Acta Cryst. (1965). **19**, 898

Structural Studies of Metal Dithiocarbamates.
III. The Crystal and Molecular Structure of Zinc Diethyldithiocarbamate*

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(*Received* 9 *June* 1965)

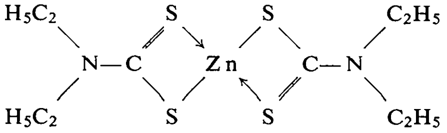
The crystal structure of zinc(II) bis(*N,N*-diethyldithiocarbamate), $[(C_2H_5)_2NCS_2]_2$ Zn, at room temperature has been determined by three-dimensional methods, including anisotropic refinement by differential Fourier synthesis (final *R* value, 0·106). There are four formula units in the monoclinic cell, $a=$ 10·015, $b=$ 10·661, $c=$ 16·357 Å, $\beta=111°58'$, with space group $P2_1/c$. Each pair of centrosymmetrically related zinc atoms share sulphur atoms, thus forming a dimeric unit in which each zinc atom is coordinated with five sulphur atoms, at distances ranging from $2{\cdot}33_1$ to $2{\cdot}81_5$ Å, in a distorted trigonal bipyramidal environment. Alternatively, it could be regarded as a distorted tetragonal pyramidal environment. One of the sulphur–zinc *intrachelate* distances is *ca.*0·4 Å longer than the corresponding *interchelate* distance. The same ligand molecule thus behaves in two very different ways in the same complex: one ligand forming a four-membered chelate ring, and a second coordinating with two different zinc atoms, whilst at the same time completing a chelate ring with a remarkably long approach distance. The four shortest bonds formed by any one zinc atom are directed to the corners of a very distorted tetrahedron. The ligand molecules are planar (obviously apart from the terminal CH_3 groups), sulphur–carbon bond lengths range from $1{\cdot}72_2$ to $1{\cdot}73_7$ Å, and the two $C(sp^2)-N(sp^2)$ bonds are 1·31 and 1·34 Å long. As expected from previous infrared work, $\cdots\overset{(-)}{S_2C}=\overset{(+)}{N}R_2$ is an important canonical form in the structure of zinc diethyldithiocarbamate. The crystal parameters of zinc diethyldithiocarbamate have values very near to those of the corresponding copper complex. However, the two compounds are only partially isostructural, because small differences in atomic positions, mainly of the metal atoms, produce a rather different coordination geometry in the two cases.

Introduction

The first paper of this series (Bonamico, Dessy, Mariani, Vaciago & Zambonelli, 1965) gave the general reasons for the investigation of the structure of metal dithiocarbamates.

The second paper (Bonamico, Dessy, Mugnoli, Vaciago & Zambonelli, 1965) dealt with the structure of copper diethyldithiocarbamate and reported earlier suggestions (Shugam & Shkol'nikova, 1958; Vaciago, Gramaccioli & Pullia, 1960) that the similarity of the crystal parameters of zinc diethyldithiocarbamate (Simonsen & Wah Ho, 1953) to those of the copper salt could indicate that these compounds were isostructural. It was, however, pointed out in the second paper of this series that the results found on the coordination geometry of the copper complex did not seem to be applicable to the case of the zinc salt but no detailed discussion was possible because no structural investigation of a zinc coordination compound of dithiocarbamic acid had been carried out previously.

For this particular reason, as well as for the more general ones, the third compound investigated in our laboratory was zinc(II) bis(*N,N*-diethyldithiocarbamate):



with the bond orders written in the conventional way. An interim report on the three-dimensional work on this structure was published in 1963 (Bonamico, Dessy, Mazzone, Mugnoli, Vaciago & Zambonelli, 1963).

Experimental

Crystal data

Zinc diethyldithiocarbamate forms transparent monoclinic prisms, stable in air and in the X-ray beam.

The unit-cell dimensions were redetermined by a modified, improved version of Christ's method (Mazzone, Vaciago & Bonamico, 1963) from zero-layer Weissenberg films about the *a* and *b* axes, using Cu $K\alpha$ radiation (λ taken as 1·5418 Å). They should replace the earlier values given by Simonsen & Wah Ho (1953).

Zinc(II) bis(N,N-diethyldithiocarbamate)
$C_{10}H_{20}N_2S_4Zn$. F.W. = 361·91.
Monoclinic prismatic, $a=10{\cdot}015\pm0{\cdot}010$, $b=10{\cdot}661\pm0{\cdot}005$, $c=16{\cdot}357\pm0{\cdot}010$ Å;
$\beta=111°\,58'\pm5'$; $U=1619{\cdot}7$ Å^3;
$D_m=1{\cdot}480\pm0{\cdot}005$ g.cm^{-3} (by flotation); $Z=4$;
$D_c=1{\cdot}485$ g.cm^{-3}; $F(000)=752$.

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* This paper was part of communication 6·27 to the I.U.Cr. Sixth International Congress held in Rome in 1963.

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Absorption coefficient for Cu radiation, 67 cm^{-1}.
Space group $P2_1/c$ (C^5_{2h}, No. 14), from systematic absences.*

Intensity measurements

The X-ray intensities were estimated visually from sets of multiple-film equi-inclination Weissenberg photographs taken about the *a* (6 layers), *b* (7 layers) and *c* axes (1 layer) for approximately square crystals, 0·02 cm thick. 2652 independent reflexions were collected (about 75% of the possible ones with Cu radiation). The intensities were corrected for Lorentz and polarization factors, and placed on a common scale by the method of Rollett & Sparks (1960). No absorption or extinction corrections were applied. Spot-size correction was applied according to Phillips (1954).

Determination of structure

A three-dimensional Patterson function was computed. Approximate positions were found for zinc and sulphur atoms. By a three-dimensional F_o synthesis, phased on the contribution of these five atoms, it was possible to locate all the atoms, apart from the hydrogen atoms. At this stage, a structure factor calculation gave a reliability index $R=0·36$.

Refinement

Refinement was done by differential Fourier synthesis. After the first cycle, the reliability index *R* was 0·19. Two other cycles lowered the *R* value to 0·167. Three cycles of anisotropic refinement, and the introduction of hydrogen atoms in positions* calculated

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* Unit-cell dimensions for the copper compound, quoted from paper II of this series, are: $a=9·907$, $b=10·627$, $c=16·591$ Å; $\beta=113°52'$; $U=1597·4$ Å^3; *space group* $P2_1/c$. As in paper II, setting $P2_1/c$ is again preferred here to the conventional $P2_1/n$ for the sake of comparison with the work of other authors.

* When the choice of the hydrogen positions is not unique, as on the methyl groups, a staggered conformation is assumed.

Table 1. *Final coordinates with standard deviations* (× 10^4)

	x/a	y/b	z/c
Zn	1697 (1)	725 (1)	540 (1)
S(1)	3408 (3)	2441 (2)	1121 (2)
S(2)	2169 (3)	725 (2)	2063 (2)
S(3)	2439 (3)	−386 (3)	−443 (2)
S(4)	535 (2)	−1714 (2)	288 (1)
N(1)	3872 (9)	2672 (8)	2834 (5)
N(2)	1352 (9)	−2624 (7)	−982 (5)
C(1)	3206 (10)	2027 (10)	2086 (5)
C(2)	4713 (11)	3776 (10)	2854 (8)
C(3)	3690 (13)	2342 (12)	3670 (7)
C(4)	3762 (16)	4937 (12)	2580 (10)
C(5)	4865 (20)	1536(23)	4258 (9)
C(6)	1416 (11)	−1687 (8)	−447 (5)
C(7)	2123 (13)	−2636 (12)	−1595 (9)
C(8)	451 (12)	−3740 (10)	−1027 (8)
C(9)	1191 (18)	−2181 (19)	−2506 (8)
C(10)	1347 (17)	−4817 (12)	−476 (13)

Table 3. *Coordinates* (× 10^4) *and isotropic temperature factors for hydrogen atoms*

	x/a	y/b	z/c	B(Å^2)
H(2)*a*	5272	3647	2402	4·7
H(2)*b*	5498	3909	3521	4·7
H(3)*a*	2672	1845	3509	4·3
H(3)*b*	3663	3205	4019	4·3
H(4)*a*	4427	5754	2601	5·3
H(4)*b*	3202	5074	9030	5·3
H(4)*c*	2976	4812	1911	5·3
H(5)*a*	4668	1329	4855	5·9
H(5)*b*	5890	2023	4430	5·9
H(5)*c*	4899	662	3919	5·9
H(7)*a*	2468	−3592	−1645	4·5
H(7)*b*	3063	−2028	−1332	4·5
H(8)*a*	−47	−4042	−1711	4·4
H(8)*b*	−384	−3492	−779	4·4
H(9)*a*	1806	−2207	−2931	5·5
H(9)*b*	844	−1221	−2464	5·5
H(9)*c*	249	−2785	−2778	5·5
H(10)*a*	653	−5623	−522	6·3
H(10)*b*	1845	−4523	210	6·3
H(10)*c*	2182	−5073	−721	6·3

Table 2. *Thermal exponent coefficients* (*with e.s.d.'s*)

b_{ij} as given here are defined by: $T=\exp\{-10^{-4}(b_{11}h^2+b_{22}k^2+b_{33}l^2+b_{12}hk+b_{13}hl+b_{23}kl)\}$.

	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
Zn	125 (2)	79 (1)	31 (0)	−3 (2)	49 (1)	−16 (1)
S(1)	150 (3)	94 (2)	35 (1)	−54 (4)	66 (2)	−14 (2)
S(2)	141 (3)	77 (2)	33 (1)	−44 (4)	45 (3)	−5 (2)
S(3)	187 (4)	78 (2)	50 (1)	−58 (4)	118 (2)	−21 (2)
S(4)	133 (3)	75 (2)	28 (1)	0 (4)	55 (2)	18 (2)
N(1)	119 (12)	94 (9)	36 (3)	−42 (16)	35 (10)	−15 (8)
N(2)	139 (11)	69 (7)	33 (3)	10 (14)	69 (8)	−20 (7)
C(1)	108 (11)	69 (8)	33 (3)	7 (15)	49 (9)	−4 (8)
C(2)	152 (19)	104 (11)	58 (6)	−98 (23)	68 (16)	−67 (13)
C(3)	174 (19)	145 (15)	36 (4)	−23 (25)	73 (12)	−37 (12)
C(4)	235 (24)	81 (10)	75 (8)	−123 (25)	136 (17)	−56 (14)
C(5)	207 (27)	162 (19)	47 (6)	−4 (33)	44 (20)	12 (16)
C(6)	128 (12)	67 (8)	35 (4)	−25 (16)	53 (10)	−24 (8)
C(7)	176 (17)	105 (12)	51 (5)	−16 (22)	112 (11)	−52 (11)
C(8)	174 (18)	72 (9)	56 (6)	−63 (21)	93 (14)	−26 (11)
C(9)	260 (28)	208 (22)	39 (5)	−63 (35)	111 (15)	−52 (15)
C(10)	206 (23)	80 (12)	106 (10)	−38 (26)	171 (18)	−1 (16)

to make the C–H bond lengths 1·09 Å and to complete tetrahedra around the carbon atoms, brought the final R index to the value of 0·106 (calculated on observed reflections only).

Table 1 gives the final atomic coordinates with their e.s.d.'s (Cruickshank, 1949). Anisotropic temperature factors with their e.s.d.'s (Cruickshank, 1956) are listed in Table 2. In Table 3 atomic coordinates and isotropic temperature factors for hydrogen atoms are given.

The numbering of atoms is included in Fig. 1 and Fig. 2, except for the hydrogen atoms, which are numbered by reference to their respective carbon atoms.

Structure factors based on final parameters are compared with the observed structure amplitude in Table 4. The e.s.d. on the electron density is $\sigma(\varrho)=0{\cdot}23$ e.Å^{-3}. Atomic scattering values were those recommended in *International Tables for X-ray Crystallography* (1962). Correction for anomalous dispersion was applied for zinc and sulphur atoms (*International Tables for X-ray Crystallography*, 1962).

The comparison of peak heights and of curvatures was made as in the previous two papers of this series (Bonamico, Dessy, Mariani, Vaciago & Zambonelli, 1965; Bonamico, Dessy, Mugnoli, Vaciago & Zambonelli, 1965), but the table is omitted for the sake of brevity.

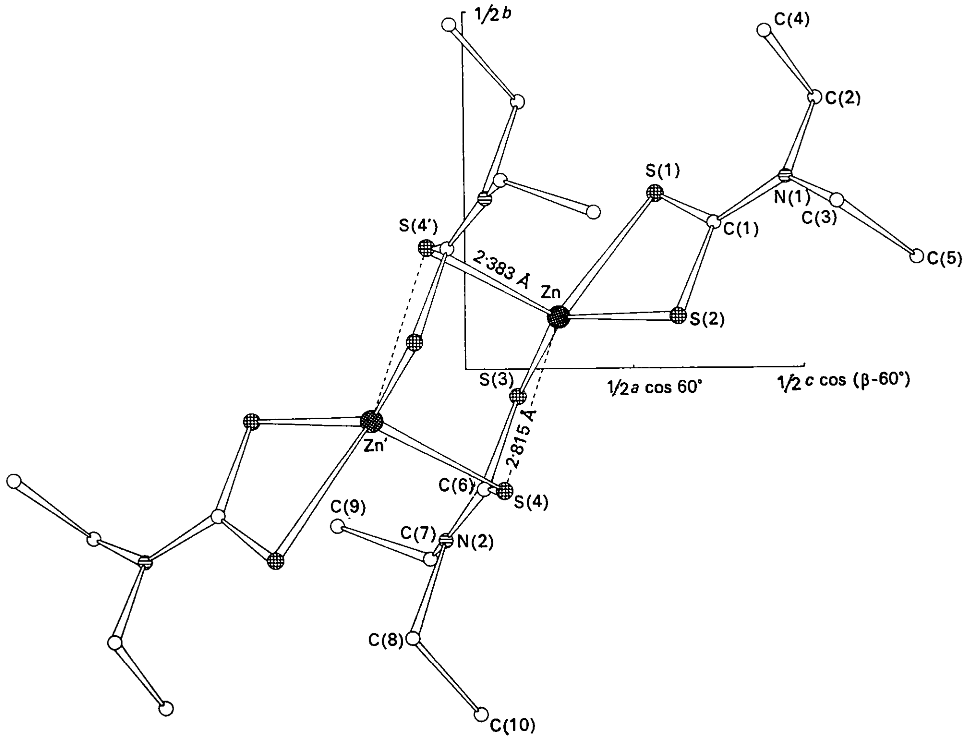

Fig. 1. Orthographic projection of the structure down the line which makes an angle of 90° with the b axis and $60°-(\beta-90°)=38°2'$ with the c axis.

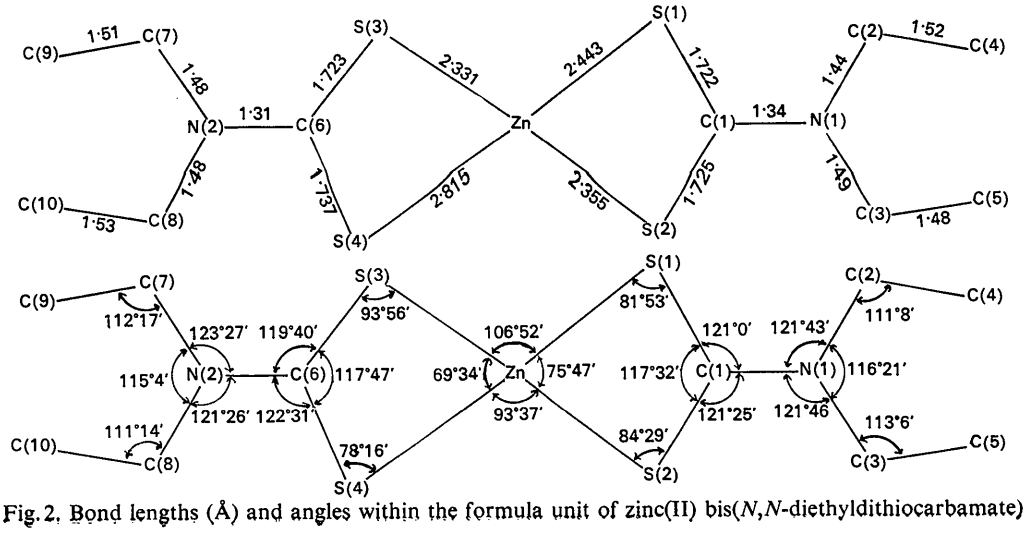

Fig. 2. Bond lengths (Å) and angles within the formula unit of zinc(II) bis(N,N-diethyldithiocarbamate).

Table 4. *Observed and calculated structure factors*

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
1	0	0	64.6	71.1	-6	0	10	19.8	18.0	3	1	2	29.1	32.0	-3	1	7	101.5	103.0	-6	1	12	12.4	15.8
2	0	0	92.8	-111.0	7	0	10	19.8	-20.1	-3	1	2	16.7	17.3	4	1	7	12.6	14.9	-9	1	12	11.5	16.1
3	0	0	68.5	-74.9	8	0	10	7.4	7.9	4	1	2	52.8	56.5	-4	1	7	35.9	-36.9	-11	1	12	2.8	4.1
4	0	0	32.3	-31.8	-8	0	10	22.7	-20.2	-4	1	2	12.1	12.3	5	1	7	7.9	-9.8	-12	1	12	2.1	2.8
5	0	0	39.9	45.1	-9	0	10	30.3	28.1	5	1	2	23.7	31.4	-5	1	7	89.9	-90.7	0	1	13	30.9	-33.5
6	0	0	44.6	47.3	-10	0	10	28.5	25.6	-5	1	2	35.9	44.5	6	1	7	17.3	-20.1	1	1	13	17.8	21.0
7	0	0	30.9	-33.2	-11	0	10	15.9	-14.1	6	1	2	11.5	-12.0	-6	1	7	6.0	-6.8	-1	1	13	47.5	-49.9
8	0	0	11.7	-11.0	-12	0	10	16.4	-12.8	-6	1	2	57.7	58.4	7	1	7	10.5	-12.4	2	1	13	24.1	30.3
9	0	0	11.7	-10.3	0	0	12	82.1	-88.6	-7	1	2	3.9	-5.2	-7	1	7	39.5	43.5	-2	1	13	7.0	-6.2
10	0	0	16.8	-19.1	-1	0	12	11.9	-12.4	-8	1	2	6.3	-7.8	-8	1	7	19.9	22.9	3	1	13	2.9	-3.3
11	0	0	7.2	-7.7	1	0	12	11.4	-12.5	9	1	2	5.6	-7.2	9	1	7	3.7	3.8	-3	1	13	27.0	28.8
0	0	2	73.7	85.1	2	0	12	63.0	64.5	-9	1	2	16.4	18.8	-9	1	7	8.1	-10.4	4	1	13	25.3	-27.2
1	0	2	104.0	106.3	-2	0	12	8.1	2.2	10	1	2	7.7	8.8	-10	1	7	8.4	-9.8	-4	1	13	24.6	24.5
-1	0	2	76.9	171.0	-3	0	12	24.3	24.0	-12	1	2	1.5	-2.9	-12	1	7	2.2	-3.6	5	1	13	12.6	-15.1
-2	0	2	6.3	-6.2	4	0	12	27.5	-26.6	0	1	3	47.2	49.0	0	1	8	30.3	31.7	-5	1	13	28.8	28.3
3	0	2	45.9	-40.3	-4	0	12	50.0	44.6	1	1	3	18.0	20.8	1	1	8	35.2	36.7	6	1	13	3.2	4.1
-3	0	2	69.9	-81.8	5	0	12	25.6	-25.8	-1	1	3	82.6	92.4	-1	1	8	23.3	-23.1	-7	1	13	8.8	-8.3
5	0	2	40.4	35.6	6	0	12	14.6	-13.8	2	1	3	51.2	-55.6	2	1	8	53.1	53.9	-8	1	13	6.5	-8.3
-5	0	2	51.2	-50.8	-6	0	12	19.1	15.6	-2	1	3	34.4	34.7	-2	1	8	53.8	49.0	-9	1	13	7.9	11.1
-6	0	2	45.5	47.4	-8	0	12	25.7	-23.0	3	1	3	70.5	-77.4	3	1	8	33.3	34.4	-10	1	13	11.5	15.2
7	0	2	24.9	-22.5	-9	0	12	12.6	10.1	-3	1	3	83.4	87.0	-3	1	8	57.7	-56.0	-11	1	13	3.7	4.4
-7	0	2	66.8	68.5	-10	0	12	33.7	30.5	4	1	3	13.3	15.8	4	1	8	20.4	-21.4	-12	1	13	4.6	-6.2
-8	0	2	19.5	-17.6	-11	0	12	9.0	7.7	-4	1	3	21.6	-21.1	-4	1	8	25.4	-24.4	0	1	14	29.9	32.2
9	0	2	16.7	-16.0	-12	0	12	13.2	-10.0	5	1	3	31.9	44.2	-5	1	8	36.4	33.9	1	1	14	3.5	-3.7
-9	0	2	44.2	-45.2	0	0	14	17.4	-19.2	-5	1	3	44.1	-49.6	6	1	8	2.1	-1.4	-1	1	14	24.0	-26.9
10	0	2	17.0	-16.1	-1	0	14	53.5	-61.4	6	1	3	9.8	11.0	-6	1	8	5.6	-7.9	2	1	14	16.1	-21.6
-10	0	2	25.7	-26.4	-2	0	14	31.3	-26.8	7	1	3	19.2	-20.9	7	1	8	4.2	-5.5	-2	1	14	19.4	-18.7
11	0	2	10.4	8.6	3	0	14	23.4	-23.6	-7	1	3	52.1	54.3	-7	1	8	28.8	33.2	3	1	14	8.8	-11.4
-11	0	2	7.9	-9.0	-3	0	14	15.4	-14.2	8	1	3	20.4	-24.6	8	1	8	2.1	-2.5	-3	1	14	12.4	-13.1
-12	0	2	13.6	10.4	4	0	14	13.3	-13.1	-8	1	3	20.9	22.7	-8	1	8	31.7	35.5	-4	1	14	4.2	4.5
0	0	4	69.5	72.4	-4	0	14	59.0	55.3	9	1	3	11.9	-14.0	-9	1	8	12.4	-14.9	5	1	14	5.6	-6.1
1	0	4	53.4	49.1	-5	0	14	70.5	64.0	-9	1	3	18.5	-22.1	-10	1	8	3.7	6.1	-5	1	14	31.2	-28.7
-1	0	4	43.2	50.4	-7	0	14	29.5	-27.2	10	1	3	4.4	5.7	-11	1	8	10.2	14.5	-6	1	14	17.3	-21.5
2	0	4	10.7	-9.0	-9	0	14	17.7	16.9	-10	1	3	26.0	-31.4	-12	1	8	1.4	-0.1	-7	1	14	7.2	8.8
-2	0	4	7.9	7.8	-10	0	14	36.2	30.7	-12	1	3	6.7	8.2	0	1	9	45.2	-47.0	-9	1	14	3.2	3.5
3	0	4	101.9	-99.2	-11	0	14	7.6	6.3	0	1	4	37.2	-37.5	1	1	9	3.7	-4.6	-10	1	14	6.3	11.0
-3	0	4	15.4	19.9	0	0	16	8.1	-8.3	1	1	4	22.2	22.8	-1	1	9	73.6	-72.2	-11	1	14	2.1	-3.1
4	0	4	40.7	37.8	1	0	16	7.4	-8.3	-1	1	4	28.9	30.2	2	1	9	20.9	22.1	0	1	15	8.4	8.8
-4	0	4	6.3	4.6	-1	0	16	5.5	-5.7	2	1	4	4.4	-1.2	-2	1	9	42.7	38.6	1	1	15	2.5	3.8
5	0	4	57.1	55.0	2	0	16	16.8	-17.8	-2	1	4	52.2	-53.4	3	1	9	4.4	5.6	-1	1	15	5.3	2.7
-5	0	4	27.0	-36.2	-2	0	16	7.3	-3.3	3	1	4	50.3	54.6	-3	1	9	68.1	85.4	2	1	15	2.5	-4.6
6	0	4	39.2	-32.1	-3	0	16	39.0	-36.6	-3	1	4	4.6	2.3	4	1	9	2.8	-2.9	-2	1	15	30.5	-29.9
-6	0	4	10.4	-10.5	-4	0	16	23.9	-21.5	4	1	4	78.1	87.2	-4	1	9	33.1	32.3	3	1	15	4.9	-5.5
7	0	4	39.5	-35.7	-5	0	16	52.8	49.2	-4	1	4	5.1	4.1	5	1	9	4.2	-6.1	-3	1	15	32.4	-34.7
-7	0	4	52.1	60.0	-6	0	16	40.2	36.4	5	1	4	11.0	-13.2	-5	1	9	33.3	-30.6	4	1	15	6.7	-7.7
8	0	4	28.5	-27.3	-7	0	16	14.3	-12.4	6	1	4	9.8	-10.2	6	1	9	9.1	-10.5	-4	1	15	13.6	14.0
-8	0	4	27.0	26.9	-10	0	16	22.0	21.8	-6	1	4	39.9	43.7	-6	1	9	29.8	-33.2	-5	1	15	44.9	48.7
-9	0	4	25.1	-26.6	-11	0	16	23.2	20.7	7	1	4	7.2	-9.2	7	1	9	15.0	-15.1	-6	1	15	19.9	26.1
10	0	4	20.5	17.8	0	0	18	11.1	13.5	-7	1	4	32.2	36.6	-7	1	9	3.5	3.8	-7	1	15	19.4	-26.1
-10	0	4	27.8	-30.5	-1	0	18	9.0	-10.1	8	1	4	11.2	-13.1	-8	1	9	19.7	24.0	-8	1	15	18.5	-26.6
-11	0	4	14.9	-13.6	-2	0	18	25.0	-23.5	-8	1	4	2.5	3.8	-9	1	9	16.4	20.4	-9	1	15	7.7	11.0
0	0	6	90.3	-94.3	-3	0	18	13.6	-12.1	9	1	4	7.7	10.2	-10	1	9	4.2	5.3	-10	1	15	19.2	22.5
1	0	6	48.2	-43.7	-4	0	18	14.0	-12.1	10	1	4	2.5	3.5	-11	1	9	5.3	-8.1	-11	1	15	2.8	3.4
-1	0	6	50.8	58.7	-5	0	18	17.8	13.9	-10	1	4	4.2	-6.3	-12	1	9	8.8	-10.7	0	1	16	22.3	25.7
2	0	6	93.8	-91.6	-6	0	18	21.3	19.4	-12	1	4	5.6	7.6	0	1	10	16.0	15.0	1	1	16	6.7	-9.7
-2	0	6	102.9	130.7	-7	0	18	6.6	-3.4	0	1	5	78.1	83.3	1	1	10	3.5	4.5	-1	1	16	11.2	-13.3
3	0	6	33.0	29.4	-8	0	18	5.9	5.0	1	1	5	24.1	-23.8	-1	1	10	54.9	-55.5	2	1	16	8.8	-10.2
-3	0	6	45.6	47.4	-9	0	18	20.1	17.4	-1	1	5	28.9	34.0	2	1	10	42.3	45.2	-2	1	16	16.0	-15.4
4	0	6	62.6	56.8	-1	0	20	16.3	23.9	2	1	5	72.3	-79.2	-2	1	10	5.2	5.0	3	1	16	3.2	-5.0
-4	0	6	24.4	21.4	-2	0	20	32.2	-25.7	-2	1	5	88.6	90.6	-3	1	10	9.3	9.6	-3	1	16	10.4	-12.5
6	0	6	57.4	-49.4	-3	0	20	44.2	-35.3	3	1	5	22.6	-22.2	4	1	10	11.2	-14.4	-4	1	16	7.4	7.2
7	0	6	37.9	-32.3	-4	0	20	15.0	-11.2	-3	1	5	26.8	26.2	-4	1	10	26.0	-25.3	-6	1	16	24.6	-32.8
-7	0	6	41.4	45.3	-5	0	20	9.1	-6.4	4	1	5	52.1	54.5	-5	1	10	33.3	-29.9	-7	1	16	7.7	-10.9
8	0	6	14.9	-14.1	-6	0	20	13.3	12.3	-4	1	5	2.8	1.0	6	1	10	10.2	-13.3	-8	1	16	4.2	-8.1
-8	0	6	19.5	19.7	-7	0	20	11.2	10.4	5	1	5	37.3	38.7	-6	1	10	5.6	8.9	-10	1	16	13.1	15.9
9	0	6	12.6	11.7	1	1	0	65.7	-58.7	-5	1	5	45.5	-46.2	-7	1	10	7.7	8.8	-11	1	16	4.4	5.9
-9	0	6	22.3	-21.8	2	1	0	132.1	165.6	6	1	5	15.2	-16.2	-8	1	10	31.9	37.9	-2	1	17	10.5	-12.4
12	0	6	10.5	-9.3	3	1	0	27.0	30.5	-6	1	5	12.4	-13.2	-9	1	10	17.3	21.2	-3	1	17	21.5	-24.0
0	0	8	59.4	-65.3	4	1	0	26.4	31.5	7	1	5	38.0	-44.2	-10	1	10	8.6	-11.7	-4	1	17	13.3	-14.1
1	0	8	7.0	-8.1	5	1	0	53.6	68.8	-7	1	5	27.2	29.5	-12	1	10	7.9	10.6	-5	1	17	21.9	21.3
-1	0	8	77.4	-85.0	6	1	0	9.5	-9.9	8	1	5	10.8	-13.9	0	1	11	65.1	-68.3	-6	1	17	13.8	19.9
2	0	8	17.3	16.5	7	1	0	16.7	-18.5	-8	1	5	21.8	24.6	1	1	11	18.0	-20.6	-8	1	17	5.6	-9.3
-2	0	8	98.8	109.8	8	1	0	16.3	19.0	9	1	5	9.1	10.3	-1	1	11	17.4	-17.1	-10	1	17	2.5	3.5
3	0	8	17.3	15.3	10	1	0	2.8	4.0	-9	1	5	4.6	-6.1	2	1	11	22.0	26.2	0	1	18	10.5	12.2
-3	0	8	166.7	227.9	0	1	1	121.6	145.8	10	1	5	5.6	6.7	-2	1	11	24.7	24.2	1	1	18	7.2	-9.0
4	0	8	23.4	-20.7	-1	1	1	94.5	108.7	-10	1	5	11.9	-13.8	3	1	11	19.7	25.2	-1	1	18	17.7	-20.2
-4	0	8	29.3	-27.6	2	1	1	170.2	-161.9	-11	1	5	10.0	-12.9	-3	1	11	36.5	37.7	-2	1	18	6.6	6.1
5	0	8	33.1	-27.5	-2	1	1	30.2	-30.6	-12	1	5	2.2	-4.1	4	1	11	10.0	-12.9	-3	1	18	6.7	-5.5
-5	0	8	41.4	-40.8	3	1	1	25.8	-28.5	0	1	6	20.4	19.3	-4	1	11	14.7	13.6	-4	1	18	14.9	-14.4
6	0	8	13.5	-11.7	-3	1	1	83.4	-93.6	1	1	6	14.2	12.9	5	1	11	17.8	-24.0	-5	1	18	12.2	3.9
-6	0	8	18.5	-18.3	4	1	1	29.9	33.3	-1	1	6	36.5	37.3	-5	1	11	7.7	8.0	-6	1	18	7.9	-11.0
7	0	8	21.1	-17.9	-4	1	1	16.4	-21.3	2	1	6	43.2	44.3	6	1	11	16.1	-18.0	-7	1	18	12.6	-17.2
-7	0	8	14.7	14.1	5	1	1	41.6	41.2	-2	1	6	103.5	-102.9	-6	1	11	17.5	19.9	-8	1	18	2.5	-4.6
8	0	8	10.5	-11.6	-5	1	1	29.8	38.9	3	1	6	47.9	51.5	-7	1	11	7.2	-9.4	-9	1	18	4.4	-6.7
-8	0	8	55.6	54.1	6	1	1	3.5	-3.9	-3	1	6	84.1	-86.2	-8	1	11	12.2	-15.1	-10	1	18	2.8	3.9
9	0	8	4.9	4.5	-6	1	1	33.8	36.3	4	1	6	2.5	-3.2	-9	1	11	8.8	12.6	0	1	19	15.7	17.2
-9	0	8	15.3	14.3	7	1	1	13.8	-13.6	-4	1	6	7.7	8.7	-10	1	11	19.4	27.1	-1	1	19	4.6	4.7
10	0	8	29.8	-26.7	-7	1	1	13.3	14.2	5	1	6	13.1	-15.1	-11	1	11	4.6	4.9	-2	1	19	22.3	-20.4
12	0	8	10.0	-8.1	8	1	1	6.5	-8.6	-5	1	6	29.9	27.3	-12	1	11	10.0	-12.7	-3	1	19	28.6	-27.2
0	0	10	38.9	-37.0	-8	1	1	12.4	-14.1	6	1	6	4.2	5.7	0	1	12	2.9	-1.4	-4	1	19	2.2	-0.7
1	0	10	43.8	-44.6	9	1	1	6.0	-7.8	-6	1	6	33.6	35.8	1	1	12	48.6	59.3	-5	1	19	12.1	12.2
-1	0	10	36.4	-37.1	-9	1	1	18.5	-21.6	-7	1	6	40.9	46.4	-1	1	12	6.3	3.4	-6	1	19	5.3	7.3
2	0	10	10.1	9.4	10	1	1	9.5	-12.2	-10	1	6	3.5	5.6	2	1	12	3.9	-4.8	-7	1	19	2.5	-4.9
-2	0	10	36.8	34.6	-10	1	1	5.6	-7.1	-12	1	6	1.8	3.6	-2	1	12	20.2	-19.5	-8	1	19	2.5	3.0
3	0	10	35.8	35.4	-12	1	1	3.7	4.1	0	1	7	84.5	-90.1	3	1	12	14.5	-18.1	-9	1	19	5.3	7.5
-3	0	10	75.0	80.7	0	1	2	79.0	-110.9	1	1	7	43.9	-43.1	-3	1	12	21.2	20.2	-2	1	20	10.0	-10.7
4	0	10	18.7	-16.4	1	1	2	16.7	-14.1	-1	1	7	15.2	15.5	4	1	12	2.8	-1.2	-3	1	20	9.3	8.8
-4	0	10	64.7	60.5	-1	1	2	87.2	92.3	2	1	7	22.3	21.7	-4	1	12	36.5	-34.5	-4	1	20	7.2	-7.5
5	0	10	21.3	-20.4	2	1	2	58.1	67.8	-2	1	7	112.6	120.7	5	1	12	8.4	-9.5	-5	1	20	6.0	-6.0
6	0	10	17.7	-16.6	-2	1	2	104.2	-122.0	3	1	7	25.6	25.6	-5	1	12	46.5	-46.9	-6	1	20	3.5	-1.8

