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Structural Studies of Metal Dithiocarbamates.
II. The Crystal and Molecular Structure of Copper Diethyldithiocarbamate*

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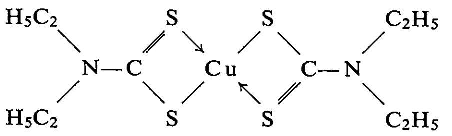
The crystal structure of copper(II) bis(*N*,*N*-diethyldithiocarbamate), $[(C_2H_5)_2NCS_2]_2Cu$, at room temperature, has been determined by three-dimensional methods, including anisotropic refinement by differential Fourier synthesis (final *R* value, 0·081). There are four formula units in the monoclinic cell, $a=9{\cdot}907$, $b=10{\cdot}627$, $c=16{\cdot}591$ Å, $\beta=113°52'$, with space group $P2_1/c$. Each pair of centrosymmetrically related copper atoms share sulphur atoms, thus forming a bimolecular unit. Copper has a distorted tetragonal-pyramidal coordination of four sulphur atoms, at a distance ranging between 2·297 and 2·339Å, and a fifth apical sulphur atom at 2·851 Å. The shortest intermolecular copper contact to a heavy atom is to a carbon atom at 3·78 Å, which implies a hydrogen atom occupying the sixth octahedral position at 2·86 Å from the copper. The ligand molecules are planar (obviously apart from the terminal CH_3 groups), the sulphur–carbon bond lengths range from 1·708 to 1·736 Å, and the two $C(sp^2)-N(sp^2)$ bonds are 1·33 and 1·35 Å long. As expected from previous infrared work, $\cdots \overset{(-)}{S_2}C=\overset{(+)}{N}R_2$ is an important canonical form in the structure of copper diethyldithiocarbamate.

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 compound investigated in our laboratory was copper(II) bis(*N*,*N*-diethyldithiocarbamate):



with the bond orders written in the conventional way.

The first structural determination of a copper salt was that of Peyronel (Pignedoli & Peyronel, 1962; and previous references quoted therein), who published a two-dimensional structure analysis of the di-n-propyl derivative. Preliminary work was also published on copper(II) bis(*N*,*N*-diethyldithiocarbamate) by several research groups (Shugam & Shkol'nikova, 1958; Vaciago, Gramaccioli & Pullia, 1960; Bally, 1963). A detailed geometrical picture of the coordination of copper and accurate data on bond lengths and angles, however, were still lacking. A further interesting point at this stage was the need for explanation of the striking similarity in the crystal parameters of copper and zinc (Simonsen & Wah Ho, 1953) diethyldithiocarbamates, which could indicate that these compounds were isostructural. An interim report on the three-dimensional work in progress in our laboratory was published in 1963 (Bonamico, Dessy, Mazzone, Mugnoli, Vaciago & Zambonelli, 1963).

As part of a programme of investigations on coinage metal dithiocarbamates the X-ray structure analysis of copper(I) *N*,*N*-diethyldithiocarbamate has also been published recently (Hesse, 1963).

Experimental

Crystal data

Copper diethyldithiocarbamate forms deep green prismatic crystals, stable in air and in the X-ray beam. Morphological and optical data can be found in a previous publication (Vaciago, Gramaccioli & Pullia, 1960).

The unit-cell dimensions were determined 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). The crystal data given below replace those reported by us in a previous publication (Vaciago, Gramaccioli & Pullia, 1960).

Copper(II) *bis*(*N*,*N-diethyldithiocarbamate*)
$C_{10}H_{20}CuN_2S_4$. F.W. = 360·08.
Monoclinic prismatic, $a=9{\cdot}907\pm0{\cdot}010$, $b=10{\cdot}627\pm0{\cdot}005$, $c=16{\cdot}591\pm0{\cdot}010$ Å;
$\beta=113°52'\pm5'$; $U=1597{\cdot}4$ Å^3;
$D_m=1{\cdot}489\pm0{\cdot}005$ g.cm^{-3} (by flotation); $Z=4$;
$D_c=1{\cdot}498$ g.cm^{-3}; $F(000)=748$;

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Absorption coefficients for Cu radiation, 66 cm^{-1}.

Space group $P2_1/c$ (C_{2h}^5, 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* axis (6 layers) and the *b* axis (7 layers) for approximately square crystals, 0·02 cm thick. 2570 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 preliminary two-dimensional investigation of the (*h*0*l*) projection (Vaciago, Gramaccioli & Pullia, 1960) gave the *x* and *z* coordinates of copper and sulphur atoms. From a three-dimensional Patterson synthesis computed from the first 2000 independent reflexions which had been collected (full data around the *b* axis and one layer around the *a* axis), the *y* coordinates of the same atoms were then found.

By a three-dimensional Fourier synthesis, phased on the contribution of the five atoms located from the Patterson and with the use of the complete set of 2570 observed reflexions, it was possible to locate all the atoms, apart from the hydrogen atoms. At this stage, a structure factor calculation gave a reliability index $R=0·32$.

Refinement

Refinement was done by differential Fourier synthesis. After the first cycle, the reliability index *R* was 0·19.

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

	x/a	*y/b*	*z/c*
Cu	1914 (1)	317 (1)	651 (1)
S(1)	3344 (2)	2116 (2)	1106 (1)
S(2)	2039 (2)	617 (2)	2051 (1)
S(3)	2462 (2)	−331 (2)	−506 (1)
S(4)	768 (2)	−1649 (2)	279 (1)
N(1)	3743 (6)	2639 (7)	2771 (4)
N(2)	1374 (5)	−2654 (5)	−1032 (3)
C(1)	3122 (8)	1881 (8)	2066 (4)
C(2)	4620 (9)	3736 (12)	2741 (6)
C(3)	3542 (9)	2420 (12)	3589 (5)
C(4)	3632 (11)	4880 (12)	2392 (8)
C(5)	4792 (14)	1630 (17)	4240 (7)
C(6)	1520 (7)	−1675 (7)	−502 (4)
C(7)	2107 (8)	−2675 (10)	−1640 (5)
C(8)	453 (8)	−3754 (9)	−1046 (5)
C(9)	1065 (12)	−2292 (14)	−2571 (5)
C(10)	1369 (14)	−4823 (13)	−489 (10)

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

	x/a	*y/b*	*z/c*	*B*(Å^2)
H(2)*a*	5179	3531	2309	5·1
H(2)*b*	5437	3935	3403	5·1
H(3)*a*	2500	1928	3432	4·8
H(3)*b*	3512	3324	3891	4·8
H(4)*a*	4300	5685	2374	5·5
H(4)*b*	3072	5089	2822	5·5
H(4)*c*	2814	4685	1728	5·5
H(5)*a*	4605	1487	4837	5·6
H(5)*b*	5838	2116	4403	5·6
H(5)*c*	4825	721	3944	5·6
H(7)*a*	2508	−3624	−1659	4·9
H(7)*b*	3035	−2023	−1402	4·9
H(8)*a*	−114	−4078	−1723	4·9
H(8)*b*	−357	−3472	−791	4·9
H(9)*a*	1653	−2320	−3001	5·6
H(9)*b*	661	−1340	−2560	5·6
H(9)*c*	134	−2941	−2816	5·6
H(10)*a*	651	−5613	−516	5·8
H(10)*b*	1935	−4509	191	5·8
H(10)*c*	2179	−5115	−740	5·8

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}
Cu	130 (1)	73 (1)	30 (0)	−23 (2)	62 (1)	−13 (1)
S(1)	138 (2)	94 (2)	37 (1)	−50 (4)	70 (1)	−10 (2)
S(2)	127 (2)	74 (2)	31 (1)	−27 (3)	58 (1)	−10 (1)
S(3)	206 (3)	85 (2)	51 (1)	−75 (4)	142 (1)	−29 (2)
S(4)	120 (2)	74 (2)	28 (1)	−13 (3)	59 (1)	−2 (1)
N(1)	115 (8)	90 (9)	34 (3)	−31 (13)	38 (5)	−31 (6)
N(2)	114 (7)	70 (7)	33 (2)	−17 (11)	58 (4)	−21 (5)
C(1)	91 (7)	77 (9)	36 (3)	10 (13)	44 (5)	−12 (7)
C(2)	141 (12)	140 (15)	49 (4)	−118 (22)	63 (8)	−50 (11)
C(3)	144 (10)	120 (12)	34 (3)	2 (17)	64 (6)	−23 (8)
C(4)	203 (17)	110 (14)	69 (6)	−92 (25)	112 (11)	−14 (12)
C(5)	190 (17)	184 (22)	45 (5)	−16 (29)	54 (11)	5 (14)
C(6)	117 (8)	66 (8)	29 (2)	−14 (13)	55 (5)	−9 (6)
C(7)	151 (10)	107 (11)	38 (3)	15 (16)	88 (6)	−21 (8)
C(8)	137 (10)	93 (10)	41 (3)	−6 (16)	61 (7)	−13 (8)
C(9)	219 (17)	158 (18)	36 (4)	−14 (26)	82 (9)	−10 (10)
C(10)	215 (18)	102 (12)	82 (7)	56 (23)	130 (12)	38 (12)

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* Note that crystals of this compound should be oriented as $P2_1/n$ (Vaciago, Gramaccioli & Pullia, 1960), but for convenience axes have been selected here according to $P2_1/c$ (see also Shugam & Shkol'nikova, 1958; Bally, 1963; Bonamico, Dessy, Mazzone, Mugnoli, Vaciago & Zambonelli, 1963).

Two other isotropic cycles lowered the *R* value to 0·147. Three cycles of anisotropic refinement, and the introduction of hydrogen atoms in positions calculated to make the C–H bond lengths 1·09 Å and to complete tetrahedra around the carbon atoms brought the final *R* index to 0·081 (calculated on observed reflexions 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 the final parameters are compared with the observed structure amplitudes in Table 4. Atomic scattering values were those recommended in *International Tables for X-ray Crystallography* (1962). Correction for anomalous dispersion was applied for copper and sulphur atoms (*International Tables for X-ray Crystallography*, 1962).

The observed and calculated values of electron density and second derivatives at the atomic peaks are compared in Table 5. Their e.s.d.'s are:

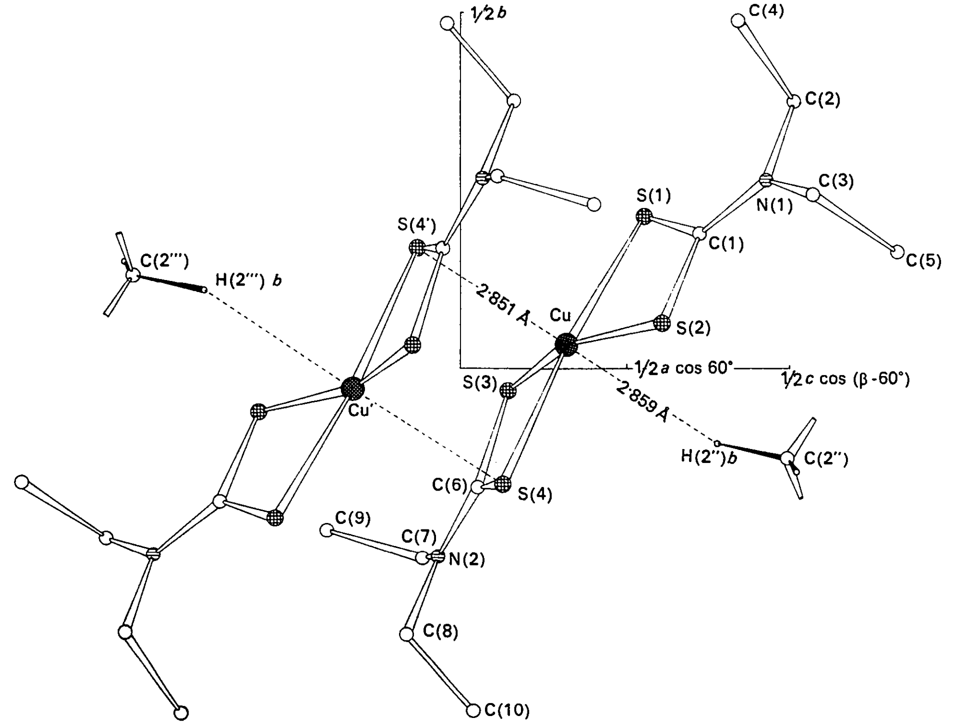

Fig. 1. Orthographic projection of the structure down the line which makes an angle of 90° with the *b* axis and 60° − (*β* − 90°) = 36° 8′ with the *c* axis.

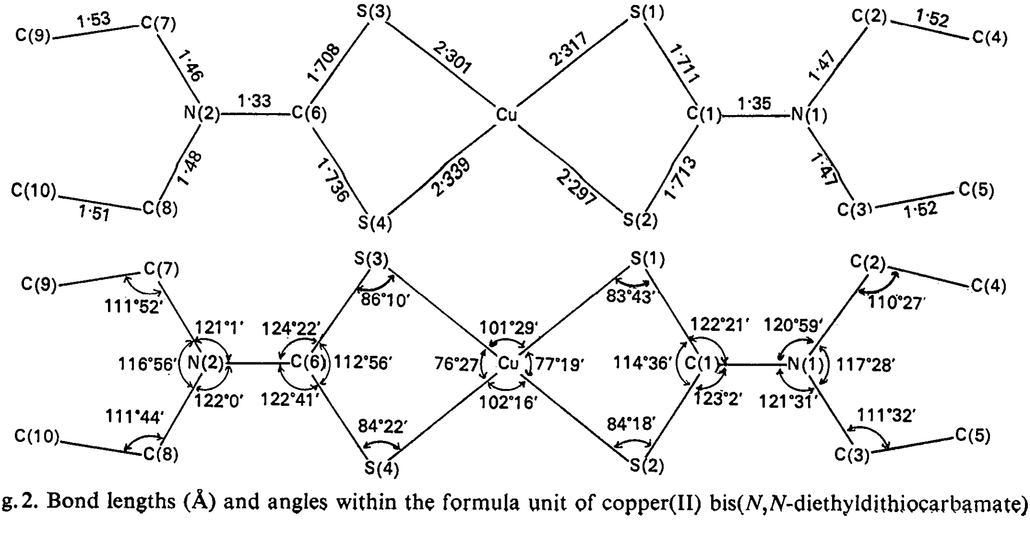

Fig. 2. Bond lengths (Å) and angles within the formula unit of copper(II) bis(*N*,*N*-diethyldithiocarbamate).

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	71.1	66.2	2	0	10	8.6	9.0	-8	1	1	33.4	-33.3	-3	1	6	50.1	-49.8	-4	1	11	17.9	16.8
2	0	0	139.5	-152.3	-2	0	10	23.4	22.8	9	1	1	14.6	17.1	4	1	6	22.3	-19.7	5	1	11	10.3	-10.4
3	0	0	85.1	-78.0	3	0	10	8.3	7.3	-9	1	1	20.7	-20.6	-4	1	6	36.0	36.7	-5	1	11	16.3	14.0
4	0	0	22.3	-20.2	-3	0	10	66.6	70.4	10	1	1	4.3	5.1	5	1	6	21.3	-19.8	6	1	11	3.0	-0.3
5	0	0	40.9	38.7	4	0	10	40.4	-35.1	-10	1	1	9.1	9.2	-5	1	6	43.0	45.4	-6	1	11	16.4	16.4
6	0	0	40.9	34.8	-4	0	10	50.7	59.5	11	1	1	1.8	0.7	-6	1	6	29.2	30.0	-7	1	11	14.6	-14.2
7	0	0	61.3	-63.5	5	0	10	14.8	-14.6	-11	1	1	13.9	15.2	7	1	6	3.6	-3.8	-8	1	11	16.4	-16.3
8	0	0	35.3	-33.6	-5	0	10	5.6	0.9	0	1	2	103.9	-95.5	-7	1	6	33.4	36.0	-9	1	11	10.3	10.0
9	0	0	9.3	8.1	6	0	10	11.6	11.0	1	1	2	17.1	15.7	8	1	6	7.8	-9.0	-10	1	11	16.4	13.8
10	0	0	5.6	5.0	-6	0	10	20.9	17.6	-1	1	2	100.2	105.6	-8	1	6	17.6	-16.1	-11	1	11	8.5	-8.4
11	0	0	4.6	4.7	-7	0	10	16.7	-16.3	2	1	2	82.9	78.7	9	1	6	2.4	-3.2	-12	1	11	10.9	-12.2
0	0	2	66.3	62.8	-8	0	10	43.2	-43.6	-2	1	2	86.9	-88.5	-9	1	6	16.4	-15.3	0	1	12	14.7	-15.3
1	0	2	58.7	67.1	-9	0	10	8.8	8.5	3	1	2	27.3	27.3	-10	1	6	3.6	3.0	1	1	12	42.3	41.4
-1	0	2	92.0	156.6	-11	0	10	27.4	-27.5	-3	1	2	36.0	37.8	-12	1	6	6.1	-5.6	-1	1	12	9.9	-11.5
2	0	2	13.2	-14.1	-12	0	10	14.8	-16.8	4	1	2	30.3	27.7	0	1	7	107.7	-106.0	2	1	12	8.5	-8.0
-2	0	2	26.9	-24.1	0	0	12	44.3	-47.7	-4	1	2	17.7	14.9	1	1	7	45.6	-38.1	-2	1	12	22.6	-23.0
3	0	2	30.2	-27.2	1	0	12	15.8	-14.2	5	1	2	3.0	3.4	-1	1	7	9.0	-9.3	3	1	12	24.3	-23.1
-3	0	2	90.6	-98.0	2	0	12	50.2	47.5	-5	1	2	15.1	16.4	2	1	7	57.9	53.8	-3	1	12	16.6	15.5
4	0	2	17.9	16.7	-2	0	12	9.7	-9.6	6	1	2	21.8	-21.8	-2	1	7	139.4	143.4	4	1	12	6.1	4.8
-4	0	2	5.6	3.2	3	0	12	19.5	-19.5	-6	1	2	40.7	40.9	3	1	7	43.8	39.9	-4	1	12	21.3	-20.2
5	0	2	16.4	16.4	-3	0	12	12.7	12.9	7	1	2	6.7	-5.8	-3	1	7	114.6	119.5	5	1	12	6.7	-6.0
-5	0	2	47.4	-44.9	4	0	12	26.9	-25.5	-7	1	2	3.6	-2.9	4	1	7	7.9	-6.9	-5	1	12	25.3	-23.2
6	0	2	42.3	-38.4	-4	0	12	57.5	58.5	8	1	2	6.1	6.1	-4	1	7	64.9	-65.0	6	1	12	7.3	-6.7
-6	0	2	24.1	23.5	-5	0	12	20.3	19.2	-8	1	2	15.8	-15.7	5	1	7	41.5	-38.5	-6	1	12	40.7	40.6
7	0	2	43.2	-37.5	-6	0	12	8.3	-5.0	9	1	2	9.7	-12.2	-5	1	7	90.1	-101.4	-7	1	12	14.6	15.5
-7	0	2	43.7	40.9	-7	0	12	8.3	-7.5	-9	1	2	7.8	7.8	6	1	7	20.7	-20.5	-9	1	12	12.8	11.0
8	0	2	9.3	8.8	-8	0	12	20.9	-22.2	10	1	2	4.3	-4.6	-6	1	7	4.3	-4.1	0	1	13	9.5	-9.6
-8	0	2	37.1	-35.8	-9	0	12	10.2	8.5	-10	1	2	9.1	-11.1	7	1	7	7.3	7.1	1	1	13	24.9	24.0
9	0	2	15.3	16.4	-10	0	12	8.3	8.3	11	1	2	4.3	5.1	-7	1	7	43.2	45.5	-1	1	13	24.3	-25.2
-9	0	2	51.6	-51.8	-11	0	12	16.7	-16.9	-11	1	2	10.9	-10.8	8	1	7	18.2	18.8	2	1	13	14.6	13.5
-10	0	2	8.3	-8.5	-12	0	12	15.8	-15.5	0	1	3	37.4	35.4	-8	1	7	21.3	19.3	-2	1	13	15.4	-16.8
-11	0	2	4.6	5.1	0	0	14	6.9	4.3	1	1	3	17.1	-16.3	9	1	7	5.4	5.8	3	1	13	23.7	-21.8
-12	0	2	14.8	18.4	1	0	14	7.8	6.2	-1	1	3	99.6	94.5	-9	1	7	29.2	-28.9	-3	1	13	3.6	2.6
0	0	4	47.9	43.4	-1	0	14	27.3	-30.6	2	1	3	35.3	-35.4	-10	1	7	28.6	-27.8	4	1	13	24.3	-22.7
1	0	4	36.2	29.4	2	0	14	21.8	-22.1	-2	1	3	25.2	26.2	-11	1	7	3.0	0.1	-4	1	13	48.1	45.8
-1	0	4	28.8	31.1	-2	0	14	25.4	-24.9	3	1	3	48.7	-44.5	-12	1	7	7.8	8.8	-5	1	13	48.3	47.7
2	0	4	18.6	17.5	3	0	14	31.6	-34.5	-3	1	3	66.4	71.5	0	1	8	46.5	44.3	-6	1	13	11.5	-10.6
-2	0	4	19.0	18.6	-3	0	14	28.0	-26.6	4	1	3	26.7	24.5	1	1	8	26.7	25.2	-7	1	13	16.4	-26.3
3	0	4	60.2	-57.6	4	0	14	7.4	-5.9	-4	1	3	17.2	-14.9	-1	1	8	43.2	-39.8	-8	1	13	5.4	-6.6
-3	0	4	4.3	-2.4	-4	0	14	63.6	65.4	5	1	3	19.6	18.8	2	1	8	32.4	33.7	-9	1	13	26.1	22.7
4	0	4	12.6	14.5	-5	0	14	79.5	84.5	-5	1	3	33.9	-39.5	-2	1	8	57.4	56.4	-10	1	13	9.1	9.8
-4	0	4	10.2	-9.4	-7	0	14	54.3	-49.5	6	1	3	24.9	-25.4	3	1	8	22.4	21.4	-11	1	13	17.6	-17.5
5	0	4	19.3	18.1	-8	0	14	8.3	-7.3	7	1	3	24.9	-26.3	-3	1	8	27.9	-26.9	-12	1	13	15.2	-16.5
-5	0	4	27.4	-27.6	-9	0	14	15.8	18.1	-7	1	3	32.8	35.4	4	1	8	24.9	-23.9	0	1	14	29.6	31.3
6	0	4	57.2	-55.2	-10	0	14	18.6	20.8	8	1	3	5.4	2.3	-4	1	8	9.0	9.1	1	1	14	10.9	-11.5
-6	0	4	8.3	-8.4	-11	0	14	12.0	-12.3	-8	1	3	3.6	-3.5	-5	1	8	55.6	55.3	-1	1	14	23.7	-25.2
7	0	4	24.1	-23.2	-12	0	14	19.0	-23.9	9	1	3	3.0	-1.0	-6	1	8	3.0	-3.0	2	1	14	23.1	-21.5
-7	0	4	21.4	22.2	0	0	16	5.1	2.4	-9	1	3	24.9	-23.7	7	1	8	7.3	-9.0	-2	1	14	27.1	-29.6
8	0	4	7.8	5.4	1	0	16	22.8	-22.0	10	1	3	3.6	4.7	-7	1	8	19.4	20.0	3	1	14	11.5	-10.6
