Computing Service Co. Ltd for their kind cooperation in calculations of full-matrix least-squares on the CDC-G20 computer.

Note added in proof: – The crystal structure of *cis*-AMCHA.HBr has recently been determined independently by Groth & Hassel (1965). The structure is essentially identical with that determined by us (see footnote, this page). We therefore do not contemplate any further work on this substance.

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The Crystal Structure of Barium Diethyl Phosphate

By Yoshimasa Kyogoku and Yoichi Iitaka

Faculty of Pharmaceutical Sciences, University of Tokyo, Hongo, Tokyo, Japan

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Crystals of barium diethyl phosphate, $Ba[(C_2H_5O)_2PO_2]_2$, are monoclinic, with space group $I2/a$, containing four molecules in a unit cell with lattice constants $a = 14·52$, $b = 18·88$, $c = 6·00$ Å and $\beta = 90·0°$. The structure was refined with anisotropic thermal parameters, using three-dimensional reflexions, by the method of least squares. The final reliability index was 0·09. The diethyl phosphate anion was found to take a configuration with the two C–O bonds in the *gauche* positions to the P–O bonds, in agreement with the conclusion reached from a spectroscopic investigation on an aqueous solution of barium dimethyl phosphate. The angles of internal rotation around the C–O and P–O bonds are compared with those of the proposed models for nucleic acids and synthetic polynucleotides.

Introduction

Natural and synthetic polynucleotides consist of chains of alternating diesterified phosphate and ribose or 2'-deoxyribose groups with a purine or pyrimidine base attached to each sugar residue. The backbone of the chains is formed by such repeating units as shown below, each consisting of six bonds: