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The Crystal and Molecular Structure of 2-Deoxy-*cis*-inosa-1,3-diamine Dihydrochloride

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The main reaction product of the hydrogenation of 4,6-dinitropyrogallol on a rhodium–platinum catalyst is a 1,3-diamino-4,5,6-trihydroxycyclohexane. Its dihydrochloride has been the subject of the present crystal-structure determination, in which the molecule is shown to have the all-*cis* configuration and to be 2-deoxy-*cis*-inosa-1,3-diamine. The space group is $P2_1$ with $a=7{\cdot}823$, $b=10{\cdot}173$, $c=13{\cdot}047$ Å, $\beta=91{\cdot}27°$. There are two molecules in the asymmetric unit. The crystal structure has been solved by the heavy-atom method, and refined by least-squares to an R index of 10·6% over 1926 observed reflections.

Introduction

In a recent investigation aimed at the synthesis of 2-deoxystreptamine and some of its configuration isomers Dijkstra (1965) has subjected 4,6-dinitropyrogallol to hydrogenation on a rhodium–platinum catalyst. The main reaction product, isolated in 40–42% yield from the reaction mixture by means of preparative chromatographic techniques, proved to be a diaminocyclohexanetriol, but differed from 2-deoxystreptamine (2-deoxymyoinosa-1,3-diamine) isolated from kanamycin. The present X-ray diffraction study was undertaken to elucidate the configuration of the dihydrochloride of the main reaction product obtained by Dijkstra.

Experimental

Crystals of 2-deoxy-*cis*-inosa-1,3-diamine dihydrochloride are colourless and elongated along [010]. They can be readily obtained from aqueous solutions. The density was measured by flotation in chloroform–bromoform. Approximate lattice constants and systematic absences were determined from Weissenberg photographs about the a and b axes. The lattice constants were refined by least-squares using 133 accurately (0·01–0·02° 2θ) measured lines of a Guinier–de Wolff powder diagram.

Crystal data (λ(Cu $K\alpha$) = 1·5418 Å).

2-Deoxy-*cis*-inosa-1,3-diamine dihydrochloride
$C_6H_7(OH)_3(NH_2)_2.2HCl$; M.W. 255·1.
m.p. > 300 °C (decomposition).

Monoclinic; $a=7{\cdot}823$ (±0·002), $b=10{\cdot}173$ (±0·002), $c=13{\cdot}047$ (±0·003) Å; $\beta=91{\cdot}27$ (±0·02°).

$U=1038{\cdot}2$ Å^3.

$D_m=1{\cdot}503$ g.cm^{-3}, $Z=4$, $D_x=1{\cdot}506$ g.cm^{-3}.

$F(000)=496$.

Absorption for X-rays, $\lambda=1{\cdot}5418$, $\mu=54{\cdot}7$ cm^{-1}.

Absent reflexions: $0k0$ when k is odd. Space group $P2_1$.

The systematic absences left $P2_1$ and $P2_1/m$ as possible choices of space group. The latter possibility was discarded when a piezoelectric effect was observed.

A crystal was ground to a cylinder of 0·21 mm diameter parallel to the b axis, and integrated reflexion intensities of the zero through ninth layers about the b axis were recorded on equi-inclination Weissenberg photographs with Cu $K\alpha$ radiation, the film holder having been loaded with six films to allow the correlation of weak and strong intensities. In the same way the zero and first layer about the a axis were recorded, this time with a spherical crystal of 0·04 cm diameter. All intensity data were obtained from photometer recorder plots, and corrections were applied for background, Lorentz and polarization factors and for specimen absorption. After scaling a set of 1926 independent structure factors was obtained, representing more than 90% of the reflexions accessible in the recorded diagrams, and more than 70% of those in the copper reflexion sphere.

Structure determination and refinement

Since the unit cell contains four molecules a trial structure had to be based on the presence of two independent molecules in the asymmetric unit. In order to solve the crystal structure a three-dimensional Patterson synthesis was computed. Despite fortuitous near-coincidences of the y parameters of three Cl^- ions, resulting in a number of non-Harker peaks in the Harker section of the Patterson synthesis, the position of the eight Cl^- ions was established. As the contribution of the Cl^- ions was expected to dominate the phases of the structure factors to such an extent as to allow the successful application of Fourier methods, further unravelling of the Patterson synthesis was discontinued and a Fourier synthesis based on the phases of the Cl^- ions was computed. This Fourier synthesis revealed some of the lighter atoms. After the inclusion of the latter atoms in the structure factors a second Fourier synthesis showed the position of all atoms.

Refinement was carried out by least-squares, initially with an overall isotropic temperature factor, and in the

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final stages with individual isotropic atomic temperature factors. The refinement program used a 3×3 block-diagonal approximation to the least-squares normal equations. Scattering factors were taken from Moore (1963), and the weighting scheme $w=1/(2{\cdot}84+0{\cdot}033\,.\,F_o+0{\cdot}0095\,.\,F_o^2)$ made $w\,.\,dF^2\simeq1$, independent of the magnitude of F_o. Refinement was continued untill the shifts were small fractions of the standard deviations. The final R index was 10·5% over all observed reflexions. Final parameters are presented in Table 1, together with their e.s.d.'s. Table 2 contains a list of observed and calculated structure factors.

Table 1. *Fractional coordinates and their e.s.d.'s* (Å) *in* 2-*deoxy-cis-inosa*-1,3-*diamine dihydrochloride*

	x	y	z	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$
C(1)	0·3429	0·6595	0·1052	0·013	0·016	0·013
C(2)	0·2357	0·7734	0·0760	0·012	0·016	0·012
C(3)	0·3329	0·8999	0·0890	0·012	0·014	0·012
C(4)	0·4008	0·9164	0·2001	0·011	0·013	0·011
C(5)	0·5077	0·8000	0·2235	0·011	0·013	0·011
C(6)	0·4227	0·6699	0·2146	0·012	0·015	0·012
C(7)	0·0254	0·3199	0·5432	0·012	0·014	0·012
C(8)	−0·1557	0·2775	0·5077	0·013	0·018	0·013
C(9)	−0·1731	0·3099	0·3935	0·013	0·015	0·013
C(10)	−0·0455	0·2302	0·3298	0·012	0·015	0·012
C(11)	0·1304	0·2644	0·3675	0·012	0·015	0·012
C(12)	0·1595	0·2439	0·4854	0·011	0·014	0·011
N(13)	0·2404	0·5346	0·0986	0·010	0·013	0·010
N(14)	0·2271	1·0156	0·0586	0·011	0·013	0·011
N(15)	0·0424	0·2873	0·6553	0·010	0·013	0·010
N(16)	−0·3540	0·2747	0·3611	0·012	0·016	0·012
O(17)	0·2573	0·9300	0·2680	0·009	0·010	0·009
O(18)	0·2926	0·6477	0·2874	0·009	0·010	0·009
O(19)	0·5914	0·8145	0·3253	0·010	0·011	0·010
O(20)	−0·0829	0·0963	0·3377	0·010	0·012	0·010
O(21)	0·1554	0·1099	0·5117	0·009	0·010	0·008
O(22)	0·2600	0·1891	0·3186	0·010	0·012	0·010
Cl(23)	−0·1523	−0·0112	0·1287	0·003	0·004	0·003
Cl(24)	0·1377	0·0367	−0·0808	0·003	0·004	0·003
Cl(25)	0·5305	0·0106	0·5169	0·003	0·004	0·003
Cl(26)	0·4497	0·2746	0·1321	0·003	0·004	0·003

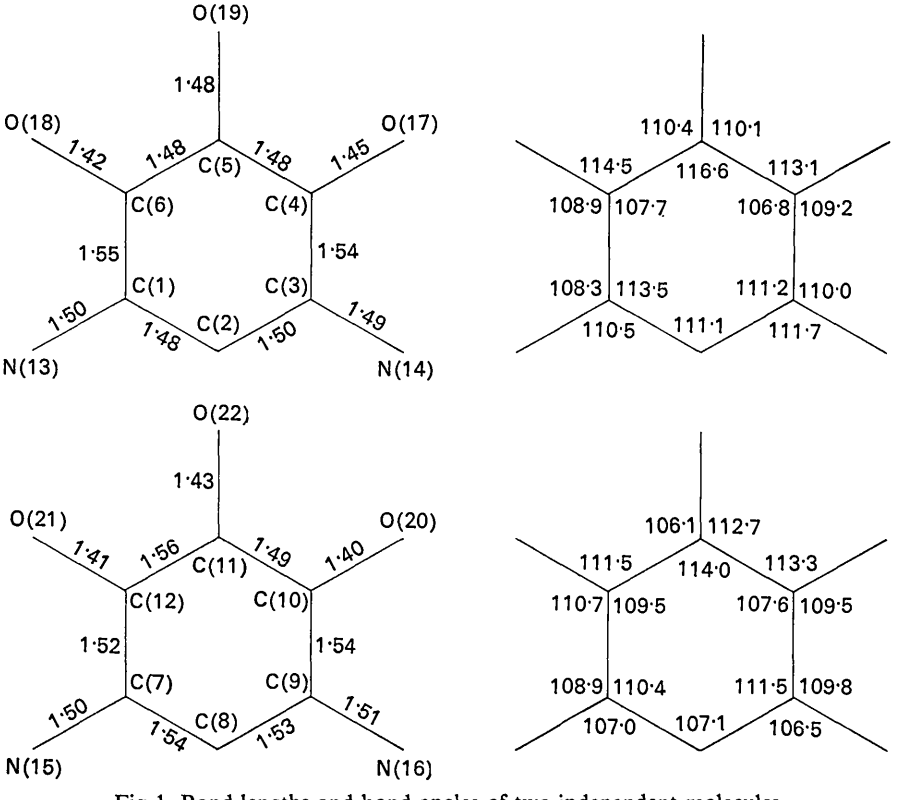

Fig. 1. Bond lengths and bond angles of two independent molecules.

Table 2. *Observed and calculated structure factors*

H	K	L	FO	FC
0	0	3	62.1	66.2
0	0	4	39.2	39.2
0	0	5	98.0	89.7
0	0	6	65.4	59.4
0	0	7	39.3	36.5
0	0	8	25.5	21.9
0	0	9	6.4	4.3
0	0	10	9.9	12.3
0	0	11	12.2	11.6
0	0	12	5.4	3.4
0	0	13	17.3	14.4
0	0	14	2.8	4.3
0	0	15	15.8	12.4
1	0	-15	10.2	8.3
1	0	-14	5.7	5.6
1	0	-13	8.7	7.8
1	0	-12	9.5	8.7
1	0	-11	22.2	19.5
1	0	-10	23.3	22.9
1	0	-9	18.9	18.3
1	0	-8	22.6	21.8
1	0	-7	18.8	17.3
1	0	-5	78.9	70.5
1	0	-4	41.9	31.9
1	0	-3	40.0	32.8
1	0	-2	42.4	30.0
1	0	2	21.0	15.6
1	0	3	21.7	28.4
1	0	4	80.8	76.4
1	0	5	53.0	41.6
1	0	6	41.4	34.7
1	0	7	18.9	14.6
1	0	8	5.8	7.8
1	0	9	6.4	5.7
1	0	11	10.2	9.5
1	0	12	13.0	12.4
1	0	13	4.3	2.3
1	0	14	15.0	13.3
1	0	15	9.9	10.5
2	0	-15	12.2	9.1
2	0	-14	21.3	17.4
2	0	-12	10.2	7.4
2	0	-11	31.2	29.9
2	0	-10	22.7	19.3
2	0	-9	23.9	23.7
2	0	-8	11.9	11.9
2	0	-7	18.7	14.4
2	0	-6	69.8	65.8
2	0	-5	51.9	43.6
2	0	-4	39.5	37.5
2	0	-3	52.4	47.5
2	0	-2	81.9	68.6
2	0	0	18.2	6.3
2	0	1	41.8	42.0
2	0	2	70.0	76.9
2	0	3	18.8	16.9
2	0	4	28.1	27.9
2	0	5	3.8	6.8
2	0	6	10.0	11.6
2	0	7	8.1	5.0
2	0	8	8.6	10.1
2	0	9	28.5	22.7
2	0	10	5.5	5.2
2	0	11	4.0	2.7
2	0	14	15.6	11.7
2	0	15	1.9	3.5
3	0	-14	5.1	6.2
3	0	-13	6.0	4.5
3	0	-12	4.7	5.9
3	0	-11	44.5	41.4
3	0	-10	2.1	4.5
3	0	-9	39.6	36.9
3	0	-8	31.2	26.0
3	0	-7	13.7	11.5
3	0	-6	29.0	25.7
3	0	-5	8.5	12.2
3	0	-4	68.2	64.5
3	0	-3	98.8	89.9
3	0	-2	2.8	3.1
3	0	-1	56.9	47.5
3	0	0	79.8	70.8
3	0	1	60.7	54.6
3	0	2	69.1	60.3
3	0	3	81.6	82.7
3	0	4	47.7	47.7
3	0	6	33.8	31.4
3	0	7	24.9	24.3
3	0	8	34.8	32.4
3	0	9	5.1	2.9
3	0	10	14.6	13.2
3	0	11	4.4	3.7
3	0	12	15.5	13.1
3	0	13	16.7	15.8
3	0	14	3.1	1.8
3	0	15	9.5	9.1
4	0	-14	14.0	12.9
4	0	-13	15.4	13.2
4	0	-12	8.9	9.0
4	0	-11	3.8	2.8
4	0	-10	12.4	10.2

H	K	L	FO	FC
4	0	-9	16.9	16.9
4	0	-8	15.9	15.1
4	0	-7	10.1	9.1
4	0	-6	31.5	27.5
4	0	-5	27.3	21.2
4	0	-4	43.4	33.6
4	0	-3	11.8	10.2
4	0	-2	12.8	13.1
4	0	-1	9.3	8.6
4	0	0	8.9	7.4
4	0	2	6.7	2.5
4	0	3	32.2	31.7
4	0	4	29.0	20.8
4	0	5	21.8	27.6
4	0	6	21.3	19.7
4	0	7	18.8	18.9
4	0	8	25.1	22.6
4	0	9	19.2	19.4
4	0	10	5.7	3.7
4	0	11	6.1	5.8
4	0	12	4.9	6.0
4	0	13	6.8	5.3
4	0	14	6.6	7.1
5	0	-14	14.0	13.8
5	0	-13	5.0	4.7
5	0	-12	11.5	10.5
5	0	-11	6.7	0.0
5	0	-9	15.9	15.9
5	0	-8	8.8	7.8
5	0	-6	27.4	24.1
5	0	-4	22.1	21.2
5	0	-3	14.4	13.3
5	0	-2	51.3	47.2
5	0	-1	50.3	44.3
5	0	0	5.1	5.6
5	0	1	32.9	32.2
5	0	2	33.6	32.2
5	0	3	7.7	10.0
5	0	4	5.6	7.3
5	0	5	16.2	14.6
5	0	6	14.8	13.3
5	0	8	20.8	17.8
5	0	9	5.2	4.5
5	0	10	4.0	0.0
5	0	11	17.3	15.0
5	0	12	3.3	5.3
5	0	13	11.4	6.7
6	0	-12	6.0	6.0
6	0	-11	4.8	5.8
6	0	-10	3.7	4.5
6	0	-9	28.8	26.8
6	0	-8	26.3	24.7
6	0	-7	4.0	5.2
6	0	-6	26.7	23.9
6	0	-4	11.6	8.1
6	0	-3	39.3	34.9
6	0	-2	50.9	48.9
6	0	-1	21.1	21.1
6	0	0	14.0	10.6
6	0	2	4.6	4.3
6	0	3	27.7	25.3
6	0	4	8.6	11.0
6	0	5	5.0	6.8
6	0	6	8.5	9.9
6	0	8	13.2	11.0
6	0	9	10.5	10.6
6	0	10	6.1	8.4
6	0	11	3.1	3.5
6	0	12	9.3	8.5
7	0	-11	1.8	1.0
7	0	-10	2.2	2.4
7	0	-8	6.2	6.3
7	0	-7	16.5	16.7
7	0	-6	4.1	2.7
7	0	-5	6.0	4.4
7	0	-4	8.4	8.3
7	0	-3	19.1	19.1
7	0	-1	8.1	6.9
7	0	0	26.0	23.6
7	0	1	6.7	7.6
7	0	2	14.2	16.0
7	0	3	27.4	24.8
7	0	4	3.5	3.6
7	0	6	28.2	25.3
7	0	7	8.0	8.9
7	0	8	6.7	5.6
7	0	9	11.5	11.9
7	0	10	8.5	5.4
7	0	11	9.2	8.4
8	0	-9	11.5	11.1
8	0	-7	7.9	7.4
8	0	-6	15.4	12.9
8	0	-5	11.5	10.6
8	0	-4	8.3	6.3
8	0	-3	26.6	23.2
8	0	-2	19.5	18.2
8	0	-1	10.8	9.4
8	0	0	6.1	5.5
8	0	1	11.6	12.4
8	0	2	12.4	12.1

H	K	L	FO	FC
8	0	3	18.4	18.5
8	0	4	3.4	4.2
8	0	6	17.3	15.2
8	0	9	7.5	2.2
9	0	-7	10.6	1.3
9	0	-6	2.7	12.1
9	0	-4	2.1	1.2
9	0	-3	4.8	3.7
9	0	-2	2.6	1.6
9	0	-1	6.9	7.6
9	0	0	5.3	2.9
9	0	1	17.3	16.2
9	0	2	14.1	11.2
9	0	3	5.4	7.6
9	0	4	17.1	18.2
9	0	5	5.1	5.8
0	1	2	41.9	34.1
0	1	3	32.5	33.1
0	1	4	54.8	54.0
0	1	5	57.7	56.6
0	1	6	6.3	2.7
0	1	7	21.8	19.4
0	1	8	19.3	17.7
0	1	9	23.9	22.5
0	1	10	33.0	32.9
0	1	11	16.1	17.3
0	1	12	8.5	8.5
0	1	13	20.8	19.7
0	1	14	8.0	5.6
0	1	15	7.3	8.5
1	1	-15	6.7	7.1
1	1	-14	11.6	10.1
1	1	-13	10.9	9.3
1	1	-12	24.6	23.2
1	1	-11	14.3	14.3
1	1	-10	10.4	10.0
1	1	-9	61.8	58.4
1	1	-8	19.2	15.4
1	1	-7	15.5	16.0
1	1	-6	35.7	36.2
1	1	-5	33.3	32.3
1	1	-4	30.4	27.9
1	1	-3	42.9	38.3
1	1	-2	44.2	35.3
1	1	-1	52.6	34.9
1	1	2	29.3	31.8
1	1	3	55.7	51.6
1	1	4	51.7	50.0
1	1	5	35.7	32.4
1	1	6	71.5	63.7
1	1	7	24.3	22.2
1	1	8	41.5	37.4
1	1	9	14.9	14.1
1	1	10	12.4	9.7
1	1	11	25.4	21.7
1	1	12	2.9	2.6
1	1	13	9.9	9.1
1	1	14	14.4	13.5
1	1	15	5.4	6.8
2	1	-15	12.2	10.4
2	1	-14	19.5	18.3
2	1	-13	3.3	1.0
2	1	-12	7.4	7.0
2	1	-11	19.1	21.0
2	1	-10	9.2	9.2
2	1	-9	15.7	12.6
2	1	-8	18.9	16.3
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2	1	-6	24.9	23.2
2	1	-5	34.2	31.7
2	1	-4	38.5	36.9
2	1	-3	30.9	33.6
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2	1	-1	39.4	25.2
2	1	0	25.7	27.6
2	1	1	25.6	25.6
2	1	2	49.7	49.9
2	1	3	29.0	32.1
2	1	4	36.3	44.1
2	1	5	10.1	8.2
2	1	6	41.9	40.2
2	1	7	38.5	39.1
2	1	8	24.8	22.7
2	1	9	37.2	38.0
2	1	10	18.1	17.4
2	1	11	20.7	17.8
2	1	12	22.8	21.1
2	1	13	6.7	7.2
2	1	14	2.1	4.6
2	1	15	11.7	12.2
3	1	-15	8.5	10.5
3	1	-14	6.0	3.2
3	1	-13	20.1	19.1
3	1	-12	5.0	2.7
3	1	-11	13.7	11.8
3	1	-10	38.9	36.5
3	1	-9	4.0	3.1
3	1	-8	18.6	17.6
3	1	-7	24.1	23.5
3	1	-6	25.1	26.4