Table 4 (*cont.*)

H	K	L	FC	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-7	1	20	19.7	-26.5	-1	2	5	1.8	-0.9	0	2	10	49.1	-53.6	0	2	16	13.2	15.4	-1	3	3	75.8	-74.5
-8	1	20	7.0	-12.0	2	2	5	81.2	83.6	1	2	10	25.7	25.7	-1	2	16	24.7	26.8	2	3	3	27.0	-25.0
0	2	0	42.1	-37.1	-2	2	5	45.5	-52.1	-1	2	10	24.6	-23.2	2	2	16	16.1	16.2	-2	3	3	52.5	-47.1
1	2	0	45.9	40.4	3	2	5	95.3	98.0	2	2	10	24.6	25.6	-2	2	16	20.9	-19.6	3	3	3	8.8	-7.8
2	2	0	85.1	-83.8	-3	2	5	55.6	-52.6	-2	2	10	22.7	22.7	-3	2	16	22.2	-22.7	-3	3	3	6.3	-7.0
3	2	0	110.1	-114.4	4	2	5	35.0	37.2	3	2	10	3.7	5.5	-4	2	16	5.5	1.1	4	3	3	21.9	22.7
4	2	0	56.0	62.3	-4	2	5	32.9	30.8	-3	2	10	4.2	1.1	-5	2	16	17.3	16.4	-4	3	3	9.1	-7.5
5	2	0	38.0	44.3	5	2	5	19.7	-17.6	4	2	10	27.4	28.1	-6	2	16	16.8	21.3	5	3	3	45.3	39.4
6	2	0	13.3	-13.5	-5	2	5	35.0	31.4	-4	2	10	8.7	7.0	-7	2	16	9.7	-12.4	-5	3	3	58.8	-55.5
7	2	0	14.2	13.5	6	2	5	21.8	-22.1	-5	2	10	1.8	-1.6	-8	2	16	24.9	-34.1	6	3	3	24.6	21.4
9	2	0	6.2	-5.8	-6	2	5	42.8	40.8	6	2	10	14.9	-13.4	-9	2	16	2.1	-2.1	-6	3	3	13.6	-12.1
10	2	0	2.8	3.6	7	2	5	7.0	-7.9	-6	2	10	35.7	-36.6	-10	2	16	7.0	7.7	-7	3	3	11.9	12.6
11	2	0	4.6	5.3	-7	2	5	24.4	25.5	7	2	10	5.1	5.7	-11	2	16	4.5	-6.6	-8	3	3	20.9	19.3
0	2	1	56.7	-58.5	8	2	5	10.8	13.3	-7	2	10	29.2	-32.9	0	2	17	9.1	7.0	9	3	3	9.5	11.0
1	2	1	56.9	-53.3	-8	2	5	22.9	23.0	-9	2	10	2.9	2.1	-1	2	17	11.1	-12.5	10	3	3	3.8	4.3
-1	2	1	31.7	-25.0	9	2	5	5.1	5.8	-10	2	10	11.4	14.2	2	2	17	8.8	-17.4	-10	3	3	4.9	4.6
2	2	1	46.2	46.5	10	2	5	3.2	-3.5	-11	2	10	7.7	8.5	-3	2	17	8.0	-8.2	-11	3	3	6.2	6.4
-2	2	1	111.2	-118.3	-10	2	5	6.0	-6.9	-12	2	10	11.0	-11.8	-5	2	17	4.4	-2.6	-12	3	3	5.6	7.0
3	2	1	55.5	54.5	-12	2	5	9.3	10.7	0	2	11	24.1	24.2	-6	2	17	6.9	-8.3	0	3	4	57.6	-54.2
-3	2	1	18.8	-19.8	0	2	6	13.1	-12.7	-1	2	11	10.5	-8.9	-7	2	17	18.1	-20.4	1	3	4	83.0	-79.5
4	2	1	59.0	64.6	1	2	6	44.6	-40.7	2	2	11	31.3	34.4	-8	2	17	14.9	-18.8	-1	3	4	3.8	-2.6
-4	2	1	63.2	66.4	-1	2	6	8.1	8.8	-2	2	11	28.2	-24.0	-10	2	17	8.1	16.9	2	3	4	38.5	36.7
5	2	1	30.6	37.2	2	2	6	11.2	9.5	3	2	11	8.6	-8.5	0	2	18	6.2	7.4	-2	3	4	16.0	-14.0
-5	2	1	73.7	80.7	-2	2	6	8.8	7.8	-3	2	11	3.8	5.2	1	2	18	12.6	16.7	3	3	4	41.3	41.9
6	2	1	9.0	-8.3	3	2	6	17.8	18.8	4	2	11	23.0	-25.4	-1	2	18	11.1	12.1	-3	3	4	84.0	-81.9
-6	2	1	10.1	10.8	-3	2	6	19.5	18.2	-4	2	11	28.1	-26.7	-3	2	18	19.5	-21.7	-4	3	4	18.7	-16.0
7	2	1	13.6	-12.1	4	2	6	20.1	22.1	5	2	11	14.0	-18.0	-4	2	18	9.8	11.6	5	3	4	9.3	9.4
-7	2	1	26.8	-28.0	-4	2	6	66.1	-62.9	-5	2	11	28.2	-25.9	-5	2	18	11.2	11.9	-5	3	4	38.9	34.5
8	2	1	3.4	-3.4	5	2	6	21.6	21.2	6	2	11	3.7	3.7	-6	2	18	4.2	-6.3	6	3	4	36.5	-36.5
-8	2	1	10.1	-10.0	-5	2	6	82.8	-94.4	-6	2	11	15.7	-17.6	-7	2	18	2.1	4.1	-6	3	4	13.9	12.1
-9	2	1	12.5	13.5	6	2	6	6.5	-6.6	7	2	11	8.4	8.8	-8	2	18	3.4	-3.9	7	3	4	35.2	-33.9
-10	2	1	7.7	9.8	-6	2	6	14.9	15.7	-7	2	11	13.6	15.2	-9	2	18	9.8	-12.7	8	3	4	22.0	20.9
0	2	2	63.5	60.5	7	2	6	9.3	-10.5	-8	2	11	18.8	19.9	-1	2	19	15.4	-16.8	9	3	4	16.0	14.1
1	2	2	4.6	-5.0	-7	2	6	33.8	36.0	-9	2	11	15.4	18.1	-2	2	19	9.1	-8.1	-9	3	4	28.9	-26.8
-1	2	2	37.6	32.6	8	2	6	7.7	8.8	0	2	12	14.6	-15.6	-3	2	19	4.4	-0.2	10	3	4	4.4	4.9
2	2	2	114.1	-122.4	-8	2	6	7.4	6.4	1	2	12	10.2	8.7	-5	2	19	4.9	-4.8	-10	3	4	10.4	-10.2
-2	2	2	4.5	4.1	9	2	6	8.4	8.1	-1	2	12	50.5	-54.3	-6	2	19	8.1	-10.9	-11	3	4	8.1	12.7
3	2	2	40.9	-42.4	-9	2	6	4.9	3.6	2	2	12	19.7	21.9	-7	2	19	16.1	-19.3	-12	3	4	7.0	7.1
-3	2	2	50.3	-47.6	-10	2	6	4.6	-5.6	-2	2	12	39.9	37.7	-8	2	19	9.0	-10.6	0	3	5	56.6	-48.2
4	2	2	44.6	50.9	-11	2	6	3.8	-3.9	3	2	12	34.5	39.2	-2	2	20	10.7	9.2	1	3	5	19.0	-17.7
-4	2	2	87.9	-87.4	-12	2	6	4.1	5.0	-3	2	12	45.2	46.9	-3	2	20	8.6	-8.7	-1	3	5	23.2	-21.5
5	2	2	18.4	21.2	0	2	7	44.5	-43.3	4	2	12	9.3	-11.5	-4	2	20	6.9	-6.5	2	3	5	49.8	-49.7
-5	2	2	5.1	-4.2	1	2	7	57.8	53.3	-4	2	12	43.2	-39.6	-5	2	20	27.4	25.3	-2	3	5	20.9	-17.8
6	2	2	10.5	10.6	-1	2	7	73.3	75.2	5	2	12	14.9	-16.4	-6	2	20	3.2	4.2	3	3	5	9.7	-8.3
-6	2	2	15.3	15.6	2	2	7	71.3	76.9	-5	2	12	3.8	4.2	-7	2	20	9.8	-14.0	4	3	5	24.4	24.9
7	2	2	16.6	16.4	-2	2	7	32.0	-27.9	6	2	12	9.8	10.7	1	3	0	60.7	-54.2	-4	3	5	45.1	-38.6
-7	2	2	19.2	17.4	3	2	7	39.0	37.4	-7	2	12	30.0	-34.9	2	3	0	165.7	-179.5	5	3	5	41.7	41.8
8	2	2	9.4	-10.2	-3	2	7	64.7	-60.5	-8	2	12	11.8	-12.0	3	3	0	24.1	23.5	-5	3	5	48.3	-41.4
-8	2	2	25.0	22.8	4	2	7	19.4	-19.5	-9	2	12	6.0	-4.3	4	3	0	117.8	115.9	6	3	5	8.1	8.7
-9	2	2	10.2	-11.7	-4	2	7	45.1	-41.7	-10	2	12	6.0	8.1	5	3	0	12.8	13.7	-6	3	5	38.5	-35.2
10	2	2	6.6	7.3	5	2	7	19.2	-20.3	-11	2	12	9.7	11.9	7	3	0	25.0	-27.8	7	3	5	2.7	1.9
-10	2	2	7.0	-7.4	-5	2	7	17.5	16.9	-12	2	12	3.7	-3.9	8	3	0	15.3	-14.9	-7	3	5	6.5	6.9
-11	2	2	12.5	12.1	6	2	7	2.9	-2.2	0	2	13	52.6	54.9	9	3	0	10.5	10.6	8	3	5	5.3	5.5
-12	2	2	3.8	5.4	-6	2	7	43.4	41.2	1	2	13	26.1	28.8	10	3	0	6.5	7.3	-8	3	5	18.8	17.8
0	2	3	48.3	-44.2	7	2	7	2.9	4.1	-1	2	13	32.2	-31.9	11	3	0	2.7	-3.0	9	3	5	7.3	6.8
1	2	3	62.9	81.2	-7	2	7	43.0	44.8	2	2	13	14.9	-17.4	0	3	1	2.9	-2.2	-9	3	5	9.0	8.5
-1	2	3	9.3	-6.9	-8	2	7	7.4	6.5	-2	2	13	23.6	22.4	1	3	1	32.9	-31.1	-11	3	5	8.4	8.6
2	2	3	23.6	24.1	9	2	7	1.8	-2.2	3	2	13	18.8	-21.3	-1	3	1	64.7	-67.8	-12	3	5	4.6	5.4
-2	2	3	22.9	-21.9	-9	2	7	6.2	-6.7	-3	2	13	17.0	15.6	2	3	1	85.8	-79.9	0	3	6	137.0	-147.6
3	2	3	70.5	70.7	-10	2	7	4.6	-5.2	4	2	13	9.7	-10.4	-2	3	1	18.4	-18.4	1	3	6	15.2	-15.9
-3	2	3	84.8	-78.8	-11	2	7	2.2	3.6	-4	2	13	19.5	-19.6	3	3	1	29.9	-28.6	-1	3	6	50.8	47.4
4	2	3	41.6	43.7	-12	2	7	3.4	3.5	5	2	13	3.4	3.8	-3	3	1	34.3	-29.8	2	3	6	106.0	117.0
-4	2	3	19.1	17.5	0	2	8	92.0	-93.2	-5	2	13	48.6	-44.6	4	3	1	53.8	52.8	-2	3	6	60.0	-55.4
5	2	3	38.6	35.2	1	2	8	12.9	-13.7	6	2	13	4.5	5.0	-4	3	1	13.6	9.1	3	3	6	47.7	49.2
-5	2	3	63.0	67.5	-1	2	8	31.9	-33.2	-6	2	13	26.8	-17.4	5	3	1	20.2	18.7	-3	3	6	52.1	-51.9
6	2	3	11.7	-13.0	2	2	8	67.3	61.5	-7	2	13	14.2	15.6	-5	3	1	13.9	11.4	4	3	6	13.6	-13.8
-6	2	3	69.6	64.3	-2	2	8	30.6	25.9	-8	2	13	12.9	15.0	6	3	1	9.8	8.0	-4	3	6	51.8	-46.1
7	2	3	20.1	-19.5	3	2	8	14.9	14.8	-9	2	13	7.0	6.6	-6	3	1	10.8	-10.5	5	3	6	46.5	-44.7
-7	2	3	16.4	17.1	-3	2	8	21.9	24.3	-10	2	13	5.1	7.8	7	3	1	5.3	5.4	-5	3	6	31.6	26.2
8	2	3	13.8	-14.4	4	2	8	8.8	9.1	-11	2	13	6.9	8.5	8	3	1	10.4	11.0	6	3	6	28.9	-27.2
-8	2	3	8.8	-8.8	-4	2	8	23.7	20.6	0	2	14	17.8	19.7	-8	3	1	11.9	11.7	-6	3	6	9.3	9.8
9	2	3	12.6	14.2	5	2	8	15.7	16.4	1	2	14	16.4	20.1	9	3	1	5.6	6.3	7	3	6	10.8	11.6
-9	2	3	8.4	-9.1	-5	2	8	71.7	-68.9	-1	2	14	8.0	8.4	-9	3	1	5.3	6.9	-7	3	6	7.9	-7.3
10	2	3	8.4	8.4	6	2	8	4.5	-3.8	2	2	14	13.2	14.8	10	3	1	4.6	6.5	8	3	6	12.2	11.5
-10	2	3	3.8	4.8	-6	2	8	38.9	-35.5	-2	2	14	24.1	-22.2	-10	3	1	4.4	4.1	-8	3	6	13.6	14.7
-11	2	3	11.2	12.7	7	2	8	4.5	-5.8	-3	2	14	10.1	-10.4	11	3	1	2.1	2.5	-9	3	6	2.7	0.7
0	2	4	89.0	90.7	-7	2	8	41.4	40.1	4	2	14	11.4	-11.6	-11	3	1	5.9	6.1	-10	3	6	17.1	-17.7
1	2	4	5.6	-5.1	8	2	8	3.4	3.7	-4	2	14	4.1	3.1	0	3	2	44.6	-42.4	-12	3	6	7.9	7.2
-1	2	4	78.3	-86.3	-9	2	8	12.5	-13.6	5	2	14	1.8	-1.3	1	3	2	46.8	-45.9	0	3	7	22.7	-23.6
2	2	4	93.6	-96.2	-10	2	8	8.1	9.4	-5	2	14	2.5	1.8	-1	3	2	62.6	62.2	1	3	7	7.2	-6.7
-2	2	4	56.4	-41.3	-11	2	8	2.9	-3.8	-6	2	14	6.0	6.6	2	3	2	15.3	13.0	-1	3	7	26.3	-24.1
3	2	4	13.8	-15.4	0	2	9	25.7	21.8	-7	2	14	23.4	-27.5	-2	3	2	43.9	-42.2	2	3	7	7.4	9.8
-3	2	4	46.3	42.0	1	2	9	16.8	17.0	-8	2	14	26.4	-29.9	3	3	2	8.6	10.6	-2	3	7	8.6	-7.8
4	2	4	12.8	12.4	-1	2	9	8.3	-8.7	-9	2	14	10.8	14.2	-3	3	2	105.4	-109.0	3	3	7	10.0	7.5
-4	2	4	47.5	-45.8	2	2	9	32.6	32.5	-10	2	14	5.8	8.5	4	3	2	3.5	2.4	-3	3	7	24.4	24.0
5	2	4	58.5	53.4	-2	2	9	21.9	19.9	0	2	15	22.6	25.2	-4	3	2	38.2	33.3	4	3	7	11.4	11.6
-5	2	4	56.7	-52.9	3	2	9	3.8	5.4	1	2	15	5.3	-7.2	5	3	2	8.7	9.3	-4	3	7	52.8	-50.1
6	2	4	38.0	40.1	-3	2	9	5.5	-4.4	-1	2	15	36.2	-37.8	-5	3	2	110.9	110.4	5	3	7	37.9	21.5
-6	2	4	15.7	-14.7	4	2	9	4.9	-5.1	2	2	15	12.1	-14.4	6	3	2	12.5	12.5	-5	3	7	77.6	-67.6
7	2	4	27.0	-30.1	-4	2	9	56.6	-51.2	-2	2	15	14.2	-13.7	7	3	2	28.6	-26.3	6	3	7	11.1	12.4
-7	2	4	18.5	19.5	5	2	9	16.1	-17.4	3	2	15	6.2	-7.8	-7	3	2	26.1	-23.2	-6	3	7	13.6	-12.2
8	2	4	8.8	-10.3	-5	2	9	61.8	-53.6	-3	2	15	23.3	22.6	8	3	2	22.6	-22.0	7	3	7	4.4	6.1
-8	2	4	36.6	38.6	6	2	9	5.6	-6.5	4	2	15	4.5	-5.9	-8	3	2	38.2	-36.2	-7	3	7	10.4	10.6
9	2	4	12.2	13.4	7	2	9	2.8	-2.7	-4	2	15	16.3	15.7	9	3	2	19.7	18.7	-8	3	7	5.3	5.3
-9	2	4	7.0	7.1	-7	2	9	43.4	46.7	-5	2	15	20.6	-19.5	-9	3	2	15.7	-13.9	-9	3	7	5.2	6.6
10	2	4	2.2	3.1	8	2	9	1.7	3.2	-6	2	15	23.3	-28.7	10	3	2	10.5	9.8	-11	3	7	4.6	5.8
-10	2	4	17.4	-19.4	-8	2	9	39.0	41.7	-7	2	15	12.5	-16.6	-10	3	2	16.3	17.4	0	3	8	37.1	-35.8
-12	2	4	5.8	6.7	-9	2	9	8.1	-8.6	-8	2	15	2.5	3.6	-11	3	2	9.5	9.1	1	3	8	69.2	64.4
0	2	5	80.6	-81.7	-10	2	9	13.2	-15.5	-9	2	15	11.4	16.3	0	3	3	28.6	-25.5	-1	3	8	74.7	69.0
1	2	5	37.3	-34.0	-12	2	9	9.0	10.5	-10	2	15	9.8	11.3	1	3	3	55.0	-52.4	2	3	8	22.6	23.3