-8	0	4	13.0	-16.0	-1	0	16	20.1	22.8	-10	1	3	17.0	-17.9	8	1	8	8.5	-8.2	-3	1	14	19.6	-17.7
9	0	4	6.9	6.2	2	0	16	37.1	-37.6	-11	1	3	4.3	4.9	-8	1	8	32.8	31.3	-4	1	14	13.7	14.7
-9	0	4	37.1	-39.4	-2	0	16	7.5	8.1	-12	1	3	9.7	11.5	-9	1	8	21.8	-21.5	5	1	14	6.7	-7.0
10	0	4	16.2	17.2	-3	0	16	40.4	-43.5	0	1	4	19.0	-17.8	-10	1	8	6.1	-4.9	-5	1	14	9.3	-7.1
-10	0	4	8.8	-10.0	-4	0	16	22.1	-22.2	1	1	4	41.1	36.4	-11	1	8	12.8	13.5	-6	1	14	5.4	-5.6
-11	0	4	9.3	8.4	-5	0	16	53.5	58.1	-1	1	4	30.9	28.7	-12	1	8	6.7	-7.5	-7	1	14	21.8	20.3
-12	0	4	6.5	6.9	-6	0	16	39.5	41.0	2	1	4	7.8	6.5	0	1	9	50.0	-45.7	-8	1	14	11.5	10.0
0	0	6	126.6	-125.7	-7	0	16	6.0	-3.7	-2	1	4	29.6	-30.0	1	1	9	26.4	24.1	-9	1	14	11.5	8.5
1	0	6	45.6	-39.0	-11	0	16	8.8	9.7	3	1	4	18.4	17.3	-1	1	9	84.4	-83.3	-10	1	14	13.9	14.1
-1	0	6	59.0	57.3	0	0	18	10.4	11.3	-3	1	4	38.4	37.3	2	1	9	38.8	37.8	-11	1	14	10.3	-9.6
2	0	6	66.1	-59.3	1	0	18	14.4	-13.3	4	1	4	65.8	66.2	-2	1	9	32.2	34.5	0	1	15	26.9	29.4
-2	0	6	104.1	144.4	-2	0	18	10.5	-11.7	-4	1	4	29.4	31.4	3	1	9	4.8	-5.4	-1	1	15	24.7	25.2
3	0	6	28.0	27.4	-5	0	18	14.5	13.8	5	1	4	21.0	-18.7	-3	1	9	83.8	85.0	2	1	15	27.3	-28.2
-3	0	6	58.5	61.3	-6	0	18	24.6	25.2	6	1	4	17.0	-16.6	4	1	9	39.9	-36.0	-2	1	15	31.7	-32.4
4	0	6	33.8	31.4	-7	0	18	5.6	5.8	-6	1	4	23.1	25.0	-4	1	9	36.2	34.2	3	1	15	13.9	-13.4
-4	0	6	10.7	-14.7	-8	0	18	16.2	15.0	7	1	4	6.7	-7.6	5	1	9	19.2	-18.0	-3	1	15	50.2	-49.6
5	0	6	26.9	-24.4	-9	0	18	15.3	14.8	-7	1	4	21.8	22.1	-5	1	9	29.1	-30.5	-4	1	15	12.6	10.7
-5	0	6	20.9	-20.8	-10	0	18	17.7	-17.1	8	1	4	22.5	-22.1	6	1	9	9.7	10.2	-5	1	15	70.0	70.4
6	0	6	55.3	-53.5	-1	0	20	15.2	16.9	-8	1	4	7.3	-6.9	-6	1	9	25.5	-27.9	-6	1	15	30.4	29.9
-6	0	6	11.1	11.6	-2	0	20	19.6	-20.5	9	1	4	4.3	-3.1	7	1	9	9.7	9.4	-7	1	15	38.9	-34.5
7	0	6	12.0	-10.9	-3	0	20	17.3	-18.0	-9	1	4	10.3	-8.8	-7	1	9	11.5	-10.8	-8	1	15	29.2	-27.2
-7	0	6	35.8	39.2	-4	0	20	7.7	-7.4	10	1	4	6.1	7.1	-8	1	9	12.2	11.4	-9	1	15	7.3	7.8
8	0	6	8.3	6.3	-5	0	20	9.1	-7.2	-10	1	4	13.9	-14.9	-9	1	9	22.5	19.8	-10	1	15	17.6	17.1
-8	0	6	7.8	-8.1	-6	0	20	21.8	18.8	-11	1	4	13.3	-13.9	-10	1	9	3.6	-0.7	0	1	16	16.8	17.7
9	0	6	23.7	21.4	-7	0	20	31.6	32.8	0	1	5	35.2	33.2	-11	1	9	18.2	-18.7	1	1	16	6.7	-6.4
-9	0	6	38.1	-54.0	1	1	0	36.5	-34.3	1	1	5	14.1	-14.1	-12	1	9	9.7	-11.0	-1	1	16	7.2	-7.5
-10	0	6	12.0	-11.7	2	1	0	179.3	192.8	-1	1	5	41.5	41.7	0	1	10	26.6	25.6	2	1	16	10.9	-10.3
-11	0	6	11.6	14.3	3	1	0	46.8	45.8	2	1	5	51.6	-51.1	1	1	10	5.4	-5.2	-2	1	16	14.4	-16.2
-12	0	6	7.4	6.1	4	1	0	8.9	9.6	-2	1	5	111.0	117.2	-1	1	10	64.5	-63.0	-3	1	16	19.8	-19.2
0	0	8	72.6	-71.6	5	1	0	44.5	45.7	3	1	5	9.0	-7.2	2	1	10	17.4	18.0	-5	1	16	3.6	3.3
1	0	8	23.0	17.4	6	1	0	17.6	-17.0	-3	1	5	8.6	7.7	-2	1	10	4.3	-3.8	-6	1	16	18.2	-18.0
-1	0	8	111.0	-106.1	7	1	0	34.7	-32.8	4	1	5	47.9	44.5	-3	1	10	24.8	23.5	-8	1	16	5.4	4.9
2	0	8	49.1	47.3	8	1	0	15.8	16.7	-4	1	5	26.5	-27.0	4	1	10	14.8	-13.7	-9	1	16	6.1	7.9
-2	0	8	106.9	124.2	10	1	0	4.8	-5.6	5	1	5	10.0	8.7	-4	1	10	4.6	-4.0	-10	1	16	20.7	20.6
3	0	8	15.9	16.6	11	1	0	3.6	-5.7	-5	1	5	36.0	-42.0	5	1	10	5.4	6.0	-11	1	16	9.1	9.5
-3	0	8	160.9	226.4	0	1	1	130.1	156.8	6	1	5	29.2	-29.2	-5	1	10	6.3	-4.7	1	1	17	15.8	-14.4
4	0	8	50.6	-51.4	1	1	1	28.8	-24.2	-6	1	5	7.3	7.1	6	1	10	12.8	-11.8	-1	1	17	9.0	10.7
-4	0	8	38.1	-37.6	-1	1	1	87.6	110.9	7	1	5	24.3	-26.1	-6	1	10	32.8	32.0	2	1	17	10.9	-10.1
5	0	8	54.2	-56.6	2	1	1	182.5	-188.8	-7	1	5	29.2	30.3	7	1	10	10.9	-10.9	-3	1	17	23.1	-23.2
-5	0	8	54.3	-53.8	-2	1	1	48.3	-51.0	-8	1	5	9.7	-8.3	-7	1	10	13.9	12.7	-4	1	17	11.9	-11.7
-6	0	8	27.9	-27.4	3	1	1	23.7	-21.8	9	1	5	16.4	16.9	-8	1	10	22.5	24.8	-5	1	17	21.7	21.1
7	0	8	12.5	13.3	-3	1	1	84.1	-93.3	-9	1	5	33.4	-33.2	-9	1	10	20.7	20.6	-6	1	17	19.4	18.7
-7	0	8	6.0	-5.7	4	1	1	56.8	58.7	10	1	5	6.1	7.0	-10	1	10	13.3	-11.5	-7	1	17	6.7	6.7
8	0	8	7.4	6.1	-4	1	1	17.2	-17.7	-10	1	5	5.4	-6.6	-11	1	10	9.1	-8.9	-9	1	17	3.0	-4.3
-8	0	8	34.4	35.1	5	1	1	47.1	49.8	-11	1	5	4.8	5.3	0	1	11	37.5	-37.8	-10	1	17	12.8	-11.6
-9	0	8	8.3	9.9	-5	1	1	37.2	40.6	0	1	6	46.6	44.4	1	1	11	11.7	-9.3	0	1	18	10.1	10.3
-10	0	8	42.3	-44.8	6	1	1	27.9	-26.7	1	1	6	29.2	27.0	-1	1	11	5.4	-5.9	1	1	18	5.4	-4.3
-11	0	8	10.7	-11.0	-6	1	1	34.7	34.6	-1	1	6	20.1	21.2	2	1	11	18.1	18.6	-1	1	18	9.0	-9.2
0	0	10	24.1	-23.2	7	1	1	51.1	-47.8	2	1	6	23.7	23.1	-2	1	11	7.6	7.2	-2	1	18	4.5	5.5
1	0	10	14.2	-13.5	-7	1	1	3.6	-4.9	-2	1	6	91.4	-87.7	-3	1	11	32.2	32.1	-3	1	18	12.5	-12.8
-1	0	10	19.6	-21.8	8	1	1	12.2	-12.1	3	1	6	27.5	28.3	4	1	11	32.2	-26.9	-4	1	18	22.0	-22.3

Table 4 (*cont.*)

H	K	L	FO	FC	H	K	L	FC	FC	H	K	L	FU	FC	H	K	L	FU	FC	H	K	L	FO	FC
-5	1	18	4.8	4.6	5	2	4	31.3	28.6	-9	2	9	10.8	-12.1	-7	2	16	13.2	-14.2	0	3	4	15.6	-15.4
-6	1	18	3.0	-2.2	-5	2	4	29.1	-30.1	-10	2	9	18.0	-19.5	-8	2	16	28.8	-30.7	1	3	4	36.0	-32.6
-7	1	18	4.3	-4.9	6	2	4	25.8	26.6	-12	2	9	2.4	3.1	-9	2	16	2.9	-2.8	-1	3	4	9.5	-9.6
-8	1	18	13.9	13.2	-6	2	4	21.6	24.6	0	2	10	43.6	-44.9	-10	2	16	13.2	13.1	2	3	4	35.0	33.5
-9	1	18	9.7	8.5	7	2	4	25.8	-25.3	1	2	10	42.1	39.0	2	2	17	6.0	-5.9	-2	3	4	2.7	0.6
-10	1	18	6.1	6.6	-7	2	4	36.0	32.8	-1	2	10	35.8	-35.9	-3	2	17	29.4	-29.3	3	3	4	17.9	17.5
0	1	19	8.1	9.5	8	2	4	12.0	-11.4	2	2	10	45.8	45.7	-4	2	17	14.2	-13.6	-3	3	4	40.4	-42.1
-1	1	19	3.9	4.7	-8	2	4	20.4	22.7	3	2	10	8.2	-8.1	-5	2	17	6.0	4.3	4	3	4	36.2	-30.0
-2	1	19	14.1	-13.7	9	2	4	14.4	16.0	-3	2	10	7.3	7.0	-7	2	17	6.0	-5.4	-4	3	4	12.3	10.8
-3	1	19	13.9	-15.1	-10	2	4	15.0	-16.0	-4	2	10	8.7	8.0	-9	2	17	5.4	6.4	-5	3	4	14.6	16.5
-5	1	19	8.1	8.1	0	2	5	35.0	-31.3	-5	2	10	7.2	1.8	-10	2	17	15.6	17.1	-6	3	4	14.4	-15.0
-6	1	19	11.5	11.0	1	2	5	2.9	-1.7	6	2	10	6.0	-5.9	0	2	18	5.4	4.2	7	3	4	21.3	-19.8
-7	1	19	4.3	4.1	-1	2	5	4.2	5.4	-6	2	10	25.2	-26.4	-1	2	18	15.8	17.0	-7	3	4	12.5	-11.6
-8	1	19	8.5	8.2	2	2	5	54.6	55.9	7	2	10	6.6	6.3	-3	2	18	19.5	-19.4	8	3	4	13.7	15.2
-2	1	20	8.6	-9.1	-2	2	5	42.2	-42.2	-7	2	10	35.4	-35.4	-4	2	18	4.4	5.4	-8	3	4	10.7	10.8
-4	1	20	15.1	-17.0	3	2	5	62.0	62.2	-8	2	10	10.2	8.9	-6	2	18	15.0	-13.8	9	3	4	5.6	7.7
-5	1	20	9.8	-8.2	-3	2	5	6.1	-6.9	-9	2	10	24.0	23.6	-9	2	18	9.6	-10.2	-9	3	4	3.7	-3.2
-7	1	20	17.0	-16.1	4	2	5	22.1	18.6	-10	2	10	15.0	16.4	-10	2	18	4.8	-6.1	-10	3	4	5.0	-6.6
-4	1	21	9.7	-10.2	-4	2	5	71.0	79.2	-11	2	10	4.2	5.7	-1	2	19	9.0	-9.1	-11	3	4	5.0	5.8
-5	1	21	12.2	-11.8	5	2	5	25.4	-23.6	-12	2	10	10.8	-11.3	-2	2	19	6.3	-6.8	0	3	5	60.4	-51.7
-6	1	21	6.1	5.7	-5	2	5	30.6	31.0	0	2	11	16.1	15.7	-3	2	19	7.8	-7.7	1	3	5	72.7	-62.3
0	2	0	4.9	5.1	6	2	5	12.0	-10.6	1	2	11	16.4	16.3	-4	2	19	14.6	-14.2	-1	3	5	5.5	4.6
1	2	0	50.4	47.3	-6	2	5	25.2	25.8	-1	2	11	39.1	-39.5	-5	2	19	6.0	-4.7	2	3	5	51.5	-48.8
2	2	0	112.6	-109.5	7	2	5	7.8	-8.6	2	2	11	11.2	12.8	-6	2	19	7.8	-6.5	-2	3	5	11.2	11.0
3	2	0	113.8	-119.0	-7	2	5	9.6	9.2	-2	2	11	37.8	-39.6	-7	2	19	12.6	-12.7	3	3	5	35.2	33.3
4	2	0	80.2	81.4	-8	2	5	3.6	4.1	3	2	11	10.8	-11.0	-8	2	19	8.4	7.9	-3	3	5	12.2	11.3
5	2	0	79.9	90.6	-11	2	5	14.4	-14.6	-3	2	11	17.3	17.8	-9	2	19	13.2	13.8	4	3	5	47.2	45.5
6	2	0	7.2	-6.1	0	2	6	47.3	-47.1	4	2	11	11.2	-11.6	-2	2	20	17.9	19.6	-4	3	5	70.0	-77.3
7	2	0	10.8	-9.2	1	2	6	59.6	-54.1	-4	2	11	13.9	-14.9	-3	2	20	4.8	-5.8	5	3	5	37.7	36.8
8	2	0	14.4	-13.4	-1	2	6	9.5	10.1	5	2	11	6.0	-7.3	-4	2	20	13.3	-12.9	-5	3	5	46.5	-48.7
9	2	0	3.6	-4.8	2	2	6	48.3	46.1	-5	2	11	7.5	6.1	-5	2	20	10.0	9.0	-6	3	5	22.6	24.2
10	2	0	12.0	12.7	-2	2	6	41.1	42.3	6	2	11	9.6	-9.2	-6	2	20	2.9	-3.6	7	3	5	16.9	-17.0
11	2	0	6.6	6.9	3	2	6	46.1	48.2	-6	2	11	21.0	18.9	-7	2	20	7.2	-7.5	-7	3	5	41.3	45.1
0	2	1	49.3	-50.4	-3	2	6	25.0	24.1	-7	2	11	18.0	17.5	1	3	0	32.8	-33.0	-8	3	5	21.9	21.3
1	2	1	19.7	-19.0	4	2	6	25.0	22.1	-9	2	11	14.4	15.0	2	3	0	141.5	-131.0	9	3	5	7.5	8.8
-1	2	1	13.1	-14.4	-4	2	6	82.7	-88.2	0	2	12	6.5	-5.8	3	3	0	24.5	21.3	-9	3	5	6.9	7.0
2	2	1	103.6	93.8	-5	2	6	89.7	-103.0	1	2	12	27.5	27.1	4	3	0	97.6	103.0	-11	3	5	4.4	5.2
-2	2	1	58.9	-58.0	6	2	6	21.6	-24.2	-1	2	12	49.5	-52.4	6	3	0	16.9	-17.3	-12	3	5	5.6	6.7
3	2	1	50.6	48.7	-6	2	6	49.8	51.0	2	2	12	7.6	8.3	7	3	0	16.3	-15.6	0	3	6	108.0	-100.9
-3	2	1	17.7	17.1	7	2	6	9.0	-10.0	-2	2	12	22.6	24.5	9	3	0	19.4	19.0	1	3	6	3.5	-2.9
4	2	1	34.1	30.6	-7	2	6	70.9	75.4	3	2	12	21.6	20.6	11	3	0	10.0	-11.6	-1	3	6	23.5	25.4
-4	2	1	35.2	37.6	8	2	6	16.2	17.0	-3	2	12	25.6	25.6	0	3	1	26.8	29.9	2	3	6	90.6	88.1
5	2	1	17.1	16.0	-8	2	6	5.4	5.0	4	2	12	13.8	-13.9	1	3	1	8.8	-8.6	-2	3	6	47.8	-46.9
-5	2	1	48.4	51.7	9	2	6	7.8	8.3	-4	2	12	31.6	-26.6	-1	3	1	30.1	-29.5	3	3	6	34.4	32.4
6	2	1	34.2	-33.2	-9	2	6	14.4	-14.4	5	2	12	14.4	-17.8	2	3	1	135.4	-119.8	-3	3	6	26.3	-25.3
7	2	1	13.8	-12.5	-10	2	6	9.6	-10.1	-5	2	12	18.0	16.9	-2	3	1	7.5	-11.3	4	3	6	21.4	-18.1
-7	2	1	34.9	-35.6	-12	2	6	8.4	9.8	6	2	12	14.4	14.7	3	3	1	60.2	-56.8	-4	3	6	26.8	-26.6
8	2	1	7.2	7.9	0	2	7	6.7	-5.0	-6	2	12	13.2	-13.0	-3	3	1	77.1	-77.5	5	3	6	29.2	-27.9
-8	2	1	10.2	-10.8	1	2	7	50.4	46.3	-7	2	12	40.8	-39.3	4	3	1	107.0	114.5	-5	3	6	24.2	24.3
-9	2	1	7.2	8.2	-1	2	7	42.4	41.5	-8	2	12	6.0	5.7	-4	3	1	10.7	7.3	6	3	6	16.3	-14.7
10	2	1	12.6	-14.6	2	2	7	43.2	42.8	-9	2	12	18.6	17.7	5	3	1	59.8	57.7	-6	3	6	9.4	10.1
11	2	1	3.6	-4.4	3	2	7	19.2	18.6	-10	2	12	11.4	11.4	-5	3	1	68.2	68.3	7	3	6	14.4	13.7
-11	2	1	7.2	-8.2	-3	2	7	33.9	-34.1	-12	2	12	2.9	-4.3	-6	3	1	18.8	20.9	-7	3	6	15.0	-16.2
0	2	2	78.6	76.9	4	2	7	34.7	-29.9	0	2	13	42.6	44.4	7	3	1	5.6	-5.4	8	3	6	5.6	6.5
1	2	2	33.4	-32.4	-4	2	7	3.3	-0.3	1	2	13	17.9	19.2	-7	3	1	5.6	1.9	-9	3	6	3.7	4.9
-1	2	2	67.1	67.4	5	2	7	19.1	-17.6	-1	2	13	28.1	-29.8	-9	3	1	6.2	-7.1	0	3	7	74.2	-69.9
2	2	2	131.1	-128.8	-5	2	7	34.9	37.9	2	2	13	22.8	-22.3	10	3	1	10.0	10.7	1	3	7	43.0	-37.7
-2	2	2	2.9	0.9	-6	2	7	34.9	34.3	3	2	13	16.2	-17.5	-10	3	1	3.1	4.0	-1	3	7	17.7	-18.1
3	2	2	16.4	-17.4	-7	2	7	39.6	41.6	-3	2	13	12.5	10.2	-11	3	1	8.1	7.7	2	3	7	47.4	47.3
-3	2	2	45.5	-48.4	8	2	7	9.0	-8.1	-4	2	13	4.4	-4.4	0	3	2	36.7	-37.9	-2	3	7	23.2	25.3
4	2	2	85.8	90.8	-8	2	7	3.6	-4.5	-5	2	13	31.3	-28.7	1	3	2	3.0	1.1	3	3	7	43.4	44.2
-4	2	2	73.8	-81.1	9	2	7	6.0	-6.7	-6	2	13	9.6	9.8	-1	3	2	60.5	61.9	-3	3	7	50.6	49.8
5	2	2	35.3	36.4	-9	2	7	28.2	-27.5	-7	2	13	33.0	31.3	2	3	2	47.0	44.0	-4	3	7	54.5	-58.6
-5	2	2	9.6	10.2	-10	2	7	6.0	-6.0	-8	2	13	17.4	16.9	3	3	2	7.8	9.6	5	3	7	8.9	7.6
6	2	2	20.4	-20.3	-11	2	7	2.9	4.6	-9	2	13	10.8	10.6	-3	3	2	54.9	-55.4	-5	3	7	95.5	-105.0
-6	2	2	39.0	41.0	-12	2	7	4.2	-6.1	-10	2	13	4.8	6.2	4	3	2	23.4	-20.2	6	3	7	3.7	-3.6
7	2	2	6.0	-6.9	0	2	8	123.8	-116.5	0	2	14	38.3	41.4	-4	3	2	21.8	22.4	-6	3	7	6.9	7.3
-7	2	2	16.2	18.9	1	2	8	4.8	-5.1	1	2	14	23.4	23.1	5	3	2	14.5	-14.3	7	3	7	3.1	3.1
-8	2	2	7.2	7.6	-1	2	8	57.6	-58.5	-1	2	14	19.1	20.7	-5	3	2	59.8	77.9	-7	3	7	61.4	67.5
-9	2	2	12.6	-14.1	2	2	8	94.8	89.1	-2	2	14	49.6	-54.6	6	3	2	8.1	7.0	8	3	7	5.0	5.2
10	2	2	9.6	8.6	-2	2	8	43.1	42.2	3	2	14	12.6	-13.5	-6	3	2	12.5	-10.5	-8	3	7	28.8	27.7
-10	2	2	6.6	-6.4	3	2	8	31.9	31.9	-3	2	14	39.1	-37.5	7	3	2	8.8	8.6	-9	3	7	8.8	9.2
-11	2	2	15.0	15.1	-3	2	8	37.0	39.6	4	2	14	10.2	-10.9	-7	3	2	18.8	-21.3	-12	3	7	3.7	3.7
0	2	3	40.9	-37.0	4	2	8	16.9	-14.8	-4	2	14	11.5	11.4	8	3	2	5.6	-5.3	1	3	8	59.6	57.4
1	2	3	135.2	134.8	-4	2	8	25.2	23.1	-5	2	14	26.9	24.2	-8	3	2	16.3	-16.6	-1	3	8	27.8	29.4
2	2	3	43.8	43.5	5	2	8	10.3	-9.7	-6	2	14	6.0	6.0	9	3	2	6.9	7.1	-2	3	8	6.0	7.5
-2	2	3	6.1	4.5	-5	2	8	60.6	-64.7	-7	2	14	48.1	-44.2	-9	3	2	10.0	-10.4	3	3	8	25.6	-28.1
3	2	3	42.1	39.9	-6	2	8	35.4	-34.4	-8	2	14	32.4	-30.8	-10	3	2	11.2	12.9	-3	3	8	6.7	6.6
-3	2	3	14.8	-12.1	7	2	8	4.2	5.8	-9	2	14	36.6	37.8	-11	3	2	8.8	8.9	4	3	8	10.4	-10.2
4	2	3	14.6	14.7	-7	2	8	52.8	54.9	-10	2	14	22.8	23.5	0	3	3	2.9	-2.0	-4	3	8	38.5	-41.5
-4	2	3	33.7	34.1	8	2	8	6.6	6.6	-11	2	14	6.6	-6.4	1	3	3	86.3	-72.7	5	3	8	9.1	9.2
5	2	3	9.1	6.8	-8	2	8	17.4	18.7	0	2	15	13.2	14.6	-1	3	3	63.9	-59.2	-5	3	8	65.4	-66.9
-5	2	3	31.2	33.0	-9	2	8	12.0	-12.3	1	2	15	9.6	-11.8	2	3	3	74.4	-66.5	6	3	8	14.4	14.7
6	2	3	13.8	-14.5	-10	2	8	3.6	5.2	-1	2	15	23.0	-25.2	-2	3	3	11.5	-11.9	-6	3	8	50.2	52.8
-6	2	3	37.8	38.6	-11	2	8	7.8	-8.7	2	2	15	15.0	-15.5	3	3	3	34.7	34.8	-7	3	8	59.6	64.5
-7	2	3	9.6	10.0	0	2	9	50.1	48.7	-2	2	15	19.5	-22.0	-3	3	3	7.5	-8.7	8	3	8	8.1	-8.5
8	2	3	15.6	-16.5	1	2	9	9.8	-7.5	-4	2	15	15.2	13.5	4	3	3	61.7	63.6	-9	3	8	15.0	-16.3
-8	2	3	8.4	-7.6	-1	2	9	45.1	-43.8	-6	2	15	12.6	-11.0	-4	3	3	38.6	-39.6	-10	3	8	16.9	-17.1
9	2	3	15.6	-7.1	2	2	9	9.4	10.0	-8	2	15	7.2	8.5	5	3	3	46.5	43.3	-12	3	8	12.5	15.3
-9	2	3	6.6	-7.3	-2	2	9	16.0	18.1	-9	2	15	24.6	24.5	-5	3	3	32.6	-33.7	0	3	9	62.1	-60.9
-10	2	3	8.4	-10.1	3	2	9	16.8	-17.4	-10	2	15	19.2	19.6	6	3	3	13.1	13.2	1	3	9	56.8	49.7
0	2	4	79.5	67.8	-3	2	9	16.2	14.9	-11	2	15	4.8	-5.6	-6	3	3	36.4	35.7	-1	3	9	16.8	-19.3
1	2	4	7.5	-8.2	4	2	9	7.3	-8.3	0	2	16	25.8	28.3	7	3	3	5.6	-5.9	2	3	9	58.7	59.1
-1	2	4	80.0	-73.4	-4	2	9	22.2	-20.6	1	2	16	7.8	-8.9	-7	3	3	28.2	30.8	-2	3	9	15.7	16.1
2	2	4	98.6	-89.9	-5	2	9	12.2	-11.2	-1	2	16	32.2	34.1	8	3	3	10.0	-10.7	3	3	9	5.0	5.5
-2	2	4	21.7	-18.9	-6	2	9	12.6	12.4	2	2	16	3.6	-4.7	-8	3	3	26.3	25.0	-3	3	9	5.7	-2.2
3	2	4	12.1	13.9	7	2	9	16.8	-15.7	-2	2	16	20.5	-21.5	9	3	3	12.5	12.6	4	3	9	9.0	-8.3
-3	2	4	32.5	28.3	-7	2	9	29.4	28.7	-3	2	16	38.8	-36.8	-9	3	3	6.9	-6.7	-4	3	9	17.5	-16.7
4	2	4	36.1	32.9	8	2	9	5.4	-5.6	-5	2	16	24.9	22.9	-10	3	3	3.7	-5.2	-5	3	9	40.4	-41.8
-4	2	4	51.3	-57.1	-8	2	9	34.9	33.3	-6	2	16	13.8	16.0	-11	3	3	5.0	7.1	6	3	9	5.6	5.6