H	K	L	FO	FC
3	1	-5	24.5	24.7
3	1	-4	22.0	21.2
3	1	-3	19.5	18.3
3	1	-2	6.2	8.7
3	1	-1	25.9	27.7
3	1	0	43.2	42.7
3	1	1	26.3	24.3
3	1	2	22.8	20.0
3	1	3	35.9	37.2
3	1	4	38.8	36.2
3	1	5	37.0	33.6
3	1	6	15.3	12.3
3	1	7	39.5	37.7
3	1	8	20.1	22.2
3	1	9	10.8	12.5
3	1	10	14.3	13.7
3	1	11	15.0	15.9
3	1	12	5.6	6.2
3	1	13	18.4	18.0
3	1	14	4.5	7.0
3	1	15	7.0	5.9
4	1	-15	6.4	8.2
4	1	-14	3.6	3.3
4	1	-13	2.5	1.6
4	1	-12	13.1	11.3
4	1	-11	4.8	5.3
4	1	-10	16.2	14.9
4	1	-9	15.1	16.7
4	1	-8	13.0	13.6
4	1	-7	24.6	22.2
4	1	-6	22.0	22.9
4	1	-5	44.8	42.5
4	1	-4	17.3	16.6
4	1	-3	7.2	6.6
4	1	-2	17.6	17.7
4	1	-1	8.8	8.7
4	1	0	28.7	30.5
4	1	1	15.3	15.7
4	1	2	33.1	24.6
4	1	3	32.0	34.2
4	1	4	17.6	18.1
4	1	5	17.1	15.1
4	1	6	30.6	28.0
4	1	7	15.6	14.8
4	1	8	26.0	27.4
4	1	9	13.7	12.7
4	1	10	19.4	17.3
4	1	11	20.6	20.0
4	1	12	4.6	4.1
4	1	13	9.9	9.5
4	1	14	8.8	9.1
5	1	-14	6.6	8.8
5	1	-12	11.0	11.0
5	1	-11	19.0	16.5
5	1	-10	4.4	3.9
5	1	-9	13.5	13.1
5	1	-8	7.7	6.0
5	1	-7	20.2	21.6
5	1	-6	16.0	17.2
5	1	-5	14.2	13.6
5	1	-4	20.2	20.7
5	1	-3	19.5	19.5
5	1	-2	17.0	17.4
5	1	-1	16.1	16.8
5	1	0	23.1	24.0
5	1	1	28.8	27.7
5	1	2	9.6	8.7
5	1	3	19.1	19.6
5	1	4	31.7	32.1
5	1	6	21.9	21.8
5	1	7	33.9	31.8
5	1	8	19.7	18.4
5	1	9	11.8	12.1
5	1	10	19.2	20.1
5	1	11	5.4	4.0
5	1	12	13.6	13.7
5	1	13	3.2	0.7
5	1	14	2.2	1.7
6	1	-13	6.4	7.4
6	1	-12	5.6	6.6
6	1	-11	13.5	13.2
6	1	-10	12.7	12.8
6	1	-9	2.7	3.5
6	1	-8	16.6	16.3
6	1	-7	13.2	14.8
6	1	-6	15.3	16.1
6	1	-5	8.5	9.1
6	1	-4	16.1	17.7
6	1	-3	16.4	17.2
6	1	-2	8.1	10.0
6	1	-1	7.3	9.0
6	1	0	18.1	18.1
6	1	1	15.2	15.4
6	1	2	28.0	27.7
6	1	3	7.6	8.4
6	1	4	16.1	18.3
6	1	5	16.8	17.9
6	1	6	10.7	10.6
6	1	7	15.5	16.0
6	1	8	12.5	12.5

H	K	L	FO	FC
6	1	9	5.6	5.5
6	1	10	11.2	12.1
6	1	11	8.8	9.7
6	1	12	7.6	7.6
7	1	-10	11.6	11.3
7	1	-9	4.1	4.1
7	1	-8	7.1	6.4
7	1	-7	14.0	15.3
7	1	-6	5.0	5.6
7	1	-5	6.9	6.8
7	1	-4	11.6	11.4
7	1	-3	19.5	22.9
7	1	-2	8.7	7.9
7	1	-1	10.9	11.7
7	1	0	17.2	17.9
7	1	2	9.5	11.6
7	1	3	18.7	18.7
7	1	4	4.7	4.7
7	1	5	2.3	4.4
7	1	6	19.0	18.8
7	1	7	11.1	12.3
7	1	8	6.2	6.5
7	1	9	12.6	12.9
7	1	10	9.9	8.7
8	1	-9	10.2	10.6
8	1	-7	10.0	11.3
8	1	-6	10.9	12.8
8	1	-5	6.0	7.4
8	1	-4	11.2	10.4
8	1	-3	9.9	10.4
8	1	-2	16.0	18.3
8	1	-1	11.7	12.2
8	1	0	7.9	8.1
8	1	1	14.1	15.9
8	1	2	6.3	3.3
8	1	3	11.4	12.3
8	1	4	14.2	14.6
8	1	5	7.3	7.5
8	1	6	9.8	10.2
8	1	7	12.7	13.9
8	1	8	4.6	4.8
9	1	-6	4.5	6.0
9	1	-5	6.7	8.2
9	1	-4	2.6	3.3
9	1	-3	4.7	6.2
9	1	-2	7.3	8.6
9	1	-1	9.6	10.6
9	1	0	7.4	7.6
9	1	2	12.4	14.6
9	1	3	9.1	8.9
9	1	4	3.2	5.4
9	1	5	10.1	12.1
0	2	1	39.4	51.2
0	2	2	22.4	21.1
0	2	3	62.3	72.0
0	2	4	31.6	34.0
0	2	5	15.7	16.1
0	2	6	21.3	22.9
0	2	7	11.5	8.9
0	2	8	13.8	11.6
0	2	9	23.5	22.4
0	2	10	15.0	15.3
0	2	11	13.8	12.3
0	2	12	8.0	6.8
0	2	13	12.9	12.2
0	2	14	8.5	9.1
0	2	15	8.1	7.7
1	2	-15	7.4	6.8
1	2	-14	7.6	7.4
1	2	-13	7.4	8.1
1	2	-12	10.8	10.2
1	2	-11	16.7	15.4
1	2	-10	17.2	17.3
1	2	-9	8.1	10.1
1	2	-8	4.5	4.1
1	2	-7	26.6	26.0
1	2	-6	16.3	15.1
1	2	-5	40.2	43.6
1	2	-4	29.6	30.9
1	2	-3	22.4	21.7
1	2	-2	91.7	107.3
1	2	-1	66.0	62.4
1	2	0	30.3	32.3
1	2	1	104.9	111.7
1	2	2	17.0	17.4
1	2	3	13.9	14.9
1	2	4	78.4	80.3
1	2	5	14.8	15.6
1	2	6	36.6	37.8
1	2	7	40.1	39.7
1	2	8	11.9	9.3
1	2	9	19.1	19.3
1	2	10	12.6	10.4
1	2	11	10.1	9.5
1	2	12	20.0	18.7
1	2	13	7.2	5.4
1	2	14	5.9	4.6
1	2	15	4.8	4.4
2	2	-15	6.4	6.4
2	2	-14	4.9	5.3