Table 4 (*cont.*)

H	K	L	FO	FC	H	K	L	FC	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-2	3	8	10.0	8.6	-4	3	14	8.3	1.9	2	4	2	30.9	26.5	5	4	7	5.1	3.2	3	4	13	22.7	-21.2
3	3	8	2.4	-3.7	5	3	14	7.0	7.9	-2	4	2	77.6	-74.7	6	4	7	8.3	6.6	-3	4	13	64.2	64.5
-3	3	8	7.7	-6.2	-5	3	14	41.1	-40.6	3	4	2	26.4	-23.1	-6	4	7	8.7	8.7	4	4	13	2.4	-0.7
4	3	8	10.1	-9.4	-6	3	14	25.4	-27.1	-3	4	2	11.5	-8.5	7	4	7	19.5	17.3	-4	4	13	5.9	-4.7
-4	3	8	68.7	-66.2	-7	3	14	9.5	-10.2	4	4	2	9.4	-8.8	8	4	7	5.5	7.0	5	4	13	18.1	14.5
5	3	8	10.4	-10.7	-8	3	14	20.8	20.7	-4	4	2	80.0	73.1	-8	4	7	11.1	-11.3	-5	4	13	43.8	-38.2
-5	3	8	88.6	-77.1	-9	3	14	2.4	4.1	-5	4	2	17.3	-15.9	9	4	7	5.5	5.7	-6	4	13	2.4	-2.7
-6	3	8	63.6	59.4	-10	3	14	4.1	-4.9	-6	4	2	15.0	-13.8	-9	4	7	22.7	-21.1	-7	4	13	9.7	17.5
7	3	8	9.0	8.6	0	3	15	14.3	14.1	7	4	2	17.1	-14.7	-10	4	7	18.1	-17.6	-8	4	13	6.9	6.8
-7	3	8	62.8	61.1	1	3	15	10.8	12.5	-7	4	2	19.9	16.1	-12	4	7	6.2	4.9	-9	4	13	6.2	-6.5
-9	3	8	8.7	-10.1	-1	3	15	12.1	14.2	8	4	2	16.4	13.7	0	4	8	39.3	35.8	-10	4	13	4.5	-4.8
-10	3	8	27.0	-26.1	2	3	15	15.3	16.5	-8	4	2	3.1	-3.8	1	4	8	11.9	12.1	-11	4	13	4.5	-4.9
-11	3	8	2.9	-3.3	-2	3	15	7.3	-3.6	9	4	2	10.8	9.8	-1	4	8	43.2	-42.1	0	4	14	8.3	-9.9
-12	3	8	13.9	13.4	3	3	15	3.8	5.5	-9	4	2	17.1	16.1	2	4	8	8.0	-6.5	1	4	14	6.9	8.2
0	3	9	19.8	-18.0	-3	3	15	14.2	-14.9	-11	4	2	5.5	-3.9	-2	4	8	7.9	-3.7	-1	4	14	15.6	15.2
1	3	9	32.7	30.6	-4	3	15	7.2	-6.1	0	4	3	73.1	-71.3	3	4	8	4.1	2.1	-2	4	14	24.4	21.4
-1	3	9	4.8	-4.9	-5	3	15	14.2	12.0	1	4	3	74.7	-68.8	-3	4	8	13.5	9.7	3	4	14	6.9	7.1
2	3	9	19.4	19.2	-6	3	15	5.6	7.2	-1	4	3	41.8	38.8	4	4	8	5.9	-5.8	-3	4	14	10.2	-8.5
-2	3	9	16.6	15.0	-7	3	15	20.5	-22.8	2	4	3	16.8	-15.8	-4	4	8	61.4	-52.7	4	4	14	6.6	6.6
3	3	9	10.1	9.7	-8	3	15	19.7	-21.5	-2	4	3	71.7	-68.9	5	4	8	7.6	6.9	-4	4	14	14.6	-12.2
-3	3	9	3.5	-3.3	-9	3	15	4.4	-5.0	3	4	3	25.1	-23.0	-5	4	8	17.7	-14.6	-5	4	14	17.1	14.6
4	3	9	2.7	3.5	-10	3	15	3.2	-4.9	-3	4	3	88.6	-91.4	6	4	8	20.9	18.1	-6	4	14	6.6	-7.9
-4	3	9	35.5	-32.7	-11	3	15	2.9	-3.0	4	4	3	4.5	0.5	-6	4	8	18.1	17.8	-8	4	14	3.8	-5.2
5	3	9	25.4	15.3	-1	3	16	17.0	-17.4	-4	4	3	25.1	-21.2	7	4	8	6.6	7.3	-9	4	14	13.6	-15.6
-5	3	9	49.4	-44.8	-2	3	16	14.7	-12.7	5	4	3	16.0	19.0	-7	4	8	31.2	-29.4	0	4	15	6.9	6.7
6	3	9	9.5	11.3	3	3	16	9.8	-10.9	-5	4	3	44.8	40.0	-8	4	8	9.0	8.4	1	4	15	13.2	-14.5
-6	3	9	64.7	-36.5	-3	3	16	19.7	21.4	6	4	3	21.6	-16.6	-9	4	8	4.8	-5.5	-1	4	15	19.9	-18.6
7	3	9	5.2	4.7	-4	3	16	6.2	5.9	-6	4	3	22.3	20.2	-11	4	8	14.3	12.2	2	4	15	12.5	-12.2
-7	3	9	6.7	5.9	-5	3	16	8.6	7.7	7	4	3	43.1	-37.6	0	4	9	13.5	-12.4	-2	4	15	9.7	8.6
-9	3	9	5.3	-6.9	-6	3	16	0.	0.6	-7	4	3	23.0	-20.4	1	4	9	13.6	11.7	3	4	15	4.8	2.9
-10	3	9	8.4	5.5	-7	3	16	22.3	-26.9	-8	4	3	50.1	-40.1	-1	4	9	41.8	39.8	-3	4	15	43.5	44.3
1	3	10	17.7	18.5	-8	3	16	10.5	-13.0	9	4	3	16.0	14.2	2	4	9	8.0	7.2	4	4	15	15.3	12.6
-1	3	10	29.5	28.9	-9	3	16	20.5	21.7	-9	4	3	21.6	-18.7	-2	4	9	62.8	57.6	-4	4	15	35.2	31.0
2	3	10	9.0	8.7	-10	3	16	12.8	13.2	10	4	3	17.1	12.7	3	4	9	5.9	1.8	-5	4	15	2.4	3.5
-2	3	10	9.5	9.4	-11	3	16	1.0	0.3	-11	4	3	12.5	9.2	-3	4	9	59.7	55.5	-6	4	15	14.6	-16.8
3	3	10	16.8	18.7	0	3	17	14.3	15.0	0	4	4	41.4	-38.1	4	4	9	21.3	-19.0	-8	4	15	9.0	10.7
-3	3	10	24.0	23.7	1	3	17	7.3	8.1	1	4	4	23.3	21.4	-4	4	9	6.9	-5.7	-9	4	15	6.2	7.3
4	3	10	10.8	-11.6	-1	3	17	14.0	14.9	-1	4	4	9.5	-8.7	5	4	9	21.3	-21.2	0	4	16	5.2	5.3
-4	3	10	16.6	15.3	2	3	17	4.9	6.1	2	4	4	54.1	46.9	-5	4	9	82.0	-76.8	1	4	16	4.5	3.8
5	3	10	56.0	-35.0	-2	3	17	11.2	11.4	-2	4	4	34.0	-31.3	6	4	9	2.7	-2.7	-1	4	16	2.0	0.8
-5	3	10	53.4	-46.7	-3	3	17	3.7	-3.3	3	4	4	10.4	-11.1	-6	4	9	23.0	-21.7	2	4	16	3.1	-4.1
6	3	10	11.7	10.7	-4	3	17	2.4	2.3	-3	4	4	4.4	1.5	7	4	9	18.8	14.2	-2	4	16	23.4	21.9
-6	3	10	33.6	-30.5	-5	3	17	8.7	8.6	4	4	4	9.4	7.1	-7	4	9	36.1	33.8	3	4	16	7.6	6.8
7	3	10	19.9	17.8	-6	3	17	2.1	2.6	-4	4	4	27.4	24.2	8	4	9	17.8	15.3	-4	4	16	15.7	-14.3
-7	3	10	41.3	39.5	-7	3	17	8.7	-11.7	5	4	4	11.5	12.9	-8	4	9	17.1	15.8	-5	4	16	10.4	5.4
-8	3	10	33.3	31.9	-8	3	17	16.8	-16.6	6	4	4	30.0	-26.3	-9	4	9	18.5	-18.3	-6	4	16	6.2	-7.6
-9	3	10	9.0	-11.2	-9	3	17	9.3	-10.1	-6	4	4	12.9	-10.3	-10	4	9	29.1	-27.7	-7	4	16	13.2	-15.7
-10	3	10	8.7	-9.9	0	3	18	10.5	10.8	7	4	4	13.2	11.1	-11	4	9	11.1	-9.5	-10	4	16	6.9	-7.1
-11	3	10	14.5	-14.8	-1	3	18	4.9	-5.3	-7	4	4	12.9	10.3	-12	4	9	6.2	5.6	0	4	17	11.9	11.5
0	3	11	5.6	3.7	-2	3	18	6.7	-6.1	8	4	4	10.4	9.7	0	4	10	13.9	7.3	-1	4	17	2.7	-3.9
1	3	11	19.1	19.8	-3	3	18	8.4	8.8	-9	4	4	13.9	-13.9	2	4	10	7.3	5.7	2	4	17	5.5	-5.9
-1	3	11	4.5	-3.9	-4	3	18	10.7	11.6	10	4	4	3.1	2.9	-2	4	10	8.3	-7.7	-2	4	17	7.9	8.9
2	3	11	32.7	34.1	-5	3	18	5.9	-5.8	-10	4	4	9.0	8.8	3	4	10	11.5	11.4	-3	4	17	12.8	13.1
-2	3	11	8.8	7.6	-6	3	18	8.4	9.8	-11	4	4	4.8	4.4	4	4	10	19.9	-19.0	-4	4	17	15.7	14.3
3	3	11	15.7	17.7	-8	3	18	18.8	-17.9	0	4	5	98.6	-104.9	-4	4	10	37.9	-31.0	-5	4	17	27.0	22.7
-3	3	11	19.4	-18.5	-1	3	19	16.7	16.8	1	4	5	68.1	-60.7	-5	4	10	31.4	-26.8	-6	4	17	22.3	20.9
4	3	11	8.4	10.1	-2	3	19	3.7	4.3	-1	4	5	29.5	29.0	6	4	10	19.2	15.9	-7	4	17	3.1	-5.0
-4	3	11	48.2	-44.9	-4	3	19	11.9	9.8	2	4	5	14.5	15.5	-6	4	10	20.9	18.8	-8	4	17	17.8	-17.2
-5	3	11	24.7	-21.9	-5	3	19	15.6	12.9	-2	4	5	83.8	-76.5	-7	4	10	23.0	22.3	-9	4	17	3.4	4.0
6	3	11	7.9	7.9	-6	3	19	2.9	-4.0	3	4	5	25.4	27.3	-8	4	10	21.3	-22.3	0	4	18	8.7	8.2
7	3	11	6.2	6.7	-7	3	19	7.6	-8.6	-3	4	5	37.2	-32.7	-12	4	10	8.7	8.1	-1	4	18	6.6	5.6
-7	3	11	12.5	-13.6	-8	3	19	5.3	-6.1	-4	4	5	18.0	15.8	0	4	11	16.4	-14.4	-2	4	18	4.5	4.0
-8	3	11	20.2	-21.6	-3	3	20	16.3	-15.5	5	4	5	55.7	-44.4	1	4	11	8.0	8.3	-3	4	18	7.9	7.7
-9	3	11	4.9	-6.1	-4	3	20	19.5	17.5	-5	4	5	15.3	14.0	-1	4	11	36.4	35.0	-4	4	18	2.4	-4.6
-12	3	11	3.5	-3.8	-5	3	20	25.8	23.1	6	4	5	31.2	-28.7	2	4	11	18.1	17.8	-5	4	18	2.4	-0.1
0	3	12	43.8	43.9	-6	3	20	2.1	-3.5	-6	4	5	15.3	-15.2	-2	4	11	61.8	54.9	-6	4	18	2.4	3.5
1	3	12	14.5	8.9	0	4	0	70.8	66.5	7	4	5	7.3	5.4	3	4	11	3.4	3.4	-7	4	18	14.3	-14.8
-1	3	12	3.1	0.9	1	4	0	47.0	-44.5	-7	4	5	9.4	-7.4	-3	4	11	37.2	34.8	-8	4	18	3.4	-3.7
2	3	12	9.0	10.0	2	4	0	83.8	-76.8	8	4	5	22.7	16.4	4	4	11	30.0	-30.0	-1	4	19	8.7	-9.5
-2	3	12	67.0	65.4	3	4	0	55.3	52.7	-8	4	5	4.8	-5.2	-4	4	11	9.1	7.4	-2	4	19	9.7	-8.1
3	3	12	16.0	-18.3	4	4	0	52.6	-49.3	9	4	5	15.7	11.2	5	4	11	14.6	-12.4	-3	4	19	10.1	8.6
-3	3	12	5.8	5.5	7	4	0	9.7	-7.0	-9	4	5	26.5	-24.9	-5	4	11	42.4	-36.2	-4	4	19	18.5	16.2
4	3	12	35.5	-39.6	8	4	0	17.5	18.7	-10	4	5	21.3	-20.2	6	4	11	19.9	15.8	-5	4	19	18.0	14.7
5	3	12	7.3	7.7	9	4	0	16.1	15.4	-12	4	5	10.4	8.2	-6	4	11	33.6	-33.6	-6	4	19	13.2	13.2
-5	3	12	10.2	-8.3	0	4	1	55.2	-56.8	0	4	6	23.4	-20.8	7	4	11	20.2	18.3	-7	4	19	4.1	4.9
6	3	12	20.2	17.7	1	4	1	85.4	-86.1	1	4	6	58.0	52.0	-7	4	11	7.6	8.3	-8	4	19	5.2	-6.2
-6	3	12	31.6	-30.9	-1	4	1	25.6	-26.5	-1	4	6	64.7	-59.2	-8	4	11	21.6	22.1	-4	4	20	14.3	12.9
-7	3	12	16.0	16.0	2	4	1	57.6	-51.1	2	4	6	9.0	8.4	-10	4	11	10.8	-10.9	-5	4	20	10.7	-9.8
-8	3	12	11.9	11.0	-2	4	1	124.8	-140.6	-2	4	6	9.5	6.6	-11	4	11	16.0	-14.1	1	5	0	75.5	-71.4
-9	3	12	5.9	-6.9	3	4	1	8.1	1.2	3	4	6	15.7	-15.6	-12	4	11	8.7	-9.2	2	5	0	7.6	-7.4
-12	3	12	7.9	-9.5	-3	4	1	92.0	-88.3	-3	4	6	16.7	-13.7	0	4	12	3.4	1.6	3	5	0	39.6	-36.6
0	3	13	14.3	14.8	4	4	1	7.6	7.1	4	4	6	24.4	22.9	-1	4	12	40.7	41.8	4	5	0	2.9	-2.4
1	3	13	16.6	17.7	-4	4	1	58.7	55.2	-4	4	6	21.5	17.8	2	4	12	17.1	17.9	5	5	0	35.1	36.0
2	3	13	24.0	27.0	5	4	1	11.5	-8.4	-5	4	6	9.7	10.0	-2	4	12	15.0	-14.0	6	5	0	39.7	-41.4
-2	3	13	8.8	1.4	-5	4	1	68.4	67.0	6	4	6	20.6	18.8	3	4	12	14.3	-15.3	7	5	0	37.3	-36.4
3	3	13	8.4	11.4	6	4	1	14.6	-11.3	-6	4	6	36.8	-34.2	-3	4	12	32.3	-32.0	8	5	0	5.3	-5.3
-3	3	13	17.3	-18.5	-6	4	1	22.7	-19.8	7	4	6	5.5	5.8	-4	4	12	4.5	2.9	9	5	0	5.6	4.7
4	3	13	2.9	-3.3	7	4	1	30.7	-26.6	-7	4	6	6.9	-7.3	5	4	12	12.9	10.4	10	5	0	4.8	3.8
-4	3	13	15.9	-14.1	-7	4	1	71.0	-56.4	-9	4	6	9.0	-8.0	-5	4	12	13.5	-11.0	11	5	0	6.6	5.8
-5	3	13	11.9	-11.6	8	4	1	18.1	-16.9	-11	4	6	12.5	9.7	6	4	12	4.8	-3.2	0	5	1	16.3	-15.0
-7	3	13	16.6	-18.2	-8	4	1	29.1	-24.9	0	4	7	86.8	-89.1	-6	4	12	16.0	16.6	1	5	1	31.6	30.9
-8	3	13	20.5	-22.4	9	4	1	6.6	5.6	1	4	7	8.4	8.4	-7	4	12	10.4	9.8	-1	5	1	34.1	-34.3
-9	3	13	11.1	-13.4	-9	4	1	4.8	4.4	-1	4	7	89.2	86.7	-8	4	12	18.5	-19.8	2	5	1	59.7	53.7
-10	3	13	2.1	2.8	10	4	1	10.1	8.6	2	4	7	62.3	61.4	-9	4	12	5.9	-5.5	-2	5	1	13.8	13.8
0	3	14	36.9	38.6	-10	4	1	12.2	11.1	-2	4	7	27.8	24.0	-10	4	12	5.5	6.1	3	5	1	49.6	47.6
-1	3	14	38.0	-40.8	11	4	1	5.5	5.9	3	4	7	4.4	-1.2	0	4	13	28.5	27.6	-3	5	1	69.2	70.6
2	3	14	15.3	-17.8	-11	4	1	2.0	2.9	-3	4	7	48.2	-44.6	1	4	13	12.9	13.9	4	5	1	3.8	-3.6
-2	3	14	38.8	37.6	0	4	2	32.4	-29.1	4	4	7	51.4	-51.3	-1	4	13	3.1	0.9	-4	5	1	47.9	47.5
3	3	14	15.6	-16.6	1	4	2	20.4	12.9	-4	4	7	55.7	-47.1	2	4	13	11.5	-11.4	5	5	1	17.4	-15.9
-3	3	14	71.2	73.9	-1	4	2	39.2	-35.9	5	4	7	29.3	-26.4	-2	4	13	68.7	64.4	-5	5	1	16.1	-13.2