Table 4 (*cont.*)

H	K	L	FC	FC	H	K	L	FC	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-6	3	9	47.6	-50.3	-8	3	16	18.8	-18.3	4	4	4	37.3	33.1	-6	4	9	31.5	-29.4	-3	4	16	25.2	-26.5
7	3	9	8.1	7.8	-9	3	16	21.3	21.0	-4	4	4	28.8	-29.4	7	4	9	10.5	9.8	-4	4	16	15.0	-14.5
-7	3	9	26.3	28.1	-10	3	16	15.0	15.6	5	4	4	33.6	32.2	-7	4	9	36.5	36.7	-5	4	16	15.9	13.6
-8	3	9	29.4	30.8	-11	3	16	3.7	-4.3	-5	4	4	14.3	-14.7	-9	4	9	14.2	-13.1	-7	4	16	27.2	-25.1
-9	3	9	10.7	9.8	0	3	17	13.2	15.0	6	4	4	27.2	-26.8	-10	4	9	11.1	-10.6	-8	4	16	13.6	-10.8
-10	3	9	11.9	12.1	-1	3	17	27.1	30.4	-6	4	4	19.8	20.3	-11	4	9	3.7	-3.3	-10	4	16	5.6	5.6
-12	3	9	7.5	-8.0	-3	3	17	22.6	-23.3	7	4	4	17.3	-16.1	-12	4	9	10.5	11.3	0	4	17	3.7	-4.8
0	3	10	10.5	11.9	-6	3	17	7.5	-7.7	-7	4	4	35.3	36.0	0	4	10	24.3	-26.3	1	4	17	5.6	4.6
-1	3	10	8.5	-7.0	-7	3	17	9.4	-9.4	8	4	4	6.8	7.4	1	4	10	9.1	7.7	-1	4	17	12.5	13.7
2	3	10	12.9	-12.8	-8	3	17	18.2	-18.8	-8	4	4	14.8	14.1	-1	4	10	28.8	-30.1	-3	4	17	5.6	6.0
-2	3	10	6.0	-3.8	-9	3	17	10.7	-10.8	-9	4	4	23.5	-21.9	2	4	10	27.6	28.9	-4	4	17	6.9	6.4
3	3	10	6.9	5.2	-10	3	17	10.0	10.6	-10	4	4	3.1	-3.1	-2	4	10	3.7	-3.6	-5	4	17	18.1	17.5
-3	3	10	31.1	29.8	-1	3	18	3.6	5.0	-11	4	4	7.4	7.9	3	4	10	13.9	14.5	-6	4	17	26.0	25.6
4	3	10	12.6	11.9	-2	3	18	4.4	-5.7	0	4	5	85.2	-82.4	-3	4	10	10.5	10.3	-7	4	17	16.1	-14.1
-4	3	10	19.7	18.6	-6	3	18	7.5	8.1	1	4	5	62.0	-54.1	4	4	10	14.5	-12.6	-8	4	17	37.1	-35.6
5	3	10	8.1	-8.3	-8	3	18	6.9	-7.9	-1	4	5	8.8	-7.7	-4	4	10	11.1	-7.9	-10	4	17	4.9	4.4
-5	3	10	16.7	-15.7	-1	3	19	18.3	20.3	2	4	5	28.1	28.8	5	4	10	13.1	-12.7	0	4	18	13.5	15.4
-6	3	10	18.8	-18.2	-2	3	19	8.8	9.0	-2	4	5	63.6	-61.7	-5	4	10	24.5	-21.9	-1	4	18	15.5	15.3
7	3	10	6.2	8.0	-3	3	19	6.2	-7.0	-3	4	5	20.2	-19.3	6	4	10	11.1	10.4	-3	4	18	8.0	-6.6
-7	3	10	19.4	19.2	-6	3	19	18.2	-17.2	4	4	5	19.3	-16.7	-6	4	10	6.8	-8.2	-4	4	18	11.3	-10.3
-8	3	10	14.4	16.0	-7	3	19	11.2	-11.4	-4	4	5	8.6	6.9	7	4	10	4.9	4.2	-7	4	18	10.5	-9.8
-9	3	10	15.0	-13.6	-9	3	19	10.7	-11.1	5	4	5	13.5	-11.6	-7	4	10	15.4	14.2	-8	4	18	8.6	-8.1
-12	3	10	3.7	-4.5	-2	3	20	8.1	-9.3	-5	4	5	20.9	22.1	-9	4	10	17.9	15.2	-9	4	18	4.3	0.8
1	3	11	41.4	40.0	-3	3	20	15.8	-16.7	6	4	5	10.5	-9.3	-10	4	10	12.9	13.3	-1	4	19	4.8	4.4
-1	3	11	37.2	-38.7	-4	3	20	14.3	13.0	-6	4	5	26.0	-27.1	-11	4	10	5.6	-6.6	-2	4	19	6.7	-6.3
2	3	11	39.0	39.1	-5	3	20	22.6	20.7	7	4	5	15.4	15.6	0	4	11	3.7	2.2	-4	4	19	23.3	21.0
3	3	11	12.0	12.5	-7	3	20	3.1	-4.0	-7	4	5	32.2	-31.0	1	4	11	12.2	-11.1	-5	4	19	19.4	16.1
-3	3	11	27.1	-24.9	0	4	0	141.0	133.0	8	4	5	22.2	22.1	-1	4	11	26.4	25.6	-8	4	19	12.4	-12.2
-4	3	11	40.4	-43.2	1	4	0	4.5	-4.2	-8	4	5	3.7	6.0	2	4	11	8.0	-6.8	-5	4	20	16.6	-15.5
5	3	11	13.4	-12.5	2	4	0	137.3	-128.4	9	4	5	4.9	4.2	-2	4	11	45.9	49.5	-7	4	20	9.3	9.2
-6	3	11	5.6	-4.3	3	4	0	19.6	-18.1	-11	4	5	14.2	13.4	3	4	11	17.7	17.8	1	5	0	69.8	-72.3
-7	3	11	25.0	-24.7	4	4	0	32.3	-25.5	-12	4	5	3.1	3.9	-3	4	11	6.1	3.3	2	5	0	35.8	-37.7
-9	3	11	19.4	19.4	5	4	0	42.4	41.5	0	4	6	62.4	-59.1	4	4	11	6.4	-6.0	3	5	0	22.1	-15.1
-10	3	11	9.4	10.5	6	4	0	27.2	27.5	1	4	6	17.3	-15.7	-4	4	11	5.6	-2.5	4	5	0	16.7	18.0
-11	3	11	6.2	7.9	7	4	0	13.6	-12.7	-1	4	6	27.6	-27.3	5	4	11	3.1	-3.5	5	5	0	23.2	21.5
-12	3	11	5.0	-4.5	8	4	0	3.7	5.2	2	4	6	17.1	16.8	-5	4	11	36.0	-33.3	6	5	0	50.9	-55.1
0	3	12	37.8	40.9	9	4	0	10.5	10.8	-2	4	6	54.5	55.7	6	4	11	14.8	14.0	7	5	0	29.4	-29.3
1	3	12	5.5	-6.5	10	4	0	3.1	3.7	3	4	6	20.4	19.7	-6	4	11	35.3	-33.7	8	5	0	11.7	12.9
-1	3	12	8.5	-9.1	0	4	1	35.6	-37.0	-3	4	6	12.2	10.4	-7	4	11	9.3	7.8	9	5	0	26.7	25.7
2	3	12	6.9	-7.3	1	4	1	69.8	-65.0	4	4	6	50.7	47.2	-8	4	11	3.7	4.1	10	5	0	9.1	9.9
-2	3	12	40.5	43.7	-1	4	1	9.7	10.1	-4	4	6	27.6	-30.7	-9	4	11	18.6	-16.8	0	5	1	73.2	75.7
3	3	12	3.7	-3.8	2	4	1	57.2	-55.4	5	4	6	3.7	2.9	-11	4	11	2.4	0.8	-1	5	1	34.0	33.0
4	3	12	22.9	-22.3	-2	4	1	130.3	-130.0	-5	4	6	35.3	-34.8	1	4	12	20.9	19.6	2	5	1	20.9	-24.1
5	3	12	4.4	5.5	3	4	1	34.2	32.6	6	4	6	3.7	-1.5	2	4	12	28.2	30.0	-2	5	1	44.9	-43.8
-5	3	12	5.1	-4.1	-3	4	1	90.3	-93.6	-6	4	6	11.1	-10.2	-2	4	12	35.3	-34.7	3	5	1	11.2	10.0
6	3	12	11.2	11.9	4	4	1	15.2	15.0	-7	4	6	27.2	28.8	3	4	12	3.7	-4.4	-3	5	1	8.8	7.1
-6	3	12	9.4	-10.5	-4	4	1	67.0	69.3	-8	4	6	12.9	10.8	-3	4	12	22.2	-20.4	4	5	1	5.4	-3.1
-7	3	12	20.0	20.8	5	4	1	44.3	-42.7	-9	4	6	4.9	-5.3	4	4	12	17.4	-16.1	-4	5	1	9.7	9.0
-9	3	12	16.3	-15.1	-5	4	1	49.7	47.5	-10	4	6	7.4	-6.6	-4	4	12	21.9	22.1	5	5	1	15.8	15.2
-11	3	12	5.0	5.7	6	4	1	12.4	-11.8	-11	4	6	6.8	5.1	-5	4	12	5.8	3.9	-5	5	1	10.4	-1.6
0	3	13	27.3	30.7	-6	4	1	32.2	-30.2	-12	4	6	2.4	3.0	-7	4	12	17.9	-17.7	6	5	1	15.6	14.9
1	3	13	34.4	35.1	-7	4	1	34.7	-34.9	0	4	7	77.2	-75.2	-8	4	12	14.2	-12.5	-6	5	1	5.8	-5.4
-1	3	13	17.4	-19.4	8	4	1	8.0	8.5	1	4	7	27.3	26.9	-9	4	12	16.1	15.2	7	5	1	30.0	-31.2
2	3	13	19.0	21.6	-8	4	1	6.1	-5.5	-1	4	7	58.1	59.5	-10	4	12	21.6	20.6	-7	5	1	6.5	-7.4
-2	3	13	35.4	-38.4	9	4	1	20.4	19.4	2	4	7	58.0	54.2	-12	4	12	2.4	-6.0	8	5	1	8.4	-8.2
-3	3	13	25.3	-26.0	-9	4	1	19.8	19.2	-2	4	7	11.8	14.1	0	4	13	21.6	23.3	-8	5	1	17.6	-18.9
4	3	13	11.9	-13.5	10	4	1	2.4	4.0	3	4	7	26.4	-25.5	1	4	13	9.4	-8.6	9	5	1	5.8	5.9
5	3	13	4.4	-4.7	-10	4	1	22.9	23.4	-3	4	7	18.5	-17.7	-1	4	13	7.3	-7.6	-10	5	1	4.5	3.9
-5	3	13	7.7	6.5	0	4	2	9.3	9.9	4	4	7	53.3	-45.9	2	4	13	8.7	-8.9	0	5	2	92.5	-94.5
-6	3	13	10.0	-8.2	1	4	2	7.8	-10.1	-4	4	7	61.5	-66.1	-2	4	13	60.6	59.9	1	5	2	23.0	-24.5
-7	3	13	43.2	-42.9	-1	4	2	5.4	6.6	5	4	7	7.7	-8.1	3	4	13	5.6	-6.6	-1	5	2	22.4	23.5
-8	3	13	11.9	-13.7	2	4	2	39.8	-38.9	-5	4	7	21.2	-20.7	-3	4	13	44.2	43.2	2	5	2	6.5	6.2
-9	3	13	24.5	22.5	-2	4	2	53.6	-51.3	6	4	7	26.0	22.8	4	4	13	6.1	7.2	-2	5	2	109.5	-110.1
-10	3	13	20.7	19.9	3	4	2	42.2	-36.3	-6	4	7	23.5	23.3	-4	4	13	23.9	-23.0	3	5	2	17.1	16.3
0	3	14	21.8	23.3	-3	4	2	66.8	-61.1	7	4	7	30.9	31.8	5	4	13	19.8	20.5	-3	5	2	96.7	-96.4
1	3	14	8.5	-10.4	4	4	2	38.7	36.1	-7	4	7	3.7	-4.9	-5	4	13	35.1	-31.9	4	5	2	25.7	-23.7
-1	3	14	28.7	-31.8	-4	4	2	32.3	28.0	8	4	7	4.3	4.5	-6	4	13	9.3	-7.0	-4	5	2	7.1	8.0
2	3	14	18.2	-19.1	5	4	2	26.1	24.2	-8	4	7	26.0	-24.8	-7	4	13	3.7	5.4	5	5	2	13.4	-12.3
-2	3	14	16.5	18.6	-5	4	2	18.6	17.0	-9	4	7	9.3	-10.4	-9	4	13	19.2	-17.1	-5	5	2	26.0	24.5
3	3	14	4.4	-6.0	-6	4	2	23.5	23.6	-10	4	7	3.1	0.3	-10	4	13	14.2	-13.5	6	5	2	8.4	-0.9
-3	3	14	50.6	52.1	7	4	2	18.6	-16.2	-11	4	7	17.9	17.3	0	4	14	11.5	12.6	-6	5	2	13.7	12.2
4	3	14	11.2	11.9	-7	4	2	42.1	41.4	-12	4	7	12.9	14.8	1	4	14	17.3	17.9	-7	5	2	33.3	-36.7
-4	3	14	5.8	-6.6	-8	4	2	8.0	-8.7	0	4	8	28.3	-29.4	-1	4	14	5.8	5.6	8	5	2	11.7	12.8
-5	3	14	29.8	-30.1	9	4	2	12.4	12.2	1	4	8	5.1	5.7	2	4	14	3.1	4.1	-8	5	2	15.0	-13.8
-6	3	14	16.9	-15.8	0	4	3	33.2	-30.1	-1	4	8	59.1	-58.5	-2	4	14	13.7	-14.1	9	5	2	6.5	6.7
-7	3	14	13.1	-13.2	1	4	3	77.8	-66.5	2	4	8	25.5	26.9	-3	4	14	17.2	-16.0	-9	5	2	20.2	21.2
-8	3	14	17.5	16.9	-1	4	3	26.7	27.8	-2	4	8	27.6	28.2	-4	4	14	8.1	6.2	-10	5	2	17.6	17.0
-9	3	14	10.0	11.5	2	4	3	7.5	7.5	3	4	8	32.4	32.2	-5	4	14	36.7	34.2	-11	5	2	6.5	6.6
-10	3	14	5.0	-5.9	-2	4	3	36.8	-38.6	-3	4	8	46.6	44.9	-6	4	14	16.1	-15.0	0	5	3	25.2	24.9
0	3	15	31.6	38.0	3	4	3	18.1	-14.4	4	4	8	9.5	-7.9	-7	4	14	31.5	-31.4	1	5	3	35.3	-32.0
-1	3	15	16.8	17.8	-3	4	3	79.9	-77.9	-4	4	8	51.7	-54.4	-8	4	14	14.8	-13.7	-1	5	3	86.0	84.3
2	3	15	5.6	5.4	4	4	3	38.9	-34.8	5	4	8	6.4	-6.1	-10	4	14	14.2	13.0	2	5	3	17.3	-17.3
-2	3	15	28.5	-31.4	-4	4	3	19.9	-17.8	-5	4	8	62.7	-62.6	-11	4	14	4.9	5.8	3	5	3	40.7	-39.3
-3	3	15	37.1	-37.8	5	4	3	11.4	8.9	6	4	8	7.4	8.5	0	4	15	10.2	-11.3	-3	5	3	36.0	-32.7
-5	3	15	24.4	21.3	-5	4	3	32.2	28.9	7	4	8	11.1	10.8	1	4	15	24.1	-25.3	4	5	3	17.0	14.4
-6	3	15	9.4	10.4	6	4	3	24.7	22.1	-8	4	8	30.9	34.7	-1	4	15	22.5	-22.9	-4	5	3	3.7	3.5
-7	3	15	41.3	-39.7	-6	4	3	14.8	-14.9	-9	4	8	10.5	9.9	2	4	15	4.3	-4.5	5	5	3	41.4	42.8
-8	3	15	32.0	-30.7	7	4	3	12.9	-11.9	-10	4	8	6.8	-7.1	3	4	15	11.1	10.7	-5	5	3	23.3	-21.7
-9	3	15	13.7	14.5	-7	4	3	11.7	-10.6	-12	4	8	3.7	3.2	-3	4	15	29.8	30.3	6	5	3	24.8	-26.2
-10	3	15	18.2	17.8	8	4	3	8.0	8.6	0	4	9	7.6	6.9	-4	4	15	18.4	18.5	7	5	3	16.3	-18.1
-11	3	15	8.1	8.6	9	4	3	11.7	11.7	1	4	9	25.8	24.1	-5	4	15	16.2	14.4	8	5	3	7.8	8.3
0	3	16	14.1	-17.4	-10	4	3	11.1	10.9	-1	4	9	26.4	27.4	-6	4	15	12.9	-12.0	-8	5	3	17.6	-20.1
1	3	16	3.1	-4.9	-11	4	3	13.6	13.2	2	4	9	26.2	-26.8	-7	4	15	34.0	-32.4	-9	5	3	10.4	-10.6
-1	3	16	8.6	-10.7	0	4	4	21.8	-24.5	-2	4	9	32.6	35.7	-8	4	15	3.1	-4.6	-11	5	3	4.5	5.2
2	3	16	5.6	6.8	1	4	4	28.8	-25.5	3	4	9	13.6	-11.6	-9	4	15	12.9	10.7	0	5	4	76.1	-77.1
-2	3	16	14.8	-18.1	-1	4	4	29.4	29.6	-3	4	9	57.6	58.2	-11	4	15	9.9	-11.1	1	5	4	22.1	-20.3
-3	3	16	7.7	-8.8	2	4	4	6.3	4.2	4	4	9	5.7	4.4	0	4	16	16.2	18.1	-1	5	4	5.8	5.3
-5	3	16	21.1	19.1	-2	4	4	6.4	3.1	-4	4	9	5.8	0.2	1	4	16	9.3	8.7	2	5	4	6.1	-6.2
-6	3	16	13.1	13.0	3	4	4	18.5	16.1	-5	4	9	91.0	-101.6	-1	4	16	12.4	13.2	-2	5	4	62.8	-60.9
-7	3	16	22.6	-22.6	-3	4	4	5.4	-5.8	6	4	9	9.3	9.2	2	4	16	8.0	-6.9	3	5	4	8.5	-6.8