Table 2 (*cont.*)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
2	2	-13	9.7	7.9	5	2	2	15.0	14.9	1	3	-9	28.7	27.3	4	3	10	12.2	13.1	1	4	-10	12.5	12.6
2	2	-12	8.0	7.8	5	2	3	6.9	6.7	1	3	-8	16.0	17.2	4	3	11	11.8	11.0	1	4	-9	9.9	10.7
2	2	-11	4.7	4.5	5	2	4	10.7	10.0	1	3	-6	23.0	24.8	4	3	12	8.4	9.7	1	4	-8	31.6	31.6
2	2	-10	32.5	30.5	5	2	5	5.0	2.0	1	3	-5	29.8	31.2	5	3	-13	10.4	8.0	1	4	-7	27.5	26.8
2	2	-9	25.0	25.9	5	2	6	14.1	14.2	1	3	-4	15.2	14.7	5	3	-12	7.4	5.4	1	4	-6	4.9	3.8
2	2	-8	13.8	15.3	5	2	7	18.4	20.2	1	3	-3	34.0	38.5	5	3	-11	19.0	17.0	1	4	-5	38.0	40.6
2	2	-7	43.8	42.4	5	2	8	16.2	18.1	1	3	-2	26.7	26.2	5	3	-10	14.4	12.7	1	4	-4	8.0	9.0
2	2	-6	15.3	14.7	5	2	9	8.8	7.4	1	3	-1	28.8	30.9	5	3	-9	5.5	5.0	1	4	-3	41.4	39.0
2	2	-5	26.2	24.3	5	2	10	7.8	10.9	1	3	0	15.5	16.3	5	3	-8	25.1	23.6	1	4	-2	38.7	45.2
2	2	-4	56.0	55.4	5	2	11	8.2	7.7	1	3	1	17.0	13.2	5	3	-7	13.0	12.6	1	4	-1	45.2	52.7
2	2	-3	19.5	17.5	5	2	12	6.8	8.9	1	3	2	50.5	52.4	5	3	-6	18.0	17.8	1	4	0	14.9	14.2
2	2	-2	34.8	33.7	5	2	13	9.0	10.2	1	3	3	20.8	20.0	5	3	-5	8.8	7.8	1	4	1	59.7	60.9
2	2	-1	93.3	93.9	6	2	-13	7.4	8.7	1	3	4	27.3	24.7	5	3	-3	14.8	13.6	1	4	2	29.8	31.0
2	2	0	44.6	39.5	6	2	-11	7.6	8.4	1	3	5	30.8	31.1	5	3	-2	14.0	14.0	1	4	3	26.2	27.5
2	2	1	34.0	30.4	6	2	-10	6.4	7.0	1	3	6	7.3	10.7	5	3	-1	6.8	3.3	1	4	4	22.4	23.6
2	2	2	48.4	44.6	6	2	-9	9.4	8.2	1	3	7	16.8	16.0	5	3	0	35.7	37.0	1	4	5	10.5	10.9
2	2	3	12.1	11.2	6	2	-8	4.3	3.0	1	3	8	30.7	29.3	5	3	1	10.7	8.5	1	4	6	15.1	15.5
2	2	4	19.0	19.3	6	2	-7	11.1	11.6	1	3	10	10.7	9.7	5	3	2	8.9	11.3	1	4	7	7.1	6.5
2	2	5	21.0	21.5	6	2	-6	10.1	9.6	1	3	11	20.5	20.7	5	3	3	18.1	20.6	1	4	8	14.7	13.9
2	2	6	15.6	18.0	6	2	-5	31.8	33.2	1	3	12	15.7	16.2	5	3	4	25.7	28.4	1	4	9	15.9	15.3
2	2	7	11.5	12.3	6	2	-4	13.4	10.7	1	3	13	7.4	7.6	5	3	5	7.2	8.1	1	4	10	10.6	10.2
2	2	8	10.4	11.6	6	2	-3	8.6	9.0	1	3	14	10.0	9.0	5	3	6	20.2	19.2	1	4	11	23.3	22.4
2	2	9	15.8	14.5	6	2	-2	36.8	39.6	2	3	-15	5.0	3.7	5	3	7	9.9	14.6	1	4	12	17.6	15.4
2	2	10	5.1	5.3	6	2	-1	9.5	7.2	2	3	-14	15.7	14.1	5	3	8	11.8	12.0	1	4	13	10.0	7.8
2	2	11	12.5	10.7	6	2	0	9.5	7.2	2	3	-13	12.3	10.3	5	3	9	11.3	10.3	1	4	14	7.1	6.0
2	2	12	16.2	14.9	6	2	1	16.1	15.3	2	3	-12	12.9	9.4	5	3	10	14.0	13.2	1	4	15	7.1	7.5
2	2	13	10.9	10.7	6	2	2	22.6	24.5	2	3	-11	27.4	26.2	5	3	11	9.9	9.1	2	4	-15	14.2	11.5
2	2	14	6.1	6.7	6	2	4	15.1	16.1	2	3	-10	26.0	24.6	5	3	12	17.9	17.3	2	4	-14	12.3	10.3
2	2	15	8.0	7.5	6	2	5	17.3	17.9	2	3	-9	28.2	28.1	5	3	13	8.6	8.9	2	4	-13	4.3	6.4
3	2	-15	3.2	3.6	6	2	6	10.9	11.7	2	3	-7	12.2	11.5	6	3	-12	7.8	7.1	2	4	-11	6.2	6.2
3	2	-14	12.1	10.0	6	2	7	8.3	8.0	2	3	-6	6.6	4.4	6	3	-11	12.5	11.0	2	4	-10	13.2	10.6
3	2	-13	17.0	18.1	6	2	8	6.1	5.7	2	3	-5	41.5	45.8	6	3	-10	17.9	15.3	2	4	-9	8.1	9.6
3	2	-12	10.0	10.6	6	2	9	9.1	10.7	2	3	-4	14.6	15.4	6	3	-9	5.2	4.1	2	4	-7	8.0	7.3
3	2	-11	15.0	13.6	6	2	10	9.0	9.5	2	3	-3	29.8	33.1	6	3	-8	8.3	6.4	2	4	-6	31.1	34.3
3	2	-9	14.4	12.9	6	2	11	5.7	5.6	2	3	-2	32.4	32.8	6	3	-7	10.9	10.1	2	4	-5	14.9	15.1
3	2	-8	10.1	11.0	6	2	12	5.8	5.9	2	3	-1	8.5	6.2	6	3	-6	17.2	15.7	2	4	-4	34.9	40.1
3	2	-7	22.3	22.3	7	2	-11	3.4	4.5	2	3	0	41.1	46.4	6	3	-5	14.6	13.8	2	4	-3	12.6	15.6
3	2	-6	21.5	21.6	7	2	-10	7.8	9.0	2	3	1	45.8	54.8	6	3	-4	8.3	8.3	2	4	-2	37.2	41.6
3	2	-5	24.3	23.8	7	2	-9	4.4	3.9	2	3	2	37.5	38.7	6	3	-3	23.5	22.4	2	4	-1	32.2	32.5
3	2	-4	29.3	26.0	7	2	-8	13.2	12.9	2	3	3	57.9	63.6	6	3	-2	23.4	21.2	2	4	0	33.7	30.7
3	2	-3	14.0	10.8	7	2	-7	14.5	14.4	2	3	4	23.9	22.8	6	3	-1	21.0	19.6	2	4	1	30.0	27.3
3	2	-2	52.2	52.3	7	2	-6	9.7	10.3	2	3	5	9.1	7.9	6	3	0	11.5	10.0	2	4	2	34.0	37.8
3	2	-1	12.9	14.7	7	2	-5	15.1	15.3	2	3	6	20.8	20.4	6	3	1	8.9	7.5	2	4	3	16.7	13.8
3	2	0	45.4	41.7	7	2	-4	9.8	8.3	2	3	7	30.0	29.0	6	3	2	19.5	18.1	2	4	4	17.5	16.0
3	2	1	26.0	27.3	7	2	-3	9.4	9.6	2	3	8	17.9	17.5	6	3	3	8.4	10.7	2	4	5	42.6	45.4
3	2	2	53.8	49.9	7	2	-2	29.1	30.6	2	3	9	28.9	28.4	6	3	4	21.2	23.7	2	4	6	12.2	11.2
3	2	3	11.6	31.0	7	2	-1	9.7	8.2	2	3	10	8.4	7.7	6	3	5	30.4	29.5	2	4	7	22.1	22.4
3	2	4	12.5	9.0	7	2	0	4.5	3.6	2	3	11	17.2	13.9	6	3	6	8.3	6.7	2	4	8	31.4	33.0
3	2	5	29.8	15.6	7	2	1	12.7	12.7	2	3	12	23.4	20.2	6	3	7	15.6	15.9	2	4	9	12.9	13.0
3	2	6	25.9	29.6	7	2	2	5.6	8.0	2	3	15	9.9	11.5	6	3	8	14.3	16.0	2	4	10	24.6	22.8
3	2	7	24.8	29.6	7	2	3	4.7	4.8	3	3	-14	10.7	7.9	7	3	-10	12.1	11.4	2	4	11	9.3	10.0
3	2	8	5.4	23.5	7	2	4	13.6	14.2	3	3	-13	12.1	10.2	7	3	-8	5.5	4.0	2	4	12	3.1	5.1
3	2	9	8.4	6.4	7	2	6	7.0	8.2	3	3	-12	10.9	9.1	7	3	-7	18.8	16.4	2	4	13	7.4	6.9
3	2	10	7.0	5.3	7	2	7	7.2	9.0	3	3	-10	20.8	22.1	7	3	-4	11.5	8.8	2	4	14	7.7	5.6
3	2	11	9.3	6.0	7	2	8	7.8	6.9	3	3	-9	37.9	35.9	7	3	-3	13.0	11.5	2	4	15	7.8	6.3
3	2	13	3.7	2.6	7	2	9	7.1	7.1	3	3	-8	11.7	10.0	7	3	-2	14.0	12.4	3	4	-14	5.6	5.5
3	2	14	9.8	3.8	7	2	10	8.3	11.1	3	3	-7	17.8	17.1	7	3	-1	8.3	6.7	3	4	-13	3.1	3.1
4	2	-14	4.1	3.1	8	2	-8	4.1	4.5	3	3	-5	13.4	16.4	7	3	0	10.3	6.7	3	4	-12	12.1	8.7
4	2	-13	10.4	10.0	8	2	-6	6.8	7.3	3	3	-4	43.2	42.8	7	3	1	25.0	26.1	3	4	-11	14.7	12.3
4	2	-12	5.3	6.3	8	2	-5	5.8	6.6	3	3	-3	20.4	32.9	7	3	2	16.3	14.7	3	4	-10	13.2	13.6
4	2	-11	16.9	15.7	8	2	-3	12.5	13.4	3	3	-2	28.0	28.1	7	3	3	12.9	12.4	3	4	-9	20.7	29.6
4	2	-9	6.8	5.4	8	2	-2	9.0	10.3	3	3	-1	15.2	16.3	7	3	4	12.1	12.3	3	4	-8	18.8	20.0
4	2	-8	15.4	16.5	8	2	-1	5.8	7.4	3	3	0	25.9	27.0	7	3	5	7.8	8.7	3	4	-7	11.7	9.1
4	2	-7	26.5	25.2	8	2	0	12.2	12.8	3	3	1	8.3	7.2	7	3	6	16.2	14.5	3	4	-6	35.3	33.8
4	2	-6	24.3	21.0	8	2	1	10.7	10.3	3	3	2	25.3	26.8	7	3	7	7.1	6.5	3	4	-5	18.1	19.3
4	2	-5	35.7	37.1	8	2	2	8.3	8.7	3	3	3	19.9	19.9	7	3	8	7.8	7.2	3	4	-4	5.5	5.1
4	2	-4	23.0	21.6	8	2	3	5.6	8.1	3	3	4	31.6	32.8	7	3	9	16.8	16.6	3	4	-3	38.1	38.8
4	2	-3	30.3	29.0	8	2	4	16.0	17.6	3	3	5	23.5	24.9	8	3	-7	11.1	8.6	3	4	-2	24.6	23.7
4	2	-2	51.1	53.7	8	2	6	5.5	6.2	3	3	6	22.3	24.7	8	3	-6	9.1	10.9	3	4	-1	24.0	23.1
4	2	-1	9.5	9.0	8	2	7	6.6	10.0	3	3	7	18.8	17.7	8	3	-5	12.3	6.3	3	4	0	58.5	67.3
4	2	0	9.3	10.2	9	2	-5	8.0	11.2	3	3	8	18.1	17.9	8	3	-4	8.0	8.1	3	4	1	12.1	12.9
4	2	1	52.8	51.9	9	2	-4	9.8	12.6	3	3	9	8.4	9.4	8	3	-3	17.1	14.1	3	4	2	9.0	11.3
4	2	2	10.1	8.3	9	2	-3	4.7	6.1	3	3	10	18.7	18.8	8	3	1	22.9	20.7	3	4	3	43.5	40.3
4	2	3	17.7	18.0	9	2	-2	5.9	8.2	3	3	11	15.7	15.5	8	3	2	8.8	11.0	3	4	4	12.6	14.1
4	2	4	25.7	27.0	9	2	-1	12.0	14.1	3	3	12	11.0	8.1	8	3	3	7.1	4.2	3	4	5	23.6	24.3
4	2	5	12.1	13.0	9	2	1	5.3	5.4	3	3	13	16.1	13.5	8	3	4	18.8	17.0	3	4	6	23.2	23.1
4	2	6	11.9	11.6	9	2	2	10.4	12.0	3	3	14	14.0	14.5	8	3	6	6.6	6.3	3	4	7	19.3	18.0
4	2	7	12.0	11.0	9	2	3	6.5	9.5	3	3	15	11.3	10.7	8	3	7	8.2	7.9	3	4	8	24.5	24.5
4	2	8	13.2	15.2	9	2	4	6.0	6.8	4	3	-12	15.4	13.2	8	3	8	9.8	8.4	3	4	9	9.8	11.6
4	2	9	22.7	24.8	9	2	5	7.7	10.3	4	3	-11	17.2	15.4	9	3	-4	15.5	4.7	3	4	10	17.4	15.0
4	2	10	11.5	12.1	0	3	1	52.6	66.4	4	3	-10	17.4	15.0	9	3	-3	6.8	4.2	3	4	11	4.3	2.9
4	2	11	9.3	9.6	0	3	2	42.8	52.6	4	3	-9	14.0	12.9	0	4	1	23.6	20.7	3	4	12	13.5	12.8
4	2	12	6.0	5.1	0	3	3	18.3	21.8	4	3	-8	16.3	15.9	0	4	2	32.9	35.9	3	4	13	7.5	6.3
4	2	13	10.1	11.0	0	3	4	21.6	22.1	4	3	-7	8.8	9.4	0	4	3	43.3	46.0	3	4	14	4.4	3.0
4	2	14	7.5	7.1	0	3	5	15.0	19.6	4	3	-6	19.7	20.0	0	4	4	35.8	40.3	4	4	-14	10.9	9.4
5	2	-14	6.1	7.6	0	3	6	23.2	24.4	4	3	-5	18.3	19.7	0	4	5	18.6	19.3	4	4	-13	10.5	8.4
5	2	-13	12.5	14.2	0	3	7	50.3	50.2	4	3	-4	9.3	9.8	0	4	6	16.3	16.4	4	4	-12	18.0	16.0
5	2	-11	3.5	5.6	0	3	8	32.3	32.4	4	3	-3	23.9	22.6	0	4	7	19.4	19.9	4	4	-11	14.0	11.4
5	2	-10	17.8	16.0	0	3	9	18.4	16.8	4	3	-2	17.8	19.7	0	4	8	25.9	23.7	4	4	-10	11.2	12.3
5	2	-9	11.2	11.1	0	3	10	20.1	19.2	4	3	-1	14.0	12.3	0	4	9	5.2	4.7	4	4	-9	5.1	5.7
5	2	-8	9.6	10.0	0	3	11	21.7	19.1	4	3	0	16.9	19.9	0	4	10	9.7	11.0	4	4	-8	12.0	9.9
5	2	-7	20.1	21.8	0	3	12	5.9	3.7	4	3	1	29.4	31.7	0	4	11	15.8	13.8	4	4	-7	17.6	18.8
5	2	-6	15.6	19.7	0	3	13	33.1	28.1	4	3	2	21.2	20.1	0	4	12	8.8	7.2	4	4	-6	11.2	9.5
5	2	-5	12.8	13.7	0	3	14	12.4	9.9	4	3	3	28.5	27.0	0	4	13	8.2	5.4	4	4	-5	19.6	20.1
5	2	-4	14.2	13.2	0	3	15	4.6	2.9	4	3	4	22.2	23.6	0	4	14	4.2	4.4	4	4	-4	14.9	15.3
5	2	-3	16.0	14.9	1	3	-15	10.0	8.7	4	3	5	20.8	20.2	0	4	15	7.6	7.0	4	4	-3	32.1	33.6
5	2	-2	5.1	5.9	1	3	-14	8.0	6.6	4	3	6	26.9	29.8	1	4	-14	5.9	5.7	4	4	-2	22.1	23.0
5	2	-1	35.7	5.0	1	3	-13	15.5	13.3	4	3	7	17.7	17.6	1	4	-13	12.0	10.6	4	4	-1	16.1	15.0
5	2	0	23.4	20.9	1	3	-12	16.8	15.7	4	3	8	32.6	31.7	1	4	-12	11.7	11.2	4	4	0	8.3	8.3
5	2	1	7.1	7.1	1	3	-10	8.4	7.9	4	3	9	19.3	18.1	1	4	-11	20.9	16.6	4	4	1	20.1	23.9