Table 4 (*cont.*)

H	K	L	FC	FC	H	K	L	FU	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
6	5	1	10.1	-7.4	-7	5	6	2.9	2.5	-6	5	12	9.8	12.1	-9	6	1	9.5	9.4	1	6	7	22.6	23.7
-6	5	1	52.5	-44.7	7	5	6	15.3	13.4	-7	5	12	7.7	7.2	10	6	1	5.6	5.0	-1	6	7	20.8	22.2
7	5	1	20.9	-18.7	8	5	6	9.3	7.3	-9	5	12	2.4	3.1	0	6	2	26.5	23.2	2	6	7	31.6	33.8
-7	5	1	15.0	-11.3	-8	5	6	7.7	-7.4	-10	5	12	4.8	-5.2	1	6	2	71.0	66.9	-2	6	7	29.3	-25.0
8	5	1	5.1	3.1	9	5	6	7.2	5.1	1	5	13	21.6	-22.0	-1	6	2	36.1	-35.5	3	6	7	13.3	15.4
-9	5	1	7.4	6.0	-9	5	6	21.6	-19.3	-1	5	13	20.5	21.1	2	6	2	29.6	28.7	-3	6	7	14.5	-13.6
10	5	1	6.2	-4.7	-10	5	6	10.1	-10.2	2	5	13	25.8	-27.2	-2	6	2	15.4	15.8	4	6	7	13.9	-14.7
-10	5	1	3.8	-3.8	-11	5	6	6.2	-5.3	-2	5	13	21.2	19.0	3	6	2	3.8	-3.4	-4	6	7	14.0	13.2
-11	5	1	8.7	-7.5	0	5	7	32.4	31.1	3	5	13	4.5	-3.8	-3	6	2	37.6	36.7	5	6	7	14.2	-13.8
0	5	2	107.3	-110.5	1	5	7	51.4	45.2	-3	5	13	20.9	-19.6	4	6	2	4.6	4.1	-5	6	7	12.8	-11.4
1	5	2	6.3	-7.3	-1	5	7	3.5	-4.2	4	5	13	9.5	8.8	-4	6	2	51.8	52.2	6	6	7	5.6	6.4
-1	5	2	17.1	15.8	2	5	7	4.6	3.5	-4	5	13	29.2	-27.5	5	6	2	22.6	-25.1	-6	6	7	5.3	-4.1
2	5	2	3.9	3.6	-2	5	7	23.9	-21.7	5	5	13	4.8	4.5	-5	6	2	33.0	33.3	-7	6	7	11.4	10.9
-2	5	2	106.6	-104.7	3	5	7	46.6	-48.9	-5	5	13	11.0	10.1	6	6	2	26.0	-24.2	-8	6	7	11.4	13.6
3	5	2	12.5	-13.2	-3	5	7	13.8	-13.5	-6	5	13	24.3	24.8	-6	6	2	41.3	-36.9	0	6	8	20.5	19.1
-3	5	2	77.2	-77.8	4	5	7	26.0	-26.8	-7	5	13	15.9	15.9	7	6	2	3.1	-2.9	1	6	8	13.8	15.9
4	5	2	8.0	-6.6	-4	5	7	51.4	45.7	-8	5	13	5.3	6.4	-7	6	2	41.7	-40.2	-1	6	8	37.6	36.9
-4	5	2	8.1	-6.4	5	5	7	7.7	-7.0	-9	5	13	2.4	-3.5	8	6	2	4.9	-4.8	2	6	8	5.2	-6.1
5	5	2	16.7	18.8	-5	5	7	43.5	38.8	-10	5	13	2.0	2.8	-8	6	2	8.4	7.5	-2	6	8	32.9	-32.5
-5	5	2	32.9	32.6	6	5	7	2.9	3.6	0	5	14	20.2	21.2	9	6	2	6.3	5.4	3	6	8	25.6	-27.7
6	5	2	22.5	-18.1	-6	5	7	19.5	17.3	1	5	14	8.0	-8.8	-9	6	2	8.4	7.3	-3	6	8	45.3	-44.8
-6	5	2	30.0	24.3	-7	5	7	2.9	-3.0	-1	5	14	9.3	-8.8	10	6	2	2.1	0.4	4	6	8	15.9	-17.1
7	5	2	24.6	-22.1	8	5	7	5.6	-4.7	2	5	14	19.5	-22.9	-11	6	2	5.3	-5.2	-4	6	8	41.0	37.8
-7	5	2	60.1	-53.5	-8	5	7	9.3	-7.5	-2	5	14	22.3	19.3	0	6	3	30.2	-25.5	-5	6	8	69.2	67.3
8	5	2	9.5	-9.0	-9	5	7	7.2	-6.4	3	5	14	2.4	2.9	1	6	3	17.3	18.8	6	6	8	13.5	-13.9
-8	5	2	28.5	-23.5	-11	5	7	6.9	5.2	-3	5	14	40.2	39.8	-1	6	3	36.8	32.5	-6	6	8	44.5	40.9
-9	5	2	9.5	8.6	0	5	8	16.1	-16.4	4	5	14	15.0	13.7	2	6	3	10.5	9.3	-7	6	8	12.8	12.0
10	5	2	16.4	13.4	1	5	8	12.9	-11.3	-4	5	14	28.9	27.7	-2	6	3	34.7	-30.6	-8	6	8	34.1	-32.8
-10	5	2	2.4	2.7	-1	5	8	43.5	42.2	-5	5	14	20.9	-18.8	3	6	3	22.5	-20.1	-9	6	8	19.5	-18.3
-11	5	2	4.5	3.9	2	5	8	34.3	34.3	-6	5	14	10.1	-9.7	-3	6	3	16.7	-17.6	-10	6	8	11.7	9.8
0	5	3	11.4	9.8	-2	5	8	65.0	64.9	-7	5	14	26.7	26.1	4	6	3	7.4	8.5	-11	6	8	4.2	4.8
1	5	3	18.7	18.5	3	5	8	11.2	-9.9	-9	5	14	2.0	-2.6	-4	6	3	11.1	8.9	0	6	9	4.6	-0.0
-1	5	3	4.9	3.5	-3	5	8	3.5	1.3	0	5	15	17.3	-16.7	5	6	3	6.0	-6.1	1	6	9	3.5	-4.7
2	5	3	27.2	26.8	4	5	8	36.4	-35.9	1	5	15	18.8	-20.1	-5	6	3	40.6	40.3	-1	6	9	17.8	-16.5
-2	5	3	16.7	-14.4	-4	5	8	32.0	-28.1	-1	5	15	5.2	5.0	6	6	3	7.7	8.3	2	6	9	17.8	19.7
3	5	3	11.4	-12.3	5	5	8	17.4	-16.0	2	5	15	12.9	-11.7	-6	6	3	10.0	9.4	-2	6	9	15.6	15.4
-3	5	3	17.5	18.2	-5	5	8	5.9	-6.0	-2	5	15	17.1	17.3	7	6	3	7.7	-7.3	3	6	9	9.4	10.6
4	5	3	6.9	6.6	6	5	8	10.4	8.8	-3	5	15	5.1	4.8	-7	6	3	14.2	-14.5	-3	6	9	17.8	18.0
-4	5	3	54.9	51.6	-6	5	8	32.7	-27.8	-4	5	15	11.7	-11.1	8	6	3	6.3	-6.1	4	6	9	5.3	-4.3
5	5	3	5.6	-5.5	7	5	8	3.2	3.4	-5	5	15	16.0	-13.9	-8	6	3	5.3	-5.7	-4	6	9	11.8	-12.2
-5	5	3	12.2	11.4	-7	5	8	14.6	14.3	-7	5	15	21.2	23.0	9	6	3	11.4	8.8	5	6	9	2.8	-2.0
6	5	3	36.6	-30.8	8	5	8	14.3	12.0	-8	5	15	11.7	12.6	-9	6	3	5.6	-6.6	-5	6	9	18.8	-17.5
-6	5	3	12.9	-10.5	-8	5	8	13.5	12.4	-9	5	15	7.4	6.6	-11	6	3	3.5	2.8	6	6	9	2.4	-1.2
-7	5	3	41.4	-37.3	-9	5	8	36.2	-32.5	0	5	16	11.1	11.3	0	6	4	38.3	36.5	-6	6	9	14.6	-13.7
8	5	3	9.3	7.7	-10	5	8	16.4	-14.6	1	5	16	11.9	-9.2	1	6	4	40.2	38.9	7	6	9	6.7	6.3
-8	5	3	12.9	-11.2	0	5	9	24.1	22.8	-1	5	16	6.7	-6.4	-1	6	4	39.3	-37.0	-7	6	9	27.1	27.6
-9	5	3	8.0	7.8	-1	5	9	11.5	11.5	2	5	16	9.0	-8.7	2	6	4	25.4	24.7	-8	6	9	26.7	25.1
10	5	3	2.9	-3.5	2	5	9	12.9	-10.2	-2	5	16	11.8	11.8	-2	6	4	6.0	-1.0	-9	6	9	6.3	-6.3
-10	5	3	3.5	3.5	-2	5	9	3.8	3.6	-3	5	16	7.4	6.6	3	6	4	33.6	38.3	-10	6	9	13.9	-10.8
0	5	4	84.0	-82.2	3	5	9	6.9	-4.7	-4	5	16	30.2	29.9	-3	6	4	42.3	42.3	-11	6	9	5.3	5.1
1	5	4	12.5	-12.5	-3	5	9	3.8	-4.4	-5	5	16	22.2	19.7	4	6	4	41.7	-46.7	0	6	10	15.2	-12.2
-1	5	4	26.7	24.5	4	5	9	20.9	-20.7	-7	5	16	2.4	-3.1	-4	6	4	20.2	18.6	1	6	10	5.6	7.7
2	5	4	27.8	-30.1	-4	5	9	22.6	-20.6	-8	5	16	2.9	-4.1	5	6	4	47.0	-54.1	-1	6	10	9.8	7.8
-2	5	4	77.5	-67.0	5	5	9	9.0	-8.8	-9	5	16	1.7	-3.1	-5	6	4	39.2	39.0	2	6	10	11.4	-10.6
3	5	4	3.7	3.4	-5	5	9	33.8	30.2	-10	5	16	10.8	12.1	6	6	4	5.3	-6.0	-2	6	10	18.7	18.4
-3	5	4	34.0	-29.9	-6	5	9	56.2	52.5	0	5	17	5.5	-6.7	-6	6	4	27.4	23.1	3	6	10	29.2	-33.2
4	5	4	34.8	34.6	7	5	9	2.7	1.5	1	5	17	13.2	-13.3	-7	6	4	30.6	-29.6	-3	6	10	8.6	-6.0
-4	5	4	3.8	-0.3	-7	5	9	16.4	14.8	-1	5	17	2.5	-1.9	8	6	4	8.4	7.6	4	6	10	8.8	-8.6
5	5	4	16.8	-18.0	-8	5	9	13.5	-12.3	-2	5	17	5.2	-1.8	-8	6	4	16.0	-16.1	-4	6	10	6.3	4.5
-5	5	4	10.5	-11.0	-9	5	9	19.5	-18.2	-3	5	17	2.9	-2.4	9	6	4	4.2	1.9	5	6	10	6.7	-6.9
6	5	4	23.3	-20.1	-11	5	9	9.0	6.3	-4	5	17	3.9	1.9	-11	6	4	1.0	1.9	-5	6	10	31.7	25.8
-6	5	4	9.8	8.7	0	5	10	18.5	-15.6	-5	5	17	3.2	4.3	0	6	5	37.3	-37.1	6	6	10	4.6	5.1
7	5	4	4.1	-3.8	1	5	10	19.0	-19.3	-8	5	17	18.0	16.0	1	6	5	17.0	-16.0	-6	6	10	23.4	24.0
-7	5	4	11.9	7.1	-1	5	10	2.7	-1.9	-9	5	17	14.6	14.4	-1	6	5	9.3	8.2	-7	6	10	23.2	26.2
8	5	4	5.3	-4.5	2	5	10	29.6	27.7	0	5	18	7.7	9.8	2	6	5	39.0	40.9	-8	6	10	4.9	5.7
-8	5	4	20.4	-17.3	-2	5	10	39.2	37.1	-1	5	18	14.0	-13.1	-2	6	5	33.8	-32.3	-9	6	10	19.5	-19.7
9	5	4	20.9	16.7	-3	5	10	62.5	60.4	-2	5	18	15.7	13.3	3	6	5	26.1	28.2	-10	6	10	9.3	-7.3
-9	5	4	13.8	-12.6	4	5	10	21.9	-20.4	-3	5	18	7.2	6.4	-3	6	5	25.0	-24.2	-11	6	10	12.1	9.8
-10	5	4	10.8	-9.9	-4	5	10	17.4	-6.0	-5	5	18	22.6	20.7	4	6	5	19.2	-18.6	0	6	11	4.6	-5.6
0	5	5	8.0	2.9	5	5	10	7.7	-8.4	-6	5	18	18.3	17.3	-4	6	5	19.4	16.2	1	6	11	8.1	9.7
1	5	5	66.3	55.1	-5	5	10	51.7	-45.4	-8	5	18	7.7	-7.6	5	6	5	8.4	-9.2	-1	6	11	16.6	-15.3
-1	5	5	52.4	-51.1	-6	5	10	33.6	-30.3	-3	5	19	9.5	9.4	-5	6	5	6.3	6.1	2	6	11	5.3	6.5
2	5	5	27.1	29.2	7	5	10	15.3	14.5	-4	5	19	2.7	-3.0	6	6	5	6.3	-6.4	-2	6	11	4.4	-1.0
-2	5	5	7.6	-6.5	-7	5	10	8.3	8.4	-5	5	19	10.7	-8.5	-6	6	5	14.6	-13.4	3	6	11	3.5	-0.4
3	5	5	2.4	2.2	-8	5	10	27.5	25.6	-6	5	19	3.2	-2.9	-7	6	5	2.1	1.8	-3	6	11	27.8	26.1
-3	5	5	40.0	36.8	-10	5	10	35.4	-29.9	0	6	0	77.9	-78.3	8	6	5	2.8	2.2	4	6	11	8.4	-7.6
4	5	5	45.8	-45.9	-11	5	10	8.0	-7.0	1	6	0	8.4	8.8	9	6	5	3.5	2.9	-4	6	11	11.5	9.7
-4	5	5	29.9	29.4	0	5	11	11.4	10.0	2	6	0	84.4	80.0	-9	6	5	7.0	6.8	5	6	11	5.6	-4.3
5	5	5	30.9	-33.9	1	5	11	4.1	-3.0	3	6	0	45.9	44.5	-10	6	5	12.8	-9.3	-5	6	11	21.9	-21.5
-5	5	5	23.0	20.2	-1	5	11	16.4	17.1	4	6	0	29.3	27.4	-11	6	5	3.1	-1.8	6	6	11	4.6	3.6
6	5	5	8.3	7.5	2	5	11	7.4	-6.2	5	6	0	33.7	-35.8	0	6	6	34.0	29.8	-6	6	11	3.1	-1.0
-6	5	5	7.4	-7.8	-2	5	11	6.6	-2.4	6	6	0	36.4	-35.6	1	6	6	67.5	60.5	-7	6	11	2.8	4.7
7	5	5	9.8	7.9	3	5	11	28.2	-28.6	8	6	0	5.6	4.3	-1	6	6	24.6	-22.9	-8	6	11	11.7	11.5
-7	5	5	9.8	9.3	4	5	11	11.1	-12.0	9	6	0	6.7	-7.0	2	6	6	48.0	51.1	-10	6	11	3.8	-3.4
-8	5	5	6.6	-5.7	-4	5	11	9.3	7.5	0	6	1	49.7	-44.4	-2	6	6	66.4	-65.3	0	6	12	22.3	22.4
9	5	5	5.1	-4.5	5	5	11	9.0	8.4	1	6	1	5.8	-4.6	3	6	6	31.6	-32.0	1	6	12	21.8	-21.6
-9	5	5	11.1	-9.3	6	5	11	9.3	7.9	-1	6	1	5.3	-3.5	-3	6	6	35.1	31.8	-1	6	12	5.6	-0.5
0	5	6	76.9	-74.0	-6	5	11	19.8	17.8	2	6	1	3.9	3.7	4	6	6	64.9	-69.6	2	6	12	44.9	-49.9
1	5	6	28.1	-23.9	-7	5	11	21.6	19.9	-2	6	1	29.5	-31.7	-4	6	6	70.5	64.6	-2	6	12	17.4	17.2
-1	5	6	70.1	70.0	-10	5	11	5.9	-6.5	3	6	1	10.1	-11.6	5	6	6	18.8	-17.8	3	6	12	11.7	-13.9
2	5	6	17.7	18.9	0	5	12	6.9	-7.7	-3	6	1	20.8	-21.6	-5	6	6	28.1	24.3	4	6	12	4.9	4.1
-2	5	6	38.3	-35.7	1	5	12	33.0	33.7	4	6	1	9.3	7.4	6	6	6	6.3	6.6	-4	6	12	17.8	-18.8
3	5	6	32.9	32.0	-1	5	12	21.8	23.0	-4	6	1	38.3	34.5	-6	6	6	20.2	18.6	5	6	12	8.4	7.7
-3	5	6	69.1	-67.5	2	5	12	2.9	1.4	5	6	1	33.6	35.7	-7	6	6	4.2	4.1	-5	6	12	28.8	25.9
4	5	6	42.4	-44.3	-2	5	12	29.1	26.5	-5	6	1	37.3	37.8	8	6	6	3.8	-2.8	-6	6	12	19.5	19.3
-4	5	6	38.3	33.9	3	5	12	16.4	-17.3	-6	6	1	10.0	9.2	-8	6	6	16.7	-16.9	-7	6	12	1.7	2.9
5	5	6	26.3	-32.8	-3	5	12	58.8	58.8	7	6	1	6.0	-4.6	-9	6	6	4.6	-4.5	-8	6	12	19.5	20.9
-5	5	6	8.0	6.7	-4	5	12	16.8	-15.1	-7	6	1	20.9	-19.5	-10	6	6	6.0	-5.8	-9	6	12	2.4	2.9
6	5	6	11.7	10.5	-5	5	12	44.1	-37.8	-8	6	1	4.2	-4.2	-11	6	6	5.3	-4.1	-10	6	12	5.3	-5.3
-6	5	6	9.0	-6.9	6	5	12	11.9	11.9	9	6	1	3.1	-0.4	0	6	7	20.5	-17.4	-11	6	12	3.1	3.4