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
-3	5	4	32.6	-32.6	0	5	10	6.5	5.6	0	6	0	33.3	34.5	-1	6	6	3.8	4.4	-2	6	12	9.0	10.8
4	5	4	14.0	13.4	1	5	10	16.1	-18.2	1	6	0	23.1	23.6	2	6	6	25.6	27.0	3	6	12	14.1	-15.1
-4	5	4	2.6	3.9	2	5	10	7.9	-8.8	2	6	0	12.4	12.1	-2	6	6	11.8	15.1	-3	6	12	13.1	12.8
-5	5	4	6.1	-5.5	-2	5	10	32.9	33.0	3	6	0	8.3	-8.9	3	6	6	5.8	-4.8	-4	6	12	24.1	23.6
6	5	4	10.4	-10.3	3	5	10	3.9	3.8	4	6	0	4.9	4.5	-3	6	6	42.6	41.7	-5	6	12	34.5	34.1
-6	5	4	18.2	-18.0	-3	5	10	48.7	47.0	5	6	0	18.9	-16.8	4	6	6	37.5	-37.4	-7	6	12	16.0	-17.3
7	5	4	10.4	10.9	-4	5	10	12.5	-11.0	6	6	0	12.2	-10.4	-4	6	6	22.7	22.2	0	6	13	28.7	30.7
-7	5	4	5.2	1.1	5	5	10	3.2	3.4	7	6	0	9.6	-9.6	5	6	6	25.0	-23.9	1	6	13	3.2	3.8
8	5	4	6.5	5.5	-5	5	10	65.5	-66.8	8	6	0	5.8	-6.7	-5	6	6	16.7	-14.6	-1	6	13	9.0	-9.8
9	5	4	9.7	10.0	6	5	10	5.8	5.0	9	6	0	5.1	-5.6	6	6	6	9.0	-8.9	2	6	13	27.8	-31.8
-10	5	4	4.5	5.5	-6	5	10	32.6	-32.2	0	6	1	75.2	-74.6	-6	6	6	14.7	-14.9	-2	6	13	15.1	18.4
-11	5	4	5.8	5.5	-7	5	10	13.7	13.3	1	6	1	53.1	-50.9	7	6	6	6.4	5.3	3	6	13	14.7	-13.8
0	5	5	39.3	-37.3	-8	5	10	10.4	9.9	-1	6	1	46.3	-47.5	-7	6	6	8.3	8.4	-3	6	13	42.1	41.0
1	5	5	7.5	6.4	-10	5	10	16.9	-16.3	2	6	1	9.9	11.7	-8	6	6	5.1	-3.1	4	6	13	12.2	10.8
-1	5	5	4.1	3.9	-11	5	10	5.8	-4.1	-2	6	1	58.4	-60.1	-9	6	6	17.3	-17.5	-5	6	13	45.4	-43.7
2	5	5	3.9	-4.1	0	5	11	7.5	-8.2	3	6	1	10.5	9.7	-10	6	6	12.2	-11.6	-6	6	13	11.5	-10.8
-2	5	5	65.9	64.1	1	5	11	7.5	-7.9	-3	6	1	14.6	-13.7	-11	6	6	5.1	-4.4	-7	6	13	24.3	20.6
3	5	5	3.2	-4.4	2	5	11	22.3	25.1	4	6	1	14.1	13.0	0	6	7	9.5	-10.3	1	6	14	17.3	-18.4
-3	5	5	13.9	10.8	-2	5	11	15.8	-16.4	-4	6	1	44.1	45.2	1	6	7	27.4	26.4	-1	6	14	10.2	11.0
4	5	5	9.5	10.7	3	5	11	6.5	-5.5	5	6	1	30.3	27.9	-1	6	7	51.7	53.8	2	6	14	15.2	-15.1
-4	5	5	22.0	-20.5	-3	5	11	29.3	29.4	-5	6	1	50.4	50.7	2	6	7	42.0	44.1	-2	6	14	5.8	5.3
5	5	5	22.8	-21.4	4	5	11	26.2	-25.2	6	6	1	27.5	-25.9	-2	6	7	5.8	6.3	3	6	14	9.6	-7.9
-5	5	5	17.4	-16.3	-4	5	11	39.6	42.2	7	6	1	14.7	-13.3	3	6	7	12.2	10.3	-3	6	14	6.4	-5.9
6	5	5	11.7	-12.3	-5	5	11	14.7	-13.7	-7	6	1	41.0	-45.2	-3	6	7	47.7	-45.8	-4	6	14	6.4	7.6
-6	5	5	22.8	-23.6	6	5	11	8.4	8.3	8	6	1	25.6	23.1	4	6	7	35.6	-34.8	-5	6	14	8.4	7.2
-7	5	5	28.7	31.8	-6	5	11	12.4	-10.8	-8	6	1	7.7	-8.0	-4	6	7	18.5	-17.3	-6	6	14	24.3	23.0
8	5	5	5.8	6.5	-7	5	11	6.5	-6.1	9	6	1	5.1	4.4	5	6	7	23.6	-23.9	-7	6	14	12.8	10.7
-8	5	5	13.7	15.0	-8	5	11	13.7	-13.2	-9	6	1	23.7	23.4	6	6	7	23.7	21.9	-8	6	14	6.4	-6.4
-9	5	5	24.1	-25.0	-9	5	11	11.7	11.8	0	6	2	77.6	78.9	-6	6	7	7.7	8.0	0	6	15	12.8	11.9
-10	5	5	5.8	-5.4	-10	5	11	5.8	5.4	1	6	2	27.5	26.6	7	6	7	9.6	7.8	1	6	15	14.7	-13.2
0	5	6	81.6	-82.5	-11	5	11	12.4	-12.7	-1	6	2	53.1	51.1	-7	6	7	26.9	26.2	-1	6	15	11.8	-13.3
1	5	6	13.7	-12.2	1	5	12	10.9	11.3	2	6	2	12.4	-13.2	-8	6	7	4.4	4.4	2	6	15	17.9	-16.4
-1	5	6	57.5	56.7	-1	5	12	15.6	17.1	-2	6	2	7.7	-6.2	-9	6	7	32.0	-31.4	-2	6	15	5.8	-5.1
2	5	6	29.8	29.3	-2	5	12	38.3	39.7	3	6	2	50.3	-44.9	-11	6	7	13.4	13.7	-3	6	15	5.8	6.1
-2	5	6	35.3	-35.7	3	5	12	11.7	-11.9	-3	6	2	22.9	-21.7	0	6	8	20.7	-22.6	-4	6	15	24.1	22.6
3	5	6	15.6	14.3	-3	5	12	42.8	44.0	4	6	2	12.9	-11.7	1	6	8	9.9	-9.6	-5	6	15	3.2	-4.1
-3	5	6	69.7	-71.4	4	5	12	9.4	9.0	-4	6	2	3.6	2.9	-1	6	8	6.8	7.0	-6	6	15	19.2	-15.2
4	5	6	48.9	-43.7	-4	5	12	35.3	-36.2	5	6	2	20.1	17.5	2	6	8	7.0	-6.0	-7	6	15	12.2	-10.0
-4	5	6	6.6	4.7	5	5	12	11.1	10.5	-5	6	2	10.5	9.7	-2	6	8	29.2	29.4	-8	6	15	5.8	-5.7
5	5	6	30.1	-29.9	-5	5	12	38.7	-39.8	6	6	2	16.6	-16.5	3	6	8	5.1	2.8	-9	6	15	11.5	10.7
-5	5	6	11.6	10.9	-6	5	12	6.5	6.9	-6	6	2	5.8	-5.8	-3	6	8	25.8	25.0	-10	6	15	13.4	15.0
6	5	6	18.2	22.9	-7	5	12	9.7	8.9	7	6	2	16.6	-17.3	4	6	8	8.4	-6.5	1	6	16	8.3	-7.0
-6	5	6	4.5	4.6	-8	5	12	9.7	-10.6	-7	6	2	24.3	-26.3	-4	6	8	19.2	17.1	-1	6	16	5.0	-6.4
-7	5	6	15.0	-15.4	-9	5	12	13.0	-12.6	8	6	2	5.8	-6.4	5	6	8	11.5	-10.8	-2	6	16	13.8	-14.9
7	5	6	31.3	30.6	-10	5	12	3.9	-4.5	-8	6	2	12.2	-12.7	-5	6	8	25.8	23.4	-4	6	16	17.9	16.6
8	5	6	14.3	14.2	0	5	13	9.9	-11.5	0	6	3	69.1	-70.8	6	6	8	12.8	-10.2	-5	6	16	19.9	19.0
-8	5	6	14.3	-14.3	-1	5	13	10.7	10.9	1	6	3	19.4	20.9	-6	6	8	5.8	4.3	-6	6	16	7.0	7.8
-9	5	6	11.1	-11.8	2	5	13	7.1	-6.7	-1	6	3	32.6	29.7	7	6	8	6.4	-5.4	-8	6	16	10.9	8.2
-10	5	6	5.8	6.6	-2	5	13	6.2	-5.6	2	6	3	26.1	25.5	-8	6	8	21.8	-20.0	-9	6	16	3.2	3.7
-11	5	6	15.0	15.4	3	5	13	13.7	-13.2	-2	6	3	63.5	-63.5	-9	6	8	21.1	-20.1	-1	6	17	2.4	1.6
0	5	7	21.5	-21.9	-3	5	13	24.5	-23.8	3	6	3	28.1	-25.8	-10	6	8	5.1	-5.8	-3	6	17	19.6	-18.2
1	5	7	5.2	4.8	-4	5	13	14.5	12.7	-3	6	3	13.2	-13.0	-11	6	8	3.2	2.8	-4	6	17	6.1	-5.9
-1	5	7	16.8	-19.3	5	5	13	7.1	8.4	4	6	3	8.3	7.6	0	6	9	20.5	21.0	-5	6	17	28.6	26.7
2	5	7	4.5	3.5	-5	5	13	29.7	29.6	-4	6	3	16.7	14.1	1	6	9	4.6	-5.8	-6	6	17	2.6	4.4
-2	5	7	62.1	60.2	-8	5	13	7.8	-7.5	5	6	3	18.1	-17.2	-1	6	9	18.5	-18.6	-7	6	17	16.0	-13.5
3	5	7	7.1	-6.3	-9	5	13	3.9	-3.8	-5	6	3	27.8	27.2	2	6	9	9.6	10.0	-8	6	17	7.0	-7.0
-3	5	7	33.1	32.1	-10	5	13	13.7	13.0	6	6	3	10.9	-10.3	-2	6	9	50.9	53.1	-3	6	18	13.2	-11.7
4	5	7	7.5	-8.3	0	5	14	12.8	14.4	-6	6	3	16.6	17.6	3	6	9	5.1	-4.8	-4	6	18	6.8	-6.5
-4	5	7	8.4	-9.2	1	5	14	17.7	-19.2	7	6	3	9.0	9.2	-3	6	9	31.5	29.9	-5	6	18	11.6	10.0
5	5	7	20.4	-20.1	-1	5	14	19.4	-22.2	-7	6	3	21.1	-23.7	4	6	9	18.3	-17.7	-6	6	18	21.1	19.3
-5	5	7	6.3	-8.3	2	5	14	23.9	-25.1	-8	6	3	18.6	-18.3	-4	6	9	37.2	-40.6	-7	6	18	14.1	12.3
6	5	7	7.1	-7.0	-2	5	14	16.3	18.6	-10	6	3	4.4	3.7	5	6	9	16.0	15.4	-5	6	19	17.5	18.8
7	5	7	5.8	5.7	3	5	14	5.8	6.2	-11	6	3	3.8	4.3	-5	6	9	29.4	-27.8	1	7	0	21.9	-23.6
-8	5	7	12.4	11.7	-3	5	14	37.9	39.7	0	6	4	27.9	27.6	6	6	9	10.9	8.5	2	7	0	20.2	-22.2
-9	5	7	8.4	-8.4	4	5	14	20.2	21.8	1	6	4	4.6	4.0	-6	6	9	6.4	-4.3	3	7	0	25.2	22.8
-10	5	7	15.0	-16.0	-4	5	14	23.7	24.6	-1	6	4	27.8	27.0	-7	6	9	31.4	33.3	4	7	0	44.6	43.6
-11	5	7	7.1	6.4	-5	5	14	14.6	-13.0	2	6	4	25.2	-25.6	-8	6	9	27.5	27.7	5	7	0	26.9	22.8
0	5	8	7.2	-6.4	-6	5	14	21.5	-22.3	-2	6	4	46.3	44.8	-9	6	9	17.3	-16.9	1	7	1	66.4	56.6
1	5	8	8.4	7.6	-10	5	14	5.2	-4.8	3	6	4	5.9	6.3	-10	6	9	26.9	-24.3	-1	7	1	13.0	-13.0
-1	5	8	46.6	46.3	-11	5	14	2.6	-12.6	-3	6	4	13.0	13.4	-11	6	9	9.0	8.5	-2	7	1	12.6	14.2
2	5	8	20.5	22.4	2	5	15	14.3	-13.0	4	6	4	5.5	-3.4	0	6	10	27.5	-29.6	3	7	1	39.2	-35.8
-2	5	8	67.6	67.6	3	5	15	9.1	-8.2	-4	6	4	22.7	-21.3	1	6	10	14.8	-15.8	-3	7	1	7.3	-4.7
3	5	8	26.4	-27.3	-3	5	15	18.6	-17.9	5	6	4	28.1	-26.7	-1	6	10	12.4	-12.6	4	7	1	9.7	-7.7
-3	5	8	17.3	14.1	-5	5	15	28.4	28.5	-5	6	4	12.3	-10.1	2	6	10	14.4	15.2	-4	7	1	12.0	11.0
4	5	8	33.5	-31.7	0	5	16	5.2	-5.1	6	6	4	16.6	-16.0	-2	6	10	14.2	17.4	5	7	1	7.7	-5.5
-4	5	8	54.3	-56.3	1	5	16	13.0	-11.5	-6	6	4	13.4	13.4	3	6	10	5.1	-4.7	-5	7	1	16.9	15.9
5	5	8	3.8	0.6	-4	5	16	25.3	26.2	7	6	4	6.4	-7.2	-3	6	10	56.0	56.1	0	7	2	47.0	-46.9
-5	5	8	43.8	-44.4	-5	5	16	29.0	26.4	-8	6	4	13.4	-13.4	4	6	10	16.7	-15.9	1	7	2	20.1	18.2
6	5	8	26.1	25.8	-7	5	16	32.0	-29.7	9	6	4	9.6	9.7	-4	6	10	34.3	31.7	-1	7	2	10.1	12.2
-6	5	8	19.6	-18.9	-8	5	16	26.1	-23.1	-9	6	4	16.0	-18.2	5	6	10	10.5	-10.6	2	7	2	60.0	54.4
7	5	8	12.4	12.1	-9	5	16	2.6	-1.2	-10	6	4	11.5	-10.7	-5	6	10	7.7	-7.7	-2	7	2	35.3	-37.8
-7	5	8	18.9	19.7	-10	5	16	9.1	10.0	0	6	5	60.6	-58.9	-6	6	10	7.7	-7.2	3	7	2	18.8	17.5
-9	5	8	30.0	-32.9	0	5	17	9.3	9.6	1	6	5	9.2	-9.4	-7	6	10	7.0	-5.2	-3	7	2	20.8	-18.4
-10	5	8	11.7	-9.4	-2	5	17	9.4	-9.8	-1	6	5	35.4	36.1	-10	6	10	12.2	-10.8	4	7	2	26.8	24.3
-11	5	8	14.3	15.1	-3	5	17	9.7	-9.3	2	6	5	26.6	27.8	-11	6	10	7.0	-6.2	-4	7	2	37.0	37.0
0	5	9	9.0	-8.5	-5	5	17	23.4	24.0	-2	6	5	63.5	-62.7	1	6	11	7.1	7.6	5	7	2	8.6	-6.5
1	5	9	11.2	-9.5	-6	5	17	20.9	19.1	3	6	5	44.1	43.0	-1	6	11	18.6	-20.5	-5	7	2	52.1	50.3
-1	5	9	24.7	-26.2	-7	5	17	10.4	-8.9	-3	6	5	50.5	-49.2	2	6	11	5.1	4.9	0	7	3	35.0	35.6
2	5	9	5.2	4.1	-9	5	17	4.5	4.6	4	6	5	20.1	-19.8	-2	6	11	15.4	15.5	1	7	3	6.5	7.0
-2	5	9	22.7	24.3	-2	5	18	10.4	10.0	-4	6	5	35.8	36.8	3	6	11	16.0	-17.0	-1	7	3	13.6	13.7
3	5	9	23.9	23.9	-4	5	18	3.8	4.1	5	6	5	33.6	-35.0	-3	6	11	49.2	48.5	2	7	3	32.2	-32.6
-3	5	9	60.7	60.4	-5	5	18	22.7	19.9	-5	6	5	7.8	5.7	-4	6	11	12.2	-11.1	-2	7	3	9.2	10.9
4	5	9	14.6	-13.6	-6	5	18	14.3	13.1	6	6	5	7.7	-7.1	5	6	11	3.2	3.2	3	7	3	12.2	10.1
-4	5	9	10.2	-9.7	-7	5	18	13.7	-13.0	-6	6	5	17.9	-17.0	-5	6	11	31.7	-31.2	4	7	3	14.8	12.6
5	5	9	21.5	-19.7	-8	5	18	18.9	-18.3	7	6	5	11.5	10.2	-6	6	11	15.4	13.8	-4	7	3	22.0	-19.7
-5	5	9	19.0	-15.5	-3	5	19	4.5	3.5	8	6	5	7.0	6.4	-10	6	11	8.3	-7.1	5	7	3	16.9	-14.4
-6	5	9	18.9	17.3	-4	5	19	8.2	-6.8	-8	6	5	15.4	-15.6	-11	6	11	3.8	-3.0	-5	7	3	28.4	26.8
-8	5	9	5.2	-4.3	-5	5	19	8.9	-7.1	-10	6	5	5.8	5.4	1	6	12	6.1	-6.7	0	7	4	30.6	-32.8
-10	5	9	10.4	-8.7	-6	5	19	15.0	14.4	0	6	6	13.5	-14.8	-1	6	12	11.2	-12.7	-1	7	4	32.6	32.2
-11	5	9	7.8	-7.9	-7	5	19	11.7	11.2	1	6	6	15.7	16.6	2	6	12	20.1	-21.8	2	7	4	64.8	60.1