Table 2 (*cont.*)

H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
4	4	2	28.8	29.7	9	4	5	4.7	7.3	4	5	-13	4.7	3.2	8	5	3	4.1	2.7	3	6	9	4.5	4.8
4	4	3	13.3	12.6	0	5	1	15.8	6.3	4	5	-12	14.8	13.4	8	5	4	7.88	6.4	3	6	10	7.4	7.7
4	4	4	21.9	22.6	0	5	2	24.1	21.4	4	5	-11	8.3	7.7	88	5	5	3.1	3.9	3	6	11	13.5	14.1
4	4	5	9.3	11.5	0	5	3	9.1	8.5	4	5	-10	5.4	4.6	8	5	6	6.8	7.5	3	6	12	3.1	3.3
4	4	6	33.7	38.8	0	5	4	26.5	27.9	4	5	- 9	24.0	21.9	8	5	7	5.3	5.0	3	6	13	7.3	6.9
4	4	7	15.6	15.4	0	5	5	7.7	5.5	4	5	- 8	24.9	24.3	9	5	- 3	7.8	10.4	4	6	-13	5.5	5.4
4	4	8	12.9	11.5	0	5	6	12.8	12.4	4	5	- 7	17.1	15.4	9	5	- 2	4.9	7.2	4	6	-12	4.1	4.8
4	4	9	25.3	26.1	0	5	7	11.5	10.5	4	5	- 6	9.7	11.6	9	5	- 1	6.6	12.1	4	6	-11	15.2	13.0
4	4	10	6.4	4.2	0	5	8	5.5	4.3	4	5	- 5	13.4	12.0	9	5	0	7.7	8.1	4	6	-10	17.1	16.2
4	4	11	6.8	5.4	0	5	9	13.9	13.1	4	5	- 4	27.8	29.2	9	5	1	7.5	8.5	4	6	- 9	6.6	6.9
4	4	12	4.3	5.8	0	5	10	21.9	21.7	4	5	- 3	17.3	19.4	9	5	2	9.0	10.4	4	6	- 8	9.8	10.0
4	4	13	8.6	6.5	0	5	11	11.0	10.3	4	5	- 2	11.2	12.5	0	6	1	11.9	13.9	4	6	- 7	22.6	22.9
4	4	14	5.4	4.9	0	5	12	12.1	10.8	4	5	- 1	15.5	15.1	0	6	2	7.4	7.2	4	6	- 6	5.4	4.5
5	4	-13	9.3	7.9	0	5	13	14.8	13.5	4	5	0	23.8	24.1	0	6	3	13.2	16.1	4	6	- 5	34.6	35.4
5	4	-12	2.8	2.0	0	5	15	4.9	5.3	4	5	1	7.6	9.5	0	6	4	13.8	13.3	4	6	- 4	20.9	24.3
5	4	-11	8.2	6.9	1	5	-15	8.0	9.0	4	5	2	21.3	20.9	0	6	5	15.4	16.3	4	6	- 3	13.3	14.5
5	4	-10	9.3	8.2	1	5	-14	10.2	9.8	4	5	3	22.8	22.3	0	6	6	4.4	1.5	4	6	- 2	28.9	29.6
5	4	- 9	8.5	9.0	1	5	-13	13.2	11.4	4	5	4	6.1	4.3	0	6	7	11.3	10.4	4	6	- 1	8.9	8.4
5	4	- 7	8.8	5.5	1	5	-12	15.8	13.9	4	5	5	19.2	18.2	0	6	8	26.0	27.1	4	6	0	10.6	8.0
5	4	- 6	23.3	22.7	1	5	-11	9.6	9.5	4	5	6	38.0	40.3	0	6	9	10.4	7.9	4	6	1	38.5	43.5
5	4	- 5	27.1	27.8	1	5	-10	11.4	9.6	4	5	7	12.1	12.3	0	6	10	12.6	11.6	4	6	2	12.4	13.1
5	4	- 4	19.8	16.9	1	5	- 9	30.9	32.1	4	5	8	11.5	11.0	0	6	11	15.2	14.9	4	6	3	5.3	7.0
5	4	- 3	44.5	48.1	1	5	- 8	12.7	11.4	4	5	9	10.3	13.0	0	6	12	16.1	13.5	4	6	4	7.5	8.4
5	4	- 2	40.6	42.5	1	5	- 7	9.7	10.3	4	5	10	9.1	9.1	0	6	13	4.6	4.1	4	6	5	16.5	10.6
5	4	- 1	28.2	28.9	1	5	- 6	29.4	28.6	4	5	11	20.8	21.2	0	6	14	13.5	13.7	4	6	6	16.6	17.3
5	4	1	12.2	14.7	1	5	- 5	10.0	10.8	4	5	12	5.2	5.5	1	6	-14	4.0	4.1	4	6	7	11.0	13.8
5	4	2	36.2	40.2	1	5	- 4	16.6	19.4	4	5	13	6.4	7.3	1	6	-13	3.4	3.9	4	6	8	11.5	12.6
5	4	3	7.5	9.7	1	5	- 3	12.1	13.8	5	5	-12	4.6	3.8	1	6	-12	16.7	15.6	4	6	9	7.8	8.1
5	4	4	4.0	5.1	1	5	- 2	31.4	28.2	5	5	-11	9.6	8.6	1	6	-10	7.9	10.0	4	6	10	8.8	7.2
5	4	5	7.5	7.8	1	5	- 1	35.8	42.1	5	5	-10	10.1	8.6	1	6	- 9	9.0	8.0	4	6	11	4.0	3.0
5	4	6	9.0	10.0	1	5	0	19.4	20.8	5	5	- 9	4.4	2.1	1	6	- 8	18.8	18.5	4	6	12	4.3	4.0
5	4	7	13.2	14.8	1	5	1	14.6	13.9	5	5	- 8	8.7	9.2	1	6	- 7	35.5	34.7	5	6	-12	7.3	6.3
5	4	9	6.7	4.9	1	5	2	39.7	39.8	5	5	- 5	17.4	4.4	1	6	- 6	10.3	9.6	5	6	-11	5.7	6.1
5	4	10	8.3	7.3	1	5	3	58.8	54.4	5	5	- 4	6.9	16.9	1	6	- 5	17.3	19.8	5	6	-10	12.6	11.4
5	4	11	4.8	4.2	1	5	4	6.6	8.8	5	5	- 3	4.4	5.8	1	6	- 4	13.3	13.2	5	6	- 9	10.3	9.3
5	4	13	4.7	4.6	1	5	5	31.7	33.8	5	5	- 2	12.1	6.1	1	6	- 3	14.3	19.7	5	6	- 8	8.8	9.2
6	4	-12	4.0	2.0	1	5	6	27.3	26.1	5	5	- 1	21.2	12.2	1	6	- 2	37.8	40.8	5	6	- 7	19.0	17.5
6	4	-11	10.4	8.7	1	5	7	16.1	16.7	5	5	0	18.5	21.4	1	6	- 1	31.3	32.1	5	6	- 6	7.7	6.1
6	4	-10	4.3	3.2	1	5	8	30.1	31.5	5	5	1	5.6	17.8	1	6	0	14.9	13.8	5	6	- 5	3.4	2.8
6	4	- 9	26.8	22.4	1	5	9	11.6	10.6	5	5	2	18.5	4.7	1	6	1	47.8	48.0	5	6	- 4	9.3	10.0
6	4	- 8	18.2	16.6	1	5	10	6.1	6.6	5	5	3	8.0	18.6	1	6	2	14.7	14.3	5	6	- 3	14.8	15.5
6	4	- 7	4.3	2.0	1	5	11	15.5	15.3	5	5	4	5.5	7.1	1	6	3	21.2	22.8	5	6	- 2	11.9	11.1
6	4	- 6	21.4	19.8	1	5	12	12.5	11.2	5	5	5	17.8	6.8	1	6	4	42.4	43.2	5	6	- 1	10.9	11.0
6	4	- 5	20.6	20.7	1	5	13	3.5	3.9	5	5	6	17.8	17.7	1	6	5	11.4	12.6	5	6	0	5.1	4.2
6	4	- 4	18.3	16.9	1	5	14	15.0	15.7	5	5	7	9.7	16.2	1	6	6	19.6	20.9	5	6	1	4.6	5.1
6	4	- 3	24.0	22.4	2	5	-14	14.2	14.5	5	5	8	8.9	9.5	1	6	7	17.3	19.8	5	6	3	11.0	12.5
6	4	- 2	9.6	6.9	2	5	-13	5.3	2.4	5	5	9	8.5	9.4	1	6	8	7.9	7.0	5	6	4	7.0	11.3
6	4	- 1	14.9	15.1	2	5	-12	7.4	7.1	5	5	10	12.5	7.5	1	6	9	8.8	9.9	5	6	5	4.6	6.4
6	4	0	14.4	13.2	2	5	-11	15.3	15.4	5	5	11	11.3	12.0	1	6	10	12.1	12.1	5	6	6	15.8	17.2