Table 4 (*cont.*)

H	K	L	FC	FC	H	K	L	FC	FC	H	K	L	FO	FC	H	K	L	FU	FC	H	K	L	FO	FC
0	6	13	22.3	22.9	0	7	5	14.7	-13.6	-3	8	1	4.4	-3.2	1	9	0	41.4	44.0	-2	9	14	8.1	-8.0
1	6	13	4.6	-4.6	1	7	5	27.9	31.0	4	8	1	11.0	-10.3	2	9	0	48.2	49.3	-3	9	14	19.9	-16.6
-1	6	13	11.5	-11.9	-1	7	5	31.2	-29.8	0	8	2	40.7	-36.2	3	9	0	26.5	-29.1	-1	9	15	1.3	3.7
2	6	13	12.1	-13.4	2	7	5	44.5	55.5	1	8	2	11.4	10.1	4	9	0	34.8	-36.1	-2	9	15	14.7	12.8
-2	6	13	11.7	12.0	-2	7	5	6.6	-2.3	-1	8	2	35.5	-38.2	0	9	1	57.0	-51.9	-3	9	15	8.8	7.1
3	6	13	5.3	-4.7	-3	7	5	14.7	15.7	2	8	2	31.2	30.7	1	9	1	22.2	-24.7	-5	9	15	16.7	-16.2
-3	6	13	20.2	19.3	4	7	5	27.5	-34.6	-2	8	2	50.4	-49.5	-1	9	1	43.2	-46.0	0	10	0	35.8	-33.4
-4	6	13	5.1	-4.4	-4	7	5	31.3	30.1	3	8	2	12.5	14.3	2	9	1	11.8	12.9	2	10	0	13.3	14.7
-5	6	13	22.2	-20.8	-5	7	5	20.9	18.4	-3	8	2	9.5	9.0	3	9	1	11.1	13.9	0	10	1	28.1	24.4
-6	6	13	9.3	-9.4	0	7	6	35.5	-31.1	4	8	2	14.7	-13.6	-3	9	1	13.3	14.8	1	10	1	19.0	20.8
-7	6	13	11.0	12.0	1	7	6	17.7	19.1	-4	8	2	35.8	38.1	4	9	1	11.0	-12.9	-1	10	1	10.8	12.0
-9	6	13	3.8	-4.9	-1	7	6	24.7	-24.9	1	8	3	15.9	15.7	-4	9	1	5.5	7.2	2	10	1	7.3	-4.7
0	6	14	11.2	-10.8	2	7	6	40.0	46.1	-1	8	3	6.3	5.3	1	9	2	16.4	16.7	-2	10	1	15.6	17.1
1	6	14	39.6	-43.1	-2	7	6	23.0	-20.0	2	8	3	28.2	31.6	-1	9	2	12.1	12.3	3	10	1	36.2	-46.1
-1	6	14	19.8	22.5	3	7	6	11.1	9.3	3	8	3	11.1	11.9	2	9	2	11.8	12.0	-3	10	1	7.3	-8.6
-2	6	14	24.3	24.4	-3	7	6	17.7	17.1	-3	8	3	6.6	-5.9	-2	9	2	13.3	14.9	4	10	1	22.0	-26.2
2	6	14	26.0	-23.4	-4	7	6	8.3	5.3	4	8	3	11.0	-12.9	3	9	2	17.0	-20.2	-4	10	1	29.5	-33.8
-4	6	14	26.5	-26.6	0	7	7	55.3	51.7	-4	8	3	24.9	25.1	-3	9	2	23.6	25.4	-5	10	1	15.3	-21.8
-3	6	14	4.1	4.1	1	7	7	28.5	30.6	-5	8	3	8.3	7.7	4	9	2	13.8	-14.6	0	10	2	23.6	-21.1
-5	6	14	25.0	-24.4	-1	7	7	5.1	-6.3	0	8	4	53.8	-48.0	-4	9	2	16.6	-17.1	1	10	2	5.6	1.2
-6	6	14	25.3	28.6	2	7	7	4.4	-2.6	1	8	4	15.2	-16.7	-5	9	2	16.7	-20.2	2	10	2	4.4	0.4
-7	6	14	24.1	28.0	-2	7	7	60.9	-62.2	-1	8	4	15.2	-16.3	0	9	3	31.0	-28.6	-2	10	2	13.3	14.2
-8	6	14	9.3	8.3	3	7	7	26.7	-30.7	2	8	4	43.0	49.1	1	9	3	20.9	-23.5	3	10	2	4.4	-0.6
-9	6	14	12.1	10.3	-3	7	7	19.2	-18.4	-2	8	4	28.2	-25.7	-1	9	3	3.1	1.8	-3	10	2	8.8	-7.7
0	6	15	13.2	13.8	4	7	7	14.7	-19.8	3	8	4	4.4	8.4	2	9	3	10.4	8.9	-4	10	2	10.1	-8.3
1	6	15	6.7	-6.5	-4	7	7	31.3	30.6	-3	8	4	31.9	-33.1	-2	9	3	22.2	-22.3	1	10	3	17.7	20.4
-1	6	15	17.3	-17.3	-5	7	7	43.4	37.2	-4	8	4	12.8	9.6	-3	9	3	10.2	-7.8	-1	10	3	11.4,	-10.6
2	6	15	9.5	-7.6	1	7	8	9.4	10.0	5	8	4	15.3	-11.8	-4	9	3	5.5	5.2	2	10	3	4.4	-7.1
-2	6	15	5.9	-0.5	-1	7	8	12.1	-14.0	-5	8	4	20.9	18.2	0	9	4	20.5	-19.1	-2	10	3	7.3	-5.7
-3	6	15	12.5	11.8	2	7	8	4.4	5.3	1	8	5	33.7	36.7	1	9	4	21.6	30.0	3	10	3	20.6	-25.2
-4	6	15	3.7	2.9	-2	7	8	55.6	-48.9	-1	8	5	10.8	-11.2	-1	9	4	15.2	15.9	-3	10	3	13.3	16.5
-5	6	15	16.1	-15.0	3	7	8	8.8	8.6	2	8	5	11.1	14.3	2	9	4	6.6	-0.5	4	10	3	19.2	-26.0
-7	6	15	1.7	0.8	-3	7	8	8.8	4.9	-2	8	5	9.5	-8.7	-2	9	4	17.0	-18.4	0	10	4	12.9	10.9
-8	6	15	7.7	-6.7	4	7	8	11.9	14.9	3	8	5	11.1	-12.4	3	9	4	23.6	-28.9	1	10	4	7.6	-7.0
0	6	16	13.5	-12.6	-4	7	8	14.7	11.1	-3	8	5	10.2	7.6	4	9	4	11.9	-12.8	-1	10	4	8.8	-8.4
1	6	16	21.8	-20.5	-5	7	8	22.3	-18.1	-4	8	5	16.6	16.5	-4	9	4	13.8	14.1	2	10	4	4.4	-3.8
-1	6	16	2.5	-0.8	0	7	9	11.9	11.2	-5	8	5	9.7	9.3	-5	9	4	11.1	-14.3	3	10	4	11.8	15.6
2	6	16	3.1	-3.5	1	7	9	5.1	-3.5	1	8	6	42.5	46.3	0	9	5	10.5	-9.1	-4	10	4	14.7	-18.7
-2	6	16	8.0	-7.2	-1	7	9	28.5	28.3	-1	8	6	42.5	-45.9	1	9	5	8.8	9.3	0	10	5	16.6	14.6
-3	6	16	8.7	8.4	2	7	9	11.1	-14.0	2	8	6	4.4	-0.6	-1	9	5	20.9	-22.9	1	10	5	7.6	5.9
-4	6	16	11.2	10.5	-2	7	9	10.4	8.2	-2	8	6	26.7	-23.8	2	9	5	11.1	11.2	-1	10	5	9.4	11.1
-5	6	16	24.6	-20.7	3	7	9	14.0	-16.8	3	8	6	13.3	-17.2	-2	9	5	7.3	-5.6	2	10	5	8.1	-7.8
-6	6	16	8.1	-8.5	-3	7	9	45.9	-45.0	-3	8	6	25.8	-26.4	3	9	5	9.5	10.7	-2	10	5	13.3	14.5
-7	6	16	16.0	15.6	-4	7	9	17.4	-15.6	4	8	6	5.5	-8.0	-3	9	5	22.2	-23.6	3	10	5	23.6	-32.0
-8	6	16	22.0	21.4	-5	7	9	22.3	16.0	-4	8	6	13.8	14.3	4	9	5	8.3	-12.5	-3	10	5	11.1	9.3
-9	6	16	17.4	17.9	0	7	10	15.0	13.0	-5	8	6	26.5	24.3	-4	9	5	11.9	-11.4	4	10	5	23.0	-23.9
0	6	17	4.6	4.9	-1	7	10	27.9	-29.6	1	8	7	6.3	-4.9	0	9	6	38.0	36.0	-4	10	5	14.7	15.9
-3	6	17	5.3	-6.5	-2	7	10	40.9	-34.5	-1	8	7	42.5	-43.6	1	9	6	5.6	-5.9	0	10	6	10.5	5.9
-4	6	17	12.8	-10.8	-3	7	10	11.1	-10.0	2	8	7	6.6	6.0	-1	9	6	5.6	-4.3	1	10	6	10.1	-12.5
-5	6	17	5.3	5.3	-4	7	10	13.8	11.4	-2	8	7	24.4	-22.4	2	9	6	25.1	-28.5	-1	10	6	12.6	15.5
-6	6	17	5.6	6.8	-5	7	10	12.5	-11.5	-3	8	7	18.5	19.2	3	9	6	11.1	-12.3	2	10	6	6.6	8.8
-8	6	17	9.5	-8.7	0	7	11	19.9	19.5	-4	8	7	24.9	25.1	-3	9	6	10.2	8.0	-2	10	6	16.3	-16.8
-2	6	18	3.8	4.6	-1	7	11	8.1	6.4	0	8	8	48.4	45.4	4	9	6	4.5	-6.7	-3	10	6	11.1	-11.5
-3	6	18	8.7	-8.3	-2	7	11	11.1	-5.6	1	8	8	3.1	-1.1	-4	9	6	20.2	23.1	4	10	6	8.3	-8.2
-6	6	18	11.0	-9.4	-3	7	11	11.1	-12.6	-1	8	8	11.4	10.6	-5	9	6	8.3	-9.9	-4	10	6	8.3	4.1
-7	6	18	7.0	7.6	-4	7	11	13.8	-13.5	2	8	8	17.0	-20.7	0	9	7	13.5	11.7	1	10	7	25.4	-27.7
1	7	0	55.6	51.3	0	7	12	31.4	30.9	-2	8	8	31.2	-29.8	1	9	7	13.3	14.6	-1	10	7	18.4	-18.7
2	7	0	9.5	-7.0	-1	7	12	36.8	-38.2	-3	8	8	28.1	-27.4	-1	9	7	8.1	7.2	-3	10	7	30.3	37.9
3	7	0	9.5	7.0	-2	7	12	11.8	-11.4	-4	8	8	25.7	-27.0	2	9	7	5.9	-6.2	-4	10	7	32.2	31.7
4	7	0	17.3	17.7	-3	7	12	14.7	-14.2	-5	8	8	23.7	24.5	-2	9	7	35.7	-32.5	-5	10	7	9.7	-11.2
6	7	0	13.5	15.6	-4	7	12	5.5	7.0	-1	8	9	20.4	-24.3	3	9	7	4.4	-1.9	1	10	8	10.1	-6.3
0	7	1	58.7	-53.5	0	7	13	10.8	10.4	-2	8	9	43.8	-39.3	-3	9	7	34.0	-36.7	-1	10	8	13.3	15.5
1	7	1	36.2	35.3	-1	7	13	32.4	33.8	-3	8	9	7.3	5.5	-4	9	7	12.8	-9.5	-2	10	8	6.6	-6.9
-1	7	1	68.0	-58.3	-2	7	13	10.4	7.7	-4	8	9	25.7	26.4	1	9	8	29.9	-31.9	-3	10	8	19.9	-24.3
2	7	1	40.0	40.4	-3	7	13	17.0	-15.7	0	8	10	25.4	23.7	-1	9	8	36.8	-41.7	-4	10	8	4.5	5.6
-2	7	1	22.2	22.7	-4	7	13	21.1	-20.3	-1	8	10	16.4	15.8	2	9	8	4.4	-3.3	0	10	9	21.6	-22.1
3	7	1	11.8	15.0	0	7	14	12.9	13.5	-2	8	10	6.6	-3.1	-2	9	8	17.0	-17.6	1	10	9	22.2	-23.5
-3	7	1	49.6	55.9	-1	7	14	26.7	-28.4	-3	8	10	19.2	-21.6	3	9	8	3.7	8.2	-1	10	9	5.1	-6.0
4	7	1	13.8	-13.9	-2	7	14	6.6	-1.9	-4	8	10	24.9	-24.9	-3	9	8	11.1	10.1	-3	10	9	3.7	0.6
-4	7	1	31.3	30.5	-3	7	14	3.7	4.6	-5	8	10	25.1	-22.4	-4	9	8	33.1	33.7	-4	10	9	17.4	17.3
5	7	1	20.9	-25.2	-4	7	14	22.0	-21.6	0	8	11	18.4	16.6	-5	9	8	19.5	18.5	-5	10	9	11.1	13.3
0	7	2	23.9	20.4	0	7	15	15.7	-16.7	-1	8	11	22.9	-25.4	0	9	9	22.5	21.2	-1	10	10	8.1	7.0
1	7	2	47.0	43.6	-1	7	15	2.5	0.2	-2	8	11	14.7	-13.4	1	9	9	8.1	-6.8	-2	10	10	3.7	0.4
-1	7	2	33.7	32.1	-2	7	15	15.6	13.9	-3	8	11	5.9	1.2	-1	9	9	11.4	8.9	-3	10	10	9.5	-8.7
2	7	2	29.6	30.4	-3	7	15	19.2	17.9	-5	8	11	11.1	-11.4	-2	9	9	16.3	-14.8	-1	10	11	2.5	-5.2
-2	7	2	13.3	13.5	-4	7	15	11.9	-9.2	0	8	12	24.1	23.2	3	9	9	8.8	9.8	-3	10	11	16.3	16.9
3	7	2	10.2	11.7	-5	7	15	32.2	-25.6	-1	8	12	33.0	34.7	-3	9	9	28.8	-31.4	0	10	12	9.3	9.4
-3	7	2	22.2	-22.5	-1	7	16	9.4	-8.7	-2	8	12	23.7	-23.2	-4	9	9	29.5	-29.7	-1	10	12	3.8	-1.8
-4	7	2	32.2	29.5	-2	7	16	8.1	-7.5	-3	8	12	23.6	-24.3	1	9	10	15.2	-17.1	-4	10	12	8.3	-5.5
-5	7	2	22.3	23.8	-3	7	16	2.9	1.1	-4	8	12	7.3	-4.6	-1	9	10	13.3	-14.2	0	10	13	19.7	-19.6
1	7	3	19.7	16.6	-4	7	16	24.9	-19.4	-5	8	12	18.1	-14.9	-2	9	10	10.4	-1.8	-4	10	13	13.8	12.1
-1	7	3	22.9	-23.2	-5	7	16	18.1	-13.9	-1	8	13	17.7	-18.7	-3	9	10	10.2	9.2	-2	10	14	2.9	-2.9
2	7	3	24.4	27.4	-3	7	17	8.1	5.4	-2	8	13	19.2	-17.9	-4	9	10	10.1	6.8	-3	10	14	8.8	8.6
-2	7	3	30.5	-26.6	-4	7	17	0.	2.6	-3	8	13	10.2	-8.0	0	9	11	15.2	14.4	1	11	0	27.8	32.0
3	7	3	27.4	33.6	-5	7	17	8.3	-7.5	-4	8	13	11.0	-9.0	-1	9	11	12.1	14.4	2	11	0	9.5	8.4
-3	7	3	13.3	14.2	-4	7	18	10.1	-9.5	0	8	14	8.0	-8.1	-2	9	11	14.7	-13.9	3	11	0	15.3	-16.7
4	7	3	13.8	-13.2	0	8	0	32.0	-31.1	-1	8	14	12.1	12.1	-3	9	11	9.5	-9.6	4	11	0	16.4	-18.8
-4	7	3	43.2	39.6	1	8	0	41.1	-43.4	-2	8	14	23.7	23.8	-5	9	11	16.7	-19.0	5	11	0	9.5	-9.9
5	7	3	20.9	-30.7	2	8	0	30.0	28.8	-3	8	14	11.1	-10.6	0	9	12	18.5	-18.4	6	11	0	8.7	9.5
-5	7	3	40.6	41.0	3	8	0	42.4	40.9	-4	8	14	16.6	-15.4	-1	9	12	12.6	-14.7	0	11	1	11.2	8.4
1	7	4	8.1	6.8	4	8	0	17.8	-20.8	-5	8	14	15.3	-13.4	-2	9	12	17.0	-16.3	1	11	1	10.8	13.1
-1	7	4	13.9	11.3	5	8	0	16.7	-17.9	-1	8	15	7.6	-4.2	-3	9	12	18.5	18.1	-1	11	1	17.1	19.5
2	7	4	56.4	66.5	8	8	0	10.5	11.2	-2	8	15	5.9	-2.5	-4	9	12	4.5	2.3	2	11	1	8.1	7.9
-2	7	4	8.8	6.4	9	8	0	8.1	8.8	-3	8	15	14.0	-12.6	0	9	13	13.5	12.9	-2	11	1	13.3	18.1
3	7	4	22.9	27.4	0	8	1	18.4	15.9	-4	8	15	27.5	-21.6	-1	9	13	14.6	15.6	3	11	1	3.7	-1.0
-3	7	4	17.0	-16.7	1	8	1	50.8	53.9	-1	8	16	6.9	-7.2	-2	9	13	8.8	8.6	-3	11	1	8.8	-9.1
4	7	4	14.7	-16.6	-1	8	1	41.3	43.5	-2	8	16	18.5	13.6	-3	9	13	8.8	-9.5	-4	11	1	10.1	-11.6
-4	7	4	11.9	8.4	2	8	1	19.2	20.1	-3	8	16	22.2	18.8	-4	9	13	13.8	-11.1	0	11	2	20.6	17.9
5	7	4	8.3	16.1	-2	8	1	32.6	32.5	-5	8	16	13.9	-10.2	0	9	14	13.8	-12.3	1	11	2	8.1	8.0
-5	7	4	43.4	41.3	3	8	1	4.4	-4.4	-4	8	17	10.1	-10.0	-1	9	14	13.9	14.5	-1	11	2	8.1	8.0