6	4	1	13.5	15.2	2	5	-10	14.2	12.7	6	5	-11	14.2	13.0	1	6	11	6.4	6.4	5	6	7	11.5	14.3
6	4	2	17.9	19.0	2	5	- 9	14.7	11.7	6	5	-10	9.9	10.6	1	6	12	12.6	11.5	5	6	8	9.4	9.2
6	4	3	4.6	4.5	2	5	- 8	13.5	14.7	6	5	- 9	16.0	13.1	1	6	14	4.2	3.5	5	6	9	10.2	11.4
6	4	4	12.2	14.2	2	5	- 6	23.6	25.1	6	5	- 8	17.7	17.6	2	6	-14	4.0	4.0	5	6	10	6.4	7.5
6	4	5	7.1	8.2	2	5	- 5	23.7	25.8	6	5	- 7	8.3	5.8	2	6	-13	12.3	9.6	5	6	11	6.1	4.7
6	4	6	8.0	8.0	2	5	- 4	8.0	9.3	6	5	- 6	6.6	6.7	2	6	-12	9.2	8.7	6	6	-10	6.5	7.0
6	4	7	8.0	8.5	2	5	- 3	14.2	14.2	6	5	- 5	13.3	12.2	2	6	-11	9.5	8.7	6	6	- 9	7.3	6.7
6	4	8	5.6	6.8	2	5	- 2	20.7	24.1	6	5	- 4	13.0	9.2	2	6	-10	21.0	19.1	6	6	- 8	11.2	9.8
6	4	9	13.5	14.1	2	5	- 1	25.0	23.5	6	5	- 3	9.8	8.8	2	6	- 9	18.0	17.7	6	6	- 7	4.1	4.1
6	4	10	8.1	8.1	2	5	0	22.6	24.2	6	5	- 2	15.3	14.6	2	6	- 8	7.0	7.5	6	6	- 6	3.4	3.1
6	4	11	4.2	3.1	2	5	1	11.1	13.0	6	5	- 1	8.3	7.0	2	6	- 7	19.3	17.0	6	6	- 5	15.3	16.3
6	4	12	8.0	9.9	2	5	2	20.0	23.9	6	5	0	24.6	23.6	2	6	- 6	10.2	10.9	6	6	- 4	5.4	4.8
7	4	-10	7.9	7.3	2	5	3	19.4	18.0	6	5	1	11.6	11.2	2	6	- 4	42.4	46.8	6	6	- 3	3.7	3.0
7	4	- 9	13.0	11.7	2	5	4	6.7	9.1	6	5	2	23.7	21.9	2	6	- 3	24.4	26.6	6	6	- 2	6.4	5.9
7	4	- 8	8.7	8.1	2	5	5	10.8	11.9	6	5	3	18.9	18.9	2	6	- 2	15.8	15.4	6	6	- 1	19.0	20.7
7	4	- 7	17.5	16.8	2	5	6	19.8	18.4	6	5	4	19.3	20.8	2	6	- 1	29.0	35.3	6	6	0	8.6	9.9
7	4	- 6	3.3	2.1	2	5	7	24.0	25.1	6	5	5	12.2	12.9	2	6	0	13.9	11.5	6	6	1	7.5	9.2
7	4	- 5	6.5	5.9	2	5	8	15.2	14.2	6	5	6	9.7	10.4	2	6	1	22.9	19.5	6	6	2	12.8	15.8
7	4	- 4	30.2	29.7	2	5	9	16.4	14.9	6	5	7	10.7	10.0	2	6	2	21.5	22.0	6	6	3	11.2	13.2
7	4	- 3	23.4	22.1	2	5	10	11.9	11.8	6	5	8	13.9	14.3	2	6	3	14.2	11.3	6	6	4	10.9	10.9
7	4	- 2	6.7	6.4	2	5	11	8.3	8.4	6	5	9	3.7	4.6	2	6	4	20.0	21.7	6	6	5	12.9	15.7
7	4	- 1	8.8	9.7	2	5	12	20.2	19.5	6	5	10	8.7	8.6	2	6	6	16.2	16.1	6	6	6	4.0	2.7
7	4	0	6.6	8.1	2	5	13	5.2	4.8	6	5	11	4.9	4.5	2	6	7	24.2	25.9	6	6	7	15.7	15.8
7	4	1	12.8	12.9	2	5	14	8.7	8.7	7	5	- 9	8.6	8.0	2	6	8	4.7	5.2	6	6	8	10.6	10.3
7	4	3	9.8	8.6	3	5	-13	11.0	11.0	7	5	- 8	5.4	5.9	2	6	9	26.5	25.6	6	6	9	3.1	3.9
7	4	4	3.4	3.6	3	5	-12	11.1	9.7	7	5	- 7	9.5	9.0	2	6	10	5.1	6.4	6	6	10	9.2	9.2
7	4	5	8.8	7.7	3	5	-11	15.0	13.2	7	5	- 5	20.5	20.3	2	6	11	17.6	16.3	7	6	- 9	3.3	4.0
7	4	6	16.4	15.6	3	5	-10	9.1	9.0	7	5	- 4	12.0	11.2	2	6	12	10.3	10.4	7	6	- 8	14.6	13.2
7	4	7	2.6	2.7	3	5	- 9	14.6	11.6	7	5	- 3	2.6	3.0	2	6	13	7.5	6.4	7	6	- 7	9.2	10.2
7	4	8	9.7	7.5	3	5	- 8	7.4	7.7	7	5	- 2	4.8	4.9	2	6	14	6.4	6.0	7	6	- 6	7.1	7.0
7	4	9	5.9	7.3	3	5	- 7	9.9	9.8	7	5	- 1	10.8	10.4	3	6	-13	9.9	9.4	7	6	- 5	20.8	18.5
7	4	10	6.0	4.0	3	5	- 6	11.9	11.4	7	5	0	19.8	19.4	3	6	-12	3.6	3.8	7	6	- 4	7.6	6.6
8	4	- 8	8.2	7.0	3	5	- 5	16.2	16.1	7	5	1	5.8	6.5	3	6	-11	18.7	17.1	7	6	- 3	18.5	18.5
8	4	- 7	18.9	16.3	3	5	- 4	17.7	15.4	7	5	2	16.2	15.8	3	6	-10	7.9	7.6	7	6	- 2	4.1	3.6
8	4	- 6	4.0	4.1	3	5	- 3	14.9	17.9	7	5	3	16.1	15.1	3	6	- 9	9.0	8.5	7	6	- 1	5.5	4.6
8	4	- 5	9.4	8.3	3	5	- 2	19.0	19.9	7	5	4	7.5	7.3	3	6	- 8	13.5	13.9	7	6	0	5.5	4.6
8	4	- 4	9.3	7.3	3	5	- 1	5.1	3.1	7	5	5	8.4	10.8	3	6	- 7	6.0	5.0	7	6	1	4.3	3.3
8	4	- 3	4.2	3.9	3	5	0	38.8	40.0	7	5	6	19.5	20.1	3	6	- 6	7.2	7.0	7	6	2	4.8	3.6
8	4	- 2	10.6	9.4	3	5	1	34.1	34.7	7	5	7	4.1	3.1	3	6	- 5	8.4	7.7	7	6	3	10.7	10.9
8	4	- 1	13.3	12.7	3	5	2	25.6	25.5	7	5	8	7.0	7.5	3	6	- 4	11.5	11.9	7	6	4	7.9	8.6
8	4	0	13.3	5.5	3	5	3	15.0	15.1	7	5	9	4.2	5.9	3	6	- 3	11.5	11.9	7	6	5	6.2	7.4
8	4	1	17.4	17.6	3	5	4	17.6	18.0	8	5	- 7	2.9	3.0	3	6	- 2	14.8	15.8	7	6	6	4.0	4.0
8	4	2	7.5	7.4	3	5	5	9.0	10.5	8	5	- 6	4.3	3.5	3	6	- 1	9.8	13.0	7	6	7	5.6	6.2
8	4	3	7.3	7.2	3	5	6	13.0	12.3	8	5	- 5	3.8	1.9	3	6	0	11.3	11.1	8	6	- 6	6.7	7.0
8	4	5	4.8	6.3	3	5	7	20.1	21.4	8	5	- 4	7.7	5.3	3	6	1	8.1	7.3	8	6	- 5	6.8	5.8
8	4	6	8.8	7.0	3	5	8	6.7	6.9	8	5	- 3	13.7	11.6	3	6	2	25.1	28.7	8	6	- 4	4.6	5.1
8	4	7	4.2	2.9	3	5	9	4.9	7.4	8	5	- 2	9.0	8.8	3	6	3	12.3	12.4	8	6	- 3	9.6	9.5
8	4	8	5.2	5.6	3	5	10	8.5	10.3	8	5	- 1	11.2	10.8	3	6	4	12.8	14.0	8	6	- 2	3.4	1.8
9	4	1	3.6	5.6	3	5	11	15.1	14.0	8	5	0	5.88	5.0	3	6	5	19.0	21.8	8	6	- 1	1.2	3.5
9	4	2	4.9	3.3	3	5	12	6.6	6.3	8	5	1	12.5	12.2	3	6	6	9.8	10.6	8	6	0	4.7	6.6
9	4	4	3.1	5.6	3	5	13	5.3	5.8	8	5	2	15.2	14.8	3	6	7	4.1	4.4	8	6	1	8.4	9.0
															3	6	8	18.7	20.3	8	6	2	1.4	3.6