Table 4 (*cont.*)

H	K	L	FO	FC
2	11	2	11.1	-14.8
-2	11	2	13.3	15.3
3	11	2	9.5	-11.4
-3	11	2	6.6	7.2
4	11	2	11.9	-15.8
-1	11	3	8.1	7.8
2	11	3	8.1	9.0
-2	11	3	14.0	18.1
3	11	3	8.1	9.3
4	11	3	9.1	-8.7
-4	11	3	4.5	-7.3
1	11	4	3.1	-2.2
2	11	4	5.9	6.8
-2	11	4	12.5	15.9
3	11	4	12.5	-14.2
-3	11	4	5.9	-5.9
4	11	4	30.3	-31.0
1	11	5	10.8	-12.2
-1	11	5	20.4	23.2
2	11	5	16.3	-6.0
-2	11	5	9.5	6.5
3	11	5	3.7	3.7
1	11	6	6.3	-5.8
-1	11	6	16.4	-17.4
-2	11	6	3.7	4.8
3	11	6	19.9	-22.5
-3	11	6	21.5	27.3
-4	11	6	4.5	-2.2
0	11	7	10.8	2.0
1	11	7	15.2	-17.9
-1	11	7	15.9	18.0
-2	11	7	9.5	8.0
-3	11	7	3.7	6.1
-4	11	7	8.3	7.6
0	11	8	12.1	-13.5
1	11	8	13.9	-14.3
-1	11	8	10.8	-10.8
-2	11	8	18.5	-20.2
-3	11	8	11.1	11.6
-4	11	8	29.5	26.1
-1	11	9	6.3	7.6
-2	11	9	5.2	7.0
-3	11	9	3.7	2.1
-4	11	9	16.6	16.4
-2	11	10	2.9	-4.9
-4	11	10	9.1	9.7
-2	11	11	2.9	-0.4
-4	11	11	9.1	7.0
-1	11	12	3.1	-3.5
-3	11	12	2.9	2.5
-4	11	12	11.0	12.2
0	12	0	22.5	24.9
1	12	0	9.7	11.5
2	12	0	5.9	-0.4
4	12	0	11.9	-14.2
0	12	1	11.5	9.5
1	12	1	13.3	16.4
-1	12	1	11.4	13.5
2	12	1	3.7	4.2
-2	12	1	11.8	14.6
3	12	1	2.9	-5.3
4	12	1	3.7	-5.3
-4	12	1	11.0	-8.2
0	12	2	5.2	6.8
1	12	2	6.3	-5.0
-1	12	2	23.4	25.8
2	12	2	8.1	10.2
-2	12	2	12.5	15.5
4	12	2	11.0	-10.4
-4	12	2	8.3	-8.5
0	12	3	5.1	7.4
2	12	3	6.6	5.9
-3	12	3	3.7	3.5
4	12	3	6.3	-7.7
-4	12	3	11.0	11.0
1	12	4	2.5	-1.7
-1	12	4	27.2	26.3
2	12	4	4.4	5.7
-2	12	4	9.5	11.6
-3	12	4	5.1	-4.8
0	12	5	10.5	10.9
1	12	5	6.9	9.1
-1	12	5	6.9	-7.8
2	12	5	10.4	0.1
-2	12	5	5.2	3.8
3	12	5	10.2	-12.2
-3	12	5	7.3	7.9
1	12	6	5.6	-7.9
-1	12	6	19.0	20.0
-2	12	6	27.4	23.7
-3	12	6	5.9	-5.2
-5	12	6	11.1	14.6
-1	12	7	19.0	-19.6
-2	12	7	2.9	-5.9
-3	12	7	12.5	13.4
-4	12	7	12.8	11.7
0	12	8	6.2	-1.0
-2	12	8	6.6	7.2
-3	12	8	15.4	16.7
-4	12	8	8.3	6.4
-2	12	9	11.1	-11.4
-4	12	9	11.0	11.9
-3	12	10	4.4	5.0
1	13	0	8.8	8.0
2	13	0	12.6	16.7
0	13	1	7.9	5.9
1	13	1	7.6	-5.3
-1	13	1	17.1	16.0
2	13	1	5.2	-5.6
-3	13	1	10.2	-12.3
1	13	2	6.9	7.2
2	13	2	10.4	12.3
-3	13	2	10.2	11.0
1	13	3	8.1	-9.7
-1	13	3	14.6	16.6
2	13	3	6.6	5.2
-4	13	3	8.3	-9.2
-2	9	3	22.2	-22.3
-3	9	3	10.2	-7.8
-4	9	3	5.5	5.2
0	9	4	20.5	-19.1
1	9	4	21.6	30.0
-2	9	14	8.1	-8.0
-3	9	14	19.9	-16.6
-1	9	15	1.3	3.7
-2	9	15	14.7	12.8
-3	9	15	8.8	7.1
-5	9	15	16.7	-16.2
0	10	0	35.8	-33.4
2	10	0	13.3	14.7
0	10	1	28.1	24.4
1	10	1	19.0	20.8
-1	10	1	10.8	12.0
2	10	1	7.3	-4.7
-2	10	1	15.6	17.1
3	10	1	36.2	-46.1
-3	10	1	7.3	-8.6
4	10	1	22.0	-26.2
-4	10	1	29.5	-33.8
-5	10	1	15.3	-21.8
0	10	2	23.6	-21.1
1	10	2	5.6	1.2
2	10	2	4.4	0.4
-2	10	2	13.3	14.2
3	10	2	4.4	-0.6
-3	10	2	8.8	-7.7
-4	10	2	10.1	-8.3
1	10	3	17.7	20.4
-1	10	3	11.4	-10.6
2	10	3	4.4	-7.1
-2	10	3	7.3	-5.7
3	10	3	20.6	-25.2

Table 5. *Bond lengths within the formula unit, with standard deviations*

Zn–S(1)	2·443 Å	(0·003)
Zn–S(2)	2·355	(0·003)
Zn–S(3)	2·331	(0·003)
Zn–S(4)	2·815	(0·002)
S(1)–C(1)	1·722	(0·010)
S(2)–C(1)	1·725	(0·010)
S(3)–C(6)	1·723	(0·010)
S(4)–C(6)	1·737	(0·009)
C(1)–N(1)	1·34	(0·013)
C(6)–N(2)	1·31	(0·012)
N(1)–C(2)	1·44	(0·014)
N(1)–C(3)	1·49	(0·015)
N(2)–C(7)	1·48	(0·015)
N(2)–C(8)	1·48	(0·014)
C(2)–C(4)	1·52	(0·018)
C(3)–C(5)	1·48	(0·022)
C(7)–C(9)	1·51	(0·021)
C(8)–C(10)	1·53	(0·020)

Table 6. *Bond angles within the formula unit, with standard deviations*

S(1)–Zn–S(2)	75°47′	(13′)
S(1)–Zn–S(3)	106 52	(14)
S(2)–Zn–S(4)	93 37	(12)
S(3)–Zn–S(4)	69 34	(12)
Zn–S(1)–C(1)	81 53	(35)
Zn–S(2)–C(1)	84 29	(35)
Zn–S(3)–C(6)	93 56	(34)
Zn–S(4)–C(6)	78 16	(34)
S(1)–C(1)–S(2)	117 32	(51)
S(1)–C(1)–N(1)	121 0	(59)
S(2)–C(1)–N(1)	121 25	(59)
S(3)–C(6)–S(4)	117 47	(49)
S(3)–C(6)–N(2)	119 40	(57)
S(4)–C(6)–N(2)	122 31	(57)
C(1)–N(1)–C(2)	121 43	(1° 9′)
C(1)–N(1)–C(3)	121 46	(1 11)
C(2)–N(1)–C(3)	116 21	(1 13)
C(6)–N(2)–C(7)	123 27	(1 3)
C(6)–N(2)–C(8)	121 26	(1 6)
C(7)–N(2)–C(8)	115 4	(1 13)
N(1)–C(2)–C(4)	111 8	(1 23)
N(1)–C(3)–C(5)	113 6	(1 36)
N(2)–C(7)–C(9)	112 17	(1 34)
N(2)–C(8)–C(10)	111 14	(1 27)

Calculations

The calculations were carried out on an IBM 1620 electronic computer.

Intensity corrections and structure factors were calculated with the use of programs of V. Scatturin and coworkers. D. van der Helm's general Fourier synthesis and E. Giglio's program for the differential Fourier syntheses were used. The least-squares planes were calculated by a program written by S. Chu (equation of the plane in the form $Ax+By+Cz=D$, referred to the crystallographic axes). Special modifications of the programs above and various minor other programs were written by one of us (L. Z.) and by A. Domenicano.

Discussion

An orthographic projection of the structure of zinc diethyldithiocarbamate, as seen down the line which makes an angle of 90° with the b axis and $60° - (\beta - 90°) = 38°2'$ with the c axis, is given in Fig. 1. The asymmetric unit is chosen so as to contain one monomer of zinc diethyldithiocarbamate. However, each pair of centrosymmetrically related zinc atoms, at the rather short distance of 3·546 Å (e.s.d.: 0·002 Å), share sulphur atoms, thus forming a dimeric unit.

The bond lengths and angles within the formula unit, with their e.s.d.'s (Cruickshank & Robertson, 1953) are listed in Tables 5 and 6 respectively, and are also shown in Fig. 2. All the relevant bond, interaction and contact distances and angles in the zinc coordination sphere are reported in Table 7, including, for the sake of completeness, some of the values already given in Tables 5 and 6.

The results of the calculation of a number of significant least-squares planes are presented in Table 8.

In zinc diethyldithiocarbamate the metal atom is five-coordinated. The geometry of this coordination is intermediate between tetragonal pyramidal and trigonal bipyramidal, although in our opinion it is more correct to consider it as a distorted example of the second case. The five zinc-sulphur distances range from $2\cdot33_1$ to $2\cdot81_5$ Å. Of these, Zn–S(2), Zn–S(3), Zn–S(4′), $2\cdot35_5$, $2\cdot33_1$, $2\cdot38_3$ Å respectively*, can be regarded as normal by comparison with the value of 2·35 Å found in dichlorobisthioureazinc (Kunchur & Truter, 1958), where the coordination is tetrahedral. On the other hand, Zn–S(1) and especially Zn–S(4), $2\cdot44_3$ and $2\cdot81_5$ Å respectively, are much longer, as would be expected if they were regarded as the axial bonds in a trigonal bipyramidal configuration.

Table 7. *Distances and angles in the zinc coordination sphere*

Zn–S(1)	=2·443 Å	S(1)–Zn–S(2)	= 75° 47′
Zn–S(2)	=2·355	S(1)–Zn–S(4′)	=105 13
Zn–S(3)	=2·331	S(1)–Zn–S(3)	=106 52
Zn–S(4)	=2·815	S(4)–Zn–S(2)	= 93 37
Zn–S(4′)	=2·383	S(4)–Zn–S(4′)	= 94 23
Zn–Zn′	=3·546	S(4)–Zn–S(3)	= 69 34
S(2)–S(4′)	=3·930	S(2)–Zn–S(4′)	=112 3
S(4′)–S(3)	=3·810	S(4′)–Zn–S(3)	=107 49
S(3)–S(2)	=4·371	S(3)–Zn–S(2)	=137 43
S(1)–S(2)	=2·948	S(1)–Zn–S(4)	=160 2
S(1)–S(4′)	=3·835	S(3)–S(2)–S(4′)	= 54 19
S(1)–S(3)	=3·835	S(2)–S(4′)–S(3)	= 68 45
S(4)–S(2)	=3·783	S(4′)–S(3)–S(2)	= 56 55
S(4)–S(4′)	=3·825	S(2)–S(1)–S(3)	= 79 4
S(4)–S(3)	=2·963	S(4)–S(2)–S(1)	= 99 51
		S(1)–S(3)–S(4)	= 98 26
		S(3)–S(4)–S(2)	= 79 46
		Zn–S(4)–Zn′	= 85 37

An arrangement of five ligand atoms about the zinc that could be regarded either as a distorted trigonal bipyramid or as a distorted tetragonal pyramid has already been found in the case of monoaquobisacetylacetonatozinc (Lippert & Truter, 1960; Montgomery & Lingafelter, 1963). However, this type of coordination in zinc diethyldithiocarbamate is attained only through the formation of a dimer in which the zinc forms a normal bond with a sulphur atom of the centrosymmetrically related monomer and a very long bond with a sulphur atom within its own monomer.

In our interim report (Bonamico, Dessy, Mazzone, Mugnoli, Vaciago & Zambonelli, 1963) we remarked that this compound was then, to our knowledge, unique in that the same ligand was engaged in bonding in two very different ways in one complex: one ligand molecule forming a four-membered chelate ring, and a second coordinating with two different zinc atoms, whilst at the same time completing a chelate ring with a remarkably long approach distance. A second similar case has recently been reported of bis(*N*-methylsalicylaldiminato)zinc(II) (Orioli, Di Vaira & Sacconi, 1965), where each zinc atom is five-coordinated in a distorted trigonal bipyramidal environment and one of the oxygen–zinc intrachelate distances is *ca.* 0·1 Å longer than the corresponding interchelate distance.

Tables 7 and 8 give all the relevant information on the deviations of zinc diethyldithiocarbamate from the ideal cases of either a regular square-pyramidal or a regular trigonal-bipyramidal coordination. It appears that the same zinc–sulphur interaction which makes it possible for zinc to be five-coordinated, and the strain in the four-membered ring, revealed by the valence

Table 8. *Least-squares planes*

Equation in the form $Ax+By+Cz=D$, referred to the crystallographic axes, calculated after Schomaker, Waser, Marsh & Bergman (1959) with all weights equal to 1. All values have been multiplied by 10^3.

Plane	*A*	*B*	*C*	*D*	Atoms defining the plane
I	700	−515	196	1596	S(1) S(2) S(3) S(4)
II	−572	76	971	0	Zn Zn′ S(1) S(1′) S(4) S(4′)
III	586	810	−196	1297	Zn S(2) S(3) S(4′)
IV	776	−583	−69	1005	S(1) S(2) C(1) N(1) C(2) C(3)
V	777	−582	−70	1010	C(1) N(1) C(2) C(3)
VI	572	−432	433	1279	S(3) S(4) C(6) N(2) C(7) C(8)
VII	556	−439	446	1256	C(6) N(2) C(7) C(8)

Deviations from planes (10^{-3} Å)

	I	II	III	IV	V	VI	VII
Zn	−631	−56	153	−197	—	−259	—
Zn′	—	56	—	—	—	—	—
S(1)	−186	26	2453	1	—	—	—
S(1′)	—	−26	—	—	—	—	—
S(2)	189	—	−57	−2	—	—	—
S(3)	185	—	−56	—	—	−18	—
S(4)	−187	13	−2554	—	—	21	—
S(4′)	—	−13	−39	—	—	—	—
C(1)	—	—	—	−8	−9	—	—
N(1)	—	—	—	25	24	—	—
C(2)	—	—	—	−10	−8	—	—
C(3)	—	—	—	−6	−8	—	—
C(6)	—	—	—	—	—	−8	−3
N(2)	—	—	—	—	—	8	9
C(7)	—	—	—	—	—	21	−3
C(8)	—	—	—	—	—	−25	−3

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* The bond distance Zn–S(4′), not reported in Table 5 because it is not within the formula unit, has an e.s.d. of 0·002 Å.

angles around the zinc atom, are largely responsible for the distortions. It is noteworthy that Zn, S(1), S(4) and the centrosymmetrically related atoms Zn′, S(1′) and S(4′) lie roughly in a plane, the maximum and mean deviations being 0·06 Å and 0·03 Å respectively, whilst in the case of the copper compound the degree of coplanarity of the corresponding atoms is higher, the six atoms all lying in a plane within less than ±0·01 Å (Bonamico, Dessy, Mugnoli, Vaciago & Zambonelli, 1965).

It is also interesting to note that the four shortest bonds formed by any one zinc atom in this dimeric complex are directed to the corners of a rather distorted tetrahedron. Some of the distances and angles reported in Table 8 are relevant to the analysis of the deviations of this tetrahedron from a regular one.

Five-coordinated zinc(II) in a distorted trigonal bipyramidal environment has been found also in the related complex bis(*N*,*N*-dimethyldithiocarbamato) pyridine-zinc(II) (Fraser & Harding, 1965), where two long zinc–sulphur bonds (*ca.* 2·60 Å) can be regarded as axial, and two short zinc–sulphur bonds (*ca.* 2·33 Å) and one zinc–nitrogen bond (*ca.* 2·07 Å) can be regarded as equatorial.

As a final remark on the coordination of zinc in the present compound it should be pointed out that the dimeric unit does not seem to be present in solution: zinc diethyldithiocarbamate has a normal molecular weight in benzene (Malatesta, 1965).

Each of the two ligand molecules is planar, except for the terminal CH_3 groups. Planarity and bond length values indicate conjugation, with sp^2 hybridization of the valence orbitals of C(1), N(1), C(6) and N(2) atoms. The strain in the four-membered ring does not result in any apparent increase in the expected values of sulphur–carbon bond lengths. Our values compare well with the values found in thiourea and several of its derivatives and coordination complexes (Lopez-Castro & Truter, 1963; Dias & Truter, 1964; and other references quoted therein) and seem to be normal for S–C(sp^2) distances.

As in the cases of the nickel compound (Bonamico, Dessy, Mariani, Vaciago & Zambonelli, 1965) and of the copper compound (Bonamico, Dessy, Mugnoli, Vaciago & Zambonelli, 1965) our present results on the coplanarity of the nitrogen valence orbitals and on the C(1)–N(1) and C(6)–N(2) bond lengths confirm the findings of previous infrared work (Chatt, Duncanson & Venanzi, 1956*a*, *b*) that $\cdots \overset{(-)}{S_2}C=\overset{(+)}{N}R_2$ is an important canonical form in the structure of the dialkyldithiocarbamates*.

All other bond distances and angles in the ligand molecules compare closely, within the e.s.d.'s, with the corresponding ones in the nickel and copper compounds.

As mentioned in the introduction, one of the reasons for the investigation of the present structure was the need for an explanation of the similarity between the crystal parameters of zinc and copper diethyldithiocarbamates†, which could indicate that these compounds were isostructural, with the same coordination geometry around the metal atoms. It is now clear that they are, indeed, isostructural to a point, but not to the extent of having the same coordination configuration around the two different metal atoms. Only small changes in atomic positions, mainly of the metal atoms, produce all the necessary differences in the coordination geometry, leaving the general size and shape of the molecules practically unchanged (compare Fig. 1 and Table 1 of this paper with Fig. 1 and Table 1 of paper II of this series). Also because of these small changes the metal intermolecular contact to C(2″), which is 3·78 Å long in the case of copper and implies a hydrogen atom in the sixth octahedral position at 2·86 Å from it, becomes 4·13 Å long for the zinc compound, with the corresponding hydrogen atom at 3·28 Å, and thus loses any significance it might have had in the former case.

It is worth noticing that the crystal parameters of cadmium diethyldithiocarbamate, as recently determined in our laboratory, are: $a=10·166\pm0·010$, $b=10·746\pm0·005$, $c=16·717\pm0·010$ Å; $\beta=111°\ 53'\pm3'$; $U=1694·6$ Å^3; space group $P2_1/c$. As can be seen, they are very near to the corresponding parameters of the zinc and the copper salts. It will be interesting to determine to what extent the cadmium compound is isostructural with the zinc and the copper complexes. For this reason the structure of cadmium diethyldithiocarbamate is now being investigated and will be discussed in a subsequent paper of this series.

References

Bonamico, M., Dessy, G., Mariani, M., Vaciago, A. & Zambonelli, L. (1965). *Acta Cryst.* **19**, 619.

Bonamico, M., Dessy, G., Mazzone, G., Mugnoli, A., Vaciago, A. & Zambonelli, L. (1963). *Rend. Accad. Lincei* VIII, **35**, 338.

Bonamico, M., Dessy, G., Mugnoli, A., Vaciago, A. & Zambonelli, L. (1965). *Acta Cryst.* **19**, 886.

Chatt, J., Duncanson, L. A. & Venanzi, L. M. (1956*a*). *Nature, Lond.* **177**, 1042.

Chatt, J., Duncanson, L. A. & Venanzi, L. M. (1956*b*). *Suomen Kem.* **B29**, 75.

Cruickshank, D. W. J. (1949). *Acta Cryst.* **2**, 65.

Cruickshank, D. W. J. (1956). *Acta Cryst.* **9**, 747.

Cruickshank, D. W. J. & Robertson, A. P. (1953). *Acta Cryst.* **6**, 698.

Dias, H. W. & Truter, M. R. (1964). *Acta Cryst.* **17**, 937.

Fraser, K. A. & Harding, M. M. (1965). Private communication.

International Tables for X-ray Crystallography (1962). Vol. III. Birmingham: Kynoch Press.

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* The LCAO-MO double bond orders of the C(1)–N(1) and C(6)–N(2) bonds, calculated as shown in paper I of this series, are $p=0·60$ and $p=0·79$ respectively.

† See values reported above under *Experimental*. Powder photographs of the two compounds resemble each other very closely.

Kunchur, N. R. & Truter, M. R. (1958). *J. Chem. Soc.* p. 3478.
Lippert, E. L. & Truter, M. R. (1960). *J. Chem. Soc.* p. 4996.
Lopez-Castro, A. & Truter, M. R. (1963). *J. Chem. Soc.* p. 1309.
Malatesta, L. (1965). Private communication.
Mazzone, G., Vaciago, A. & Bonamico, M. (1963). *Ric. Sci.* **33(II-A)**, 1113.
Montgomery, H. & Lingafelter, E. C. (1963). *Acta Cryst.* **16**, 748.
Orioli, P. L., Di Vaira, M. & Sacconi, L. (1965). *Chem. Comm.* p. 103.
Phillips, D. C. (1954). *Acta Cryst.* **7**, 746.
Rollett, J. S. & Sparks, R. A. (1960). *Acta Cryst.* **13**, 273.
Schomaker, V., Waser, J., Marsh, R. E. & Bergman, G. (1959). *Acta Cryst.* **12**, 600.
Shugam, E. A. & Shkol'nikova, L. M. (1958). *Kristallografiya*, **3**, 749 (English translation (1960) in *Soviet Phys. Crystallogr.* **3**, 756).
Simonsen, S. H. & Wah Ho, J. (1953). *Acta Cryst.* **6**, 430.
Vaciago, A., Gramaccioli, C. M. & Pullia, A. (1960). *Ric. Sci.* **30**, 2528.

Acta Cryst. (1965). **19**, 909

On Hydrogen Bonds in Crystalline Hydrates

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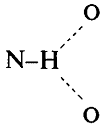
(*Received* 28 *October* 1964 *and in revised form* 11 *February* 1965)

According to the results of recent neutron and X-ray diffraction studies of crystalline hydrates linear hydrogen bonds are not as common in these compounds as has been hitherto assumed. Bent and bifurcated hydrogen bonds, as well as hydrogen atoms in positions in which they do not form hydrogen bonds, have been found to occur even in cases where arrangements with more linear hydrogen bonds would have been geometrically possible. These observations are at variance with the notion that the coordination number of the hydrogen atom in a hydrogen bond is necessarily two. It seems that the orientation of the water molecules, and hence the geometry of the hydrogen bonds, is determined by the electrostatic interactions between the water molecules and the surrounding atoms. This view is supported by the good agreement found in several hydrates between the positions of the hydrogen atoms (*a*) as determined experimentally and (*b*) as calculated theoretically to have the least electrostatic energy. The calculation of the electrostatic energy was done for different orientations of the water molecule until the position with the extreme value of the electrostatic energy was found. The shape of the molecule and the position of the water oxygen atom were held fixed throughout the calculations.

Introduction

Hydrogen bonds are formed between the most electronegative elements like F, O, N, Cl and S. Usually the hydrogen atom is connected more closely with one of the atoms, the donor atom X(*d*), and is at a larger distance from the second atom, the acceptor atom Y(*a*) of the hydrogen bond: X(*d*)–H · · · Y(*a*). Until the advent of neutron diffraction methods this arrangement was believed to be more or less linear, the angle X(*d*)–H · · · Y(*a*) being close to 180°. According to Pauling (1960) the hydrogen bond is largely ionic in character, since the hydrogen atom with its one stable orbital is capable of forming one covalent bond only (to the donor atom). Coulson & Danielsson (1954) estimated the relative magnitudes of the ionic and covalent contributions to the hydrogen bond. They concluded that the electrostatic contribution seems to be dominant, and is the more so the longer the hydrogen bond is. Pimentel & McClellan (1960) emphasized the difficulties in reconciling the electrostatic description of the hydrogen bond with some of its properties and stressed the importance of the covalent contribution to the hydrogen bond. It is generally accepted that the coordination number of a hydrogen atom in a hydrogen bond is two. There are a few exceptions to this rule; one of these is glycine (Albrecht & Corey, 1939; Marsh, 1957; Burns & Levy, 1958), where a hydrogen atom from the $-NH_3^+$ group has the coordination number three:  $\mathrm{N{-}H}\begin{array}{l}\cdot\cdot\,\mathrm{O}\\ \cdot\cdot\,\mathrm{O}\end{array}$. Such an arrangement is called a bifurcated hydrogen bond.

Since C. A. Beevers, H. Lipson and coworkers in the early 1930's determined the crystal structures of several salt hydrates it is known that the oxygen atoms of the water molecules, O(*w*), in these structures can act as

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