Tabel 2 (*cont.*)

H	K	L	FO	FC
8	6	3	7.5	8.7
8	6	4	8.9	10.5
8	6	5	5.0	4.8
0	7	1	33.2	35.3
0	7	2	25.9	27.2
0	7	3	19.8	23.0
0	7	4	13.3	15.3
0	7	5	20.7	30.5
0	7	6	9.0	9.9
0	7	7	19.9	20.0
0	7	8	23.2	20.9
0	7	9	14.5	15.6
0	7	10	15.7	14.8
0	7	11	5.5	5.1
0	7	12	6.7	4.6
0	7	13	16.2	15.4
1	7	-12	14.4	14.4
1	7	-11	12.8	13.5
1	7	-10	12.0	10.7
1	7	- 9	8.7	7.4
1	7	- 8	18.6	16.3
1	7	- 7	11.6	10.2
1	7	- 6	12.2	12.9
1	7	- 5	4.2	3.7
1	7	- 4	10.5	13.2
1	7	- 3	13.7	12.8
1	7	- 2	16.8	13.9
1	7	- 1	17.1	15.8
1	7	0	24.4	28.8
1	7	1	8.3	9.1
1	7	2	16.3	18.0
1	7	3	8.6	5.2
1	7	4	14.5	13.9
1	7	5	30.0	30.4
1	7	6	6.6	6.4
1	7	7	7.3	7.2
1	7	8	21.4	22.0
1	7	9	7.1	8.3
1	7	10	16.7	15.1
1	7	11	11.6	11.3
1	7	12	6.6	6.8
1	7	13	6.9	6.4
2	7	-13	7.9	6.0
2	7	-12	12.4	12.7
2	7	-11	12.9	12.8
2	7	-10	5.5	2.7
2	7	- 9	8.6	7.3
2	7	- 8	26.4	27.7
2	7	- 7	15.8	19.1
2	7	- 6	12.2	13.9
2	7	- 5	7.7	9.5
2	7	- 4	3.6	5.0
2	7	- 3	20.6	23.5
2	7	- 2	23.6	24.8
2	7	- 1	32.1	33.9
2	7	0	9.9	10.8
2	7	1	9.0	11.2
2	7	2	9.4	7.0
2	7	3	19.3	23.7
2	7	4	21.1	20.3
2	7	5	4.1	5.0
2	7	6	13.7	14.1
2	7	7	28.6	27.7
2	7	8	4.3	4.9
2	7	9	4.8	5.2
2	7	10	6.5	7.0
2	7	11	11.9	9.7
2	7	12	10.0	11.1
2	7	13	8.1	7.0
3	7	-13	8.2	8.7
3	7	-12	6.0	6.5
3	7	-11	5.2	4.4
3	7	-10	4.7	5.8
3	7	- 9	7.1	5.0
3	7	- 8	14.9	12.8
3	7	- 6	9.6	12.6
3	7	- 5	26.9	28.3
3	7	- 4	6.1	4.7
3	7	- 3	20.7	22.8
3	7	- 2	24.8	27.9
3	7	- 1	21.3	23.3
3	7	0	13.2	13.0
3	7	1	17.7	18.9
3	7	2	28.5	29.3
3	7	3	6.7	5.6
3	7	4	21.7	23.7
3	7	5	8.8	8.9
3	7	6	7.8	10.1
3	7	7	30.0	28.4
3	7	8	9.9	10.5
3	7	9	6.8	5.0
3	7	10	16.7	16.9
3	7	11	8.3	9.5
3	7	12	6.1	6.1
4	7	-12	5.4	4.3
4	7	- 9	8.3	9.4
4	7	- 8	5.2	3.3
4	7	- 7	10.4	10.1
4	7	- 6	4.3	4.6
4	7	- 5	6.8	6.9
4	7	- 4	9.9	9.2
4	7	- 3	6.3	4.6
4	7	- 2	7.1	6.0
4	7	- 1	22.1	22.9
4	7	0	14.4	13.8
4	7	1	22.5	25.2
4	7	2	18.7	16.8
4	7	3	8.6	6.8
4	7	4	4.6	4.9
4	7	5	18.0	19.5
4	7	6	16.8	17.4
4	7	7	9.6	9.9
4	7	8	11.8	11.8
4	7	9	7.7	7.2
4	7	10	6.3	5.9
4	7	11	6.6	8.0
4	7	12	10.9	11.5
5	7	-11	3.6	3.9
5	7	-10	7.5	7.0
5	7	- 9	9.4	8.3
5	7	- 8	8.9	10.2
5	7	- 7	13.3	12.0
5	7	- 6	7.5	8.6
5	7	- 5	26.7	28.7
5	7	- 4	17.1	18.2
5	7	- 3	3.7	5.4
5	7	- 2	19.8	21.5
5	7	- 1	14.6	15.5
5	7	0	20.0	20.2
5	7	1	8.3	8.5
5	7	2	15.1	17.0
5	7	3	18.6	21.2
5	7	4	4.4	5.0
5	7	5	5.6	7.9
5	7	6	8.5	9.0
5	7	7	12.4	12.8
5	7	8	9.4	9.0
5	7	9	4.4	6.3
5	7	10	2.6	3.81
6	7	- 8	10.3	8.1
6	7	- 7	3.5	1.9
6	7	- 6	4.0	4.7
6	7	- 5	7.7	7.6
6	7	- 4	9.7	8.2
6	7	- 2	12.8	12.9
6	7	- 1	20.5	18.6
6	7	0	8.8	8.9
6	7	1	9.4	9.9
6	7	2	5.9	3.5
6	7	3	2.88	3.3
6	7	4	16.5	15.2
6	7	5	17.0	15.7
6	7	6	8.6	6.5
6	7	7	8.6	9.2
6	7	8	2.8	3.8
6	7	9	5.1	4.6
7	7	- 7	9.6	9.2
7	7	- 6	8.6	7.4
7	7	- 5	11.7	10.6
7	7	- 4	6.5	7.5
7	7	- 3	6.0	6.1
7	7	- 2	21.4	20.6
7	7	- 1	12.4	11.3
7	7	0	7.3	7.1
7	7	1	11.9	12.5
7	7	2	9.6	9.7
7	7	3	11.4	11.0
7	7	4	6.7	7.1
7	7	5	4.7	6.0
7	7	6	8.7	9.2
8	7	- 4	6.1	7.9
8	7	- 3	3.3	5.7
8	7	- 2	11.9	11.5
8	7	- 1	6.2	6.7
8	7	0	5.5	6.5
8	7	1	9.3	10.1
8	7	2	3.1	3.9
8	7	3	6.8	7.7
0	8	1	16.0	14.8
0	8	2	25.2	27.2
0	8	3	26.7	25.7
0	8	4	6.4	7.3
0	8	5	19.1	21.8
0	8	6	8.8	9.8
0	8	7	9.0	9.8
0	8	8	18.3	18.8
1	8	-12	3.1	5.4
1	8	-11	17.1	17.1
1	8	-10	6.6	7.9
1	8	- 9	8.4	9.0
1	8	- 8	18.5	19.2
1	8	- 7	11.9	12.5
1	8	- 6	17.6	17.1
1	8	- 5	21.5	21.9
1	8	- 4	19.8	20.0
1	8	- 3	27.9	28.0
1	8	- 2	18.8	20.1
1	8	- 1	12.8	13.1
1	8	0	23.5	24.9
1	8	1	21.5	19.3
1	8	2	20.0	15.8
1	8	3	3.8	2.4
1	8	4	10.7	11.3
1	8	5	11.4	9.4
1	8	6	12.8	15.7
1	8	7	9.4	10.5
1	8	8	7.6	5.9
1	8	9	14.1	15.7
1	8	10	8.5	9.3
1	8	11	9.3	7.5
1	8	12	9.2	10.4
2	8	-12	12.1	12.9
2	8	-11	17.5	15.3
2	8	-10	5.2	5.6
2	8	- 9	15.6	17.3
2	8	- 8	11.8	11.7
2	8	- 7	3.9	4.3
2	8	- 6	23.5	24.2
2	8	- 5	4.4	3.9
2	8	- 4	10.9	11.9
2	8	- 3	12.3	11.7
2	8	- 2	16.6	18.0
2	8	- 1	16.8	18.8
2	8	0	5.1	2.9
2	8	1	9.0	9.4
2	8	2	21.2	20.7
2	8	3	20.9	20.9
2	8	4	14.5	14.5
2	8	5	10.5	11.8
2	8	6	14.8	14.9
2	8	7	5.1	7.0
2	8	8	15.8	15.5
2	8	9	5.9	5.5
2	8	10	13.3	12.6
2	8	11	6.2	7.2
2	8	12	1.8	1.7
3	8	-12	7.0	7.3
3	8	-11	10.2	9.5
3	8	-10	13.2	12.4
3	8	- 9	16.9	14.9
3	8	- 8	13.0	13.1
3	8	- 7	5.3	5.1
3	8	- 6	24.1	23.6
3	8	- 5	20.3	23.0
3	8	- 4	9.1	10.9
3	8	- 3	19.9	20.0
3	8	- 2	22.3	23.3
3	8	- 1	16.6	14.1
3	8	0	20.6	19.2
3	8	1	4.2	2.2
3	8	2	10.1	8.2
3	8	3	16.3	19.9
3	8	4	6.6	4.3
3	8	5	18.0	19.7
3	8	7	3.7	3.4
3	8	8	8.7	12.7
3	8	9	5.8	6.2
3	8	10	11.7	10.2
3	8	11	3.1	5.3
4	8	-11	11.1	12.4
4	8	-10	10.3	10.0
4	8	- 9	11.6	11.1
4	8	- 8	10.5	11.8
4	8	- 7	9.4	10.0
4	8	- 6	4.8	2.6
4	8	- 5	11.7	11.9
4	8	- 4	6.8	7.6
4	8	- 3	8.5	7.2
4	8	- 2	9.4	10.6
4	8	- 1	5.1	3.6
4	8	0	6.7	7.0
4	8	1	7.6	6.3
4	8	2	16.6	16.7
4	8	3	8.5	8.9
4	8	4	5.1	6.4
4	8	5	17.7	20.6
4	8	6	6.9	9.6
4	8	8	9.3	10.9
4	8	9	9.4	12.7
5	8	- 9	9.7	9.1
5	8	- 8	3.7	3.4
5	8	- 7	3.4	3.5
5	8	- 6	11.9	13.3
5	8	- 4	8.6	8.2
5	8	- 3	11.5	10.9
5	8	- 2	8.3	9.9
5	8	- 1	16.4	16.7
5	8	0	6.5	7.3
5	8	1	9.9	11.4
5	8	2	11.6	13.5
5	8	3	7.8	10.0
5	8	4	3.1	2.9
5	8	5	4.1	6.5
5	8	6	4.2	6.3
5	8	7	8.2	9.4
5	8	8	5.9	4.9
5	8	9	8.6	9.0
6	8	- 8	7.2	7.4
6	8	- 7	4.0	3.8
6	8	- 6	15.0	14.7
6	8	- 5	10.8	11.0
6	8	- 4	7.3	6.4
6	8	- 3	4.1	3.1
6	8	- 2	3.3	2.0
6	8	- 1	11.1	9.8
6	8	0	10.1	10.9
6	8	2	2.8	3.6
6	8	3	8.7	9.9
6	8	4	10.8	3.3
6	8	5	10.7	11.2
6	8	6	7.2	8.9
6	8	7	6.3	9.3
7	8	- 5	3.6	3.2
7	8	- 4	6.8	7.5
7	8	- 3	3.0	5.0
7	8	- 2	3.3	3.5
7	8	- 1	5.3	5.2
7	8	2	11.7	13.6
7	8	3	6.2	7.7
7	8	4	4.1	3.3
7	8	5	8.3	11.3
0	9	1	8.6	9.3
0	9	2	11.1	13.7
0	9	4	11.1	8.4
0	9	5	8.1	8.7
0	9	6	13.3	12.8
0	9	7	5.7	2.4
0	9	8	6.7	7.2
0	9	9	17.0	15.9
0	9	10	5.7	5.1
1	9	-10	4.7	5.3
1	9	- 9	18.3	18.7
1	9	- 8	6.3	6.7
1	9	- 7	17.1	17.8
1	9	- 6	8.3	9.6
1	9	- 5	7.5	10.0
1	9	- 4	8.7	10.9
1	9	- 3	13.7	17.0
1	9	- 2	11.2	12.2
1	9	- 1	17.4	24.1
1	9	0	8.7	10.6
1	9	1	15.6	13.4
1	9	2	19.9	20.1
1	9	3	12.8	14.0
1	9	4	9.2	9.7
1	9	5	24.5	27.8
1	9	6	18.3	18.0
1	9	7	5.6	7.4
1	9	8	5.7	4.6
1	9	9	7.9	8.6
1	9	10	11.9	12.5
2	9	- 9	6.4	6.7
2	9	- 8	6.8	2.3
2	9	- 7	8.8	5.7
2	9	- 6	4.1	2.1
2	9	- 5	16.2	16.1
2	9	- 4	7.5	7.2
2	9	- 3	10.5	14.0
2	9	- 2	6.7	7.5
2	9	- 1	15.7	15.0
2	9	0	18.6	21.0
2	9	1	13.5	15.0
2	9	2	3.4	1.5
2	9	4	16.4	19.0
2	9	5	11.5	12.0
2	9	6	15.8	16.5
2	9	7	4.1	2.4
2	9	8	7.5	5.1
2	9	9	14.1	15.8
2	9	10	9.2	9.3
3	9	-10	8.2	9.0
3	9	- 9	6.1	3.6
3	9	- 6	5.9	4.0
3	9	- 5	9.8	11.0
3	9	- 4	7.6	6.4
3	9	- 3	8.7	11.1
3	9	- 2	8.9	11.9
3	9	- 1	6.1	5.4
3	9	0	15.8	16.7
3	9	1	13.5	15.0
3	9	2	7.5	7.4
3	9	3	8.3	8.3
3	9	4	10.5	21.3
3	9	5	7.7	9.2
3	9	6	11.3	10.7
3	9	7	5.9	4.8
3	9	8	7.4	8.9
4	9	- 8	5.4	4.4
4	9	- 8	9.8	12.0
4	9	- 7	12.2	11.9
4	9	- 6	11.1	13.0
4	9	- 5	6.8	7.1
4	9	- 4	21.6	22.1
4	9	- 3	11.9	12.8
4	9	- 2	11.0	13.3
4	9	- 1	12.9	14.0
4	9	0	10.9	13.0
4	9	2	9.5	13.5
4	9	3	12.1	14.1
4	9	5	5.4	6.4
4	9	6	8.4	9.2
4	9	7	8.3	10.8
4	9	8	7.4	9.3
4	9	9	3.6	4.7
5	9	- 8	8.9	8.4
5	9	- 7	4.6	7.0
5	9	- 6	10.5	10.9
5	9	- 5	13.1	11.1
5	9	- 3	8.7	9.5
5	9	- 2	5.6	6.0
5	9	- 1	9.7	11.0
5	9	0	20.7	20.2
5	9	1	13.3	12.4
5	9	2	5.4	5.9
5	9	3	8.9	7.1
5	9	4	3.7	5.2
5	9	5	15.3	14.5
5	9	6	10.0	11.5
5	9	7	11.8	13.1
5	9	8	9.1	10.6

Results and discussion

The main stereochemical questions raised at the outset of the present study could be answered by inspection of the second Fourier synthesis. The cyclohexane ring was found to have the energetically most preferred 'chair' conformation, while the five substituents could be distinguished in two groups: those at carbon atoms 1 and 3 (7 and 9 in the second molecule) being represented by a considerably lower electron density than those at carbon atoms 4, 5 and 6 (10, 11 and 12 in the second molecule). Evidently the former are nitrogen atoms and the latter oxygen.

The configuration of the substituents is as follows: the nitrogen atoms at carbon atoms 1,3,7 and 9 and the oxygen atoms at C(5) and C(11) are equatorial substituents, while the oxygen atoms at C(4), C(6), C(10) and C(12) are axial substituents. Consequently both molecules in the asymmetric unit have the same configuration, as was to be expected since the starting material was a single chemical compound. In the nomenclature of Wolfrom, Radell, Husband & McGasland (1957) and Fletcher, Anderson & Lardy (1951) the subject of the present study is evidently the dihydrochloride of 2-deoxy-*cis*-inosa-1,3-diamine, the substituents having the 'all-*cis*' configuration.

Bond lengths and bond angles are given in Fig. 1. Since the standard deviations of the atomic coordinates of the carbon atoms are rather high (0·014 Å), owing to the presence of the heavy Cl^- ions and the non-centrosymmetric nature of the structure, it is felt that discussion of differences in bond lengths in the two independent molecules is not justified.

Fig. 2 shows the *a*- and *b*-axis projections of the structure. The molecular arrangement is such that the majority of the hydroxyl and amino hydrogen atoms take part in hydrogen bonding: a systematically generated list of all intermolecular distances reveals that 15 out of the 18 shortest intermolecular distances between N, O and Cl^- may be assumed to be hydrogen bonds (Table 3). The three exceptions are placed in

Table 3. *Short intermolecular distances involving hydrogen atoms*

1	N(13)–Cl^-(23)	3·06 Å	C(1)—N(13)–Cl^-(23)	107·0°
2	N(13)–Cl^-(24)	3·17	C(1)—N(13)–Cl^-(24)	118·4
3	N(13)–Cl^-(26)	3·14	C(1)—N(13)–Cl^-(26)	115·4
4	N(14)–Cl^-(23)	3·14	C(2)—N(14)–Cl^-(23)	112·2
5	N(14)–Cl^-(24)	3·19	C(2)—N(14)–Cl^-(24)	115·0
6	N(14)–Cl^-(26)	3·29	C(2)—N(14)–Cl^-(26)	105·6
7	N(15)–O(17)	2·95	C(7)—N(15)–O(17)	99·7
8	N(15)–O(18)	3·09	C(7)—N(15)–O(18)	106·3
9	N(15)–O(19)	2·88	C(7)—N(15)–O(19)	99·5
10	N(16)–Cl^-(25)	3·21	C(9)—N(16)–Cl^-(25)	95·5
11	[N(16)–Cl^-(26)	3·33	C(9)—N(16)–Cl^-(26)	131·4]
12	[N(16)–Cl^-(25′)	3·50	C(9)—N(16)–Cl^-(25′)	105·7]
13	O(17)–O(22)	2·72	C(4)—O(17)–O(22)	103·8
14	O(18)–Cl^-(25)	3·20	C(6)—O(18)–Cl^-(25)	107·4
15	[O(19)–Cl^-(25′)	3·24	C(5)—O(19)–Cl^-(25′)	133·4]
16	O(20)–Cl^-(23)	2·98	C(10)–O(20)–Cl(23)	108·9
17	O(21)–Cl^-(25)	3·10	C(12)–O(21)–Cl^-(25)	107·1
18	O(22)–Cl^-(26)	3·01	C(11)–O(22)–Cl^-(26)	125·0

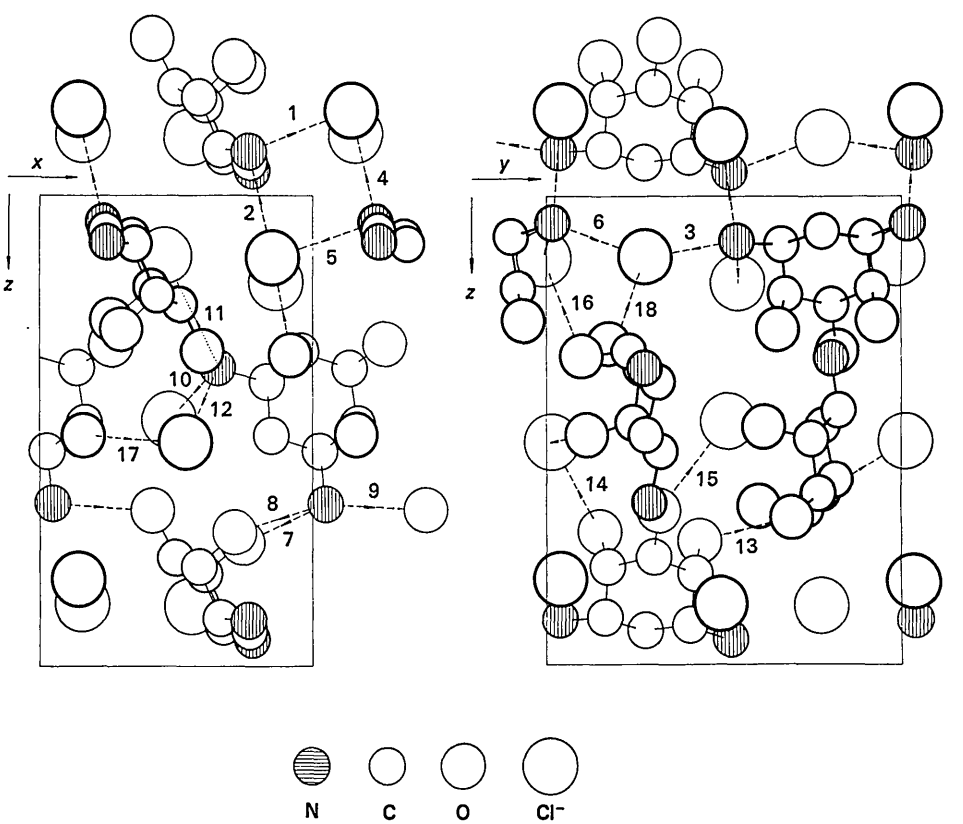

Fig. 2. *b*- and *a*-axis projections of the structure.

parentheses. The enumeration of the 18 distances corresponds to the numbers in Fig. 2.

The nitrogen atoms N(13) and N(14) of molecule 1 [with carbon ring atoms C(1) through C(6)] are tetrahedrally surrounded by three Cl^- ions Cl(23), Cl(24) and Cl(26), with the formation of six hydrogen bonds. Two of these, 3 and 6 in Table 3 and Fig. 2, take part in a strong periodic bond chain in the general direction of the *b* axis at $z \simeq 0{\cdot}1$: N(14′)–H···Cl(26)···H–N(13)–C(1)–C(2)–C(3)–N(14). This chain and its screw symmetric equivalent at $z = -0{\cdot}1$ are connected, at $y \simeq 0$ and $y \simeq \frac{1}{2}$, by the square arrangement of hydrogen bonds 1,2,4 and 5 depicted in the *b*-axis projection at $x = 1$, $z = 0$.

The nitrogen atoms of the second molecule [with carbon ring atoms C(7) through C(12)] have a different environment: N(15) takes part in the formation of the three N–H···O hydrogen bonds 7, 8 and 9, while for N(16) spatial conditions are unfavourable for hydrogen bond formation, only distance 10 being a hydrogen bond. In conclusion, Table 3 shows that five out of the six hydroxyl hydrogen atoms take part in O–H···Cl^- or O–H···O hydrogen bonds.

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The Crystal Structure of Orthanilic Acid

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Crystals of orthanilic acid, $NH_3^+C_6H_4SO_3^-$, are monoclinic, space group $P2_1/c$, with cell dimensions $a = 7{\cdot}935$, $b = 6{\cdot}570$, $c = 14{\cdot}225$ Å, $\beta = 105°\,54'$, $Z = 4$.

The structure was determined by three-dimensional X-ray techniques in order to study the N–H···O$^-$ bond system, which contains a 'bifurcated' bond of intra- and inter-molecular character. The hydrogen positions were confirmed by a neutron diffraction analysis of the 0*kl* projection. The final *R* index on the X-ray data is 0·064. The residual electron density map contains features which are due to bonding electrons. For the majority of the C–C bonds these consist of dumbell-shaped peaks which extend approximately 1 Å above and below the plane of the benzene ring.

Introduction

The investigation of the structure of orthanilic acid was undertaken as part of the programme of research on the structural properties of the anilinesulphonic acids (Fig. 1) which is in progress in this laboratory. The three compounds are similar in constitution, differing only in the point of attachment of the ions to the benzene ring. This enables a useful comparison to be made of the molecular packing and hydrogen bonding in the structures.

Sulphanilic (aniline-*p*-sulphonic) acid and metanilic (aniline-*m*-sulphonic) acid have been investigated by Rae & Maslen (1962) and Hall & Maslen (1965). Orthanilic acid was selected for a more accurate analysis because of the possibility of the structure containing an internal hydrogen bond. Large crystals of the material can be prepared quite readily, enabling a neutron-diffraction analysis to be carried out to confirm the hydrogen positions from the X-ray structure.

Experimental

Crystal data

Orthanilic (aniline-*o*-sulphonic) acid, $NH_3^+C_6H_4SO_3^-$
$a = 7{\cdot}935 \pm 0{\cdot}004$, $b = 6{\cdot}570 \pm 0{\cdot}006$, $c = 14{\cdot}225 \pm 0{\cdot}005$ Å
$\beta = 105°\,54' \pm 6'$, $U = 713{\cdot}1$ Å^3, M.W. 173·1.
$D_m = 1{\cdot}617 \pm 0{\cdot}010$, $Z = 4$, $D_x = 1{\cdot}613 \pm 0{\cdot}002$ gm.cm^{-3}.
Absent reflexions: *h*0*l* when *l* is odd, 0*k*0 when *k* is odd.
Space group: $P2_1/c$.
Crystal habit: Colourless monoclinic prisms.
Linear absorption coefficient: $\mu = 35{\cdot}84$ cm^{-1} (Cu $K\alpha$).