Table 4 (*cont.*)

H	K	L	FC	FC	H	K	L	FC	FC	H	K	L	FO	FC	H	K	L	FO	FC	H	K	L	FO	FC
-2	7	4	35.1	-37.8	-3	7	17	15.0	-13.8	2	8	11	9.2	-10.9	1	9	8	13.0	13.9	4	10	7	11.4	-9.6
3	7	4	55.9	48.8	-4	7	17	9.7	10.0	-2	8	11	13.5	17.7	2	9	8	13.0	16.6	-4	10	7	8.3	-7.8
-3	7	4	29.0	-27.4	-5	7	17	10.7	9.7	-3	8	11	12.4	12.5	-3	9	8	7.1	7.3	5	10	7	4.8	-5.8
4	7	4	8.8	-6.6	-3	7	18	13.2	-14.3	-4	8	11	7.7	-7.7	4	9	8	10.0	-8.0	-5	10	7	12.2	-11.6
-4	7	4	25.4	23.9	-4	7	18	7.3	-7.3	-5	8	11	22.8	-23.6	-4	9	8	6.9	-5.8	0	10	8	14.7	17.0
5	7	4	19.5	-17.7	-5	7	18	10.1	9.0	0	8	12	19.1	22.9	5	9	8	7.8	-6.8	2	10	8	9.4	-13.0
-5	7	4	50.9	46.0	0	8	0	14.2	-15.6	1	8	12	8.9	10.9	-5	9	8	15.9	-14.2	-2	10	8	8.8	-12.6
1	7	5	19.0	-19.7	1	8	0	7.1	-7.7	2	8	12	5.4	-6.0	0	9	9	9.8	10.8	-3	10	8	23.9	-22.6
-1	7	5	5.9	7.6	2	8	0	17.7	19.7	-2	8	12	21.8	-26.2	1	9	9	8.9	-9.7	4	10	8	12.9	10.5
2	7	5	17.0	18.4	3	8	0	8.6	6.2	-3	8	12	12.4	-11.7	-2	9	9	11.3	-13.5	-4	10	8	11.8	-10.7
-2	7	5	28.4	30.2	4	8	0	7.4	-7.9	-5	8	12	7.0	6.4	3	9	9	21.8	21.1	-5	10	8	14.8	16.0
3	7	5	18.8	18.1	5	8	0	5.4	-1.3	0	8	13	24.6	28.7	-3	9	9	21.8	-19.2	0	10	9	7.7	-8.8
-3	7	5	49.3	43.8	0	8	1	9.3	-10.5	1	8	13	5.3	-7.3	4	9	9	9.8	8.5	-1	10	9	10.7	12.2
4	7	5	17.1	-15.9	-1	8	1	17.8	19.8	-1	8	13	27.3	-31.2	-4	9	9	25.6	-28.1	2	10	9	6.1	8.4
5	7	5	23.2	-20.5	-2	8	1	24.6	-27.6	2	8	13	13.9	-15.5	-5	9	9	11.4	-8.6	-2	10	9	17.5	22.3
-5	7	5	35.6	-30.4	3	8	1	38.7	37.0	-2	8	13	7.3	8.2	0	9	10	20.2	24.1	-4	10	9	20.7	-20.5
0	7	6	54.1	-52.8	-3	8	1	13.7	-10.7	-3	8	13	13.2	13.2	1	9	10	9.5	10.8	-5	10	9	19.7	-19.2
1	7	6	18.4	18.7	4	8	1	31.7	28.2	-4	8	13	8.6	-9.2	-1	9	10	8.9	10.6	0	10	10	7.7	7.8
-1	7	6	29.6	30.0	-4	8	1	51.3	53.8	-5	8	13	7.4	-7.5	2	9	10	6.3	-7.3	1	10	10	4.7	-5.8
2	7	6	65.9	64.5	-5	8	1	37.9	34.3	1	8	14	10.1	-10.5	-2	9	10	15.4	17.5	-2	10	10	12.8	-14.6
-2	7	6	24.2	-28.4	0	8	2	6.0	-5.0	-2	8	14	4.8	4.7	-3	9	10	15.8	13.8	-5	10	10	18.3	-17.7
3	7	6	34.1	33.2	1	8	2	37.3	33.8	-4	8	14	10.7	-12.2	-4	9	10	6.2	-5.5	0	10	11	10.9	10.4
-3	7	6	28.4	-24.5	-1	8	2	20.1	-21.8	-5	8	14	10.1	-11.0	-5	9	10	31.8	-32.0	-1	10	11	5.9	-6.3
4	7	6	20.5	-17.1	2	8	2	10.1	-12.3	-1	8	15	30.8	-29.3	0	9	11	10.9	12.5	2	10	11	7.3	-9.1
-4	7	6	10.7	9.9	-2	8	2	21.8	-23.6	-2	8	15	8.2	-9.2	1	9	11	7.1	8.1	-2	10	11	23.3	23.3
5	7	6	25.6	-24.4	-3	8	2	17.5	-16.7	-4	8	15	6.0	-6.5	2	9	11	5.9	7.7	-3	10	11	32.3	29.7
-5	7	6	23.7	19.8	4	8	2	11.8	10.7	0	8	16	1.0	1.6	-2	9	11	20.6	-24.7	-4	10	11	17.1	-13.0
0	7	7	14.7	13.9	-4	8	2	15.0	14.5	-4	8	16	5.9	5.3	-4	9	11	4.5	4.3	-5	10	11	30.8	-27.7
1	7	7	7.1	-6.8	5	8	2	7.7	6.6	1	9	0	5.9	6.6	-5	9	11	19.3	-19.9	0	10	12	9.3	10.6
-1	7	7	14.8	16.3	-5	8	2	24.1	21.7	2	9	0	4.2	-4.3	0	9	12	17.5	18.6	-1	10	12	9.5	9.1
2	7	7	5.9	6.4	0	8	3	30.6	-32.2	4	9	0	24.5	23.0	1	9	12	4.1	-6.1	-2	10	12	5.0	-6.0
-2	7	7	17.3	-19.7	1	8	3	16.5	-18.1	5	9	0	9.6	8.7	-1	9	12	15.4	-19.0	-3	10	12	13.7	-12.3
3	7	7	12.4	-11.8	-1	8	3	8.9	10.7	0	9	1	33.3	-33.8	2	9	12	12.8	-14.4	-1	10	13	5.3	-5.2
-3	7	7	15.5	14.8	2	8	3	37.0	37.0	1	9	1	17.2	-19.6	-2	9	12	18.9	18.8	-2	10	13	6.3	7.7
4	7	7	22.3	-19.5	-2	8	3	23.3	-25.7	-1	9	1	42.7	-41.6	-3	9	12	21.8	21.1	-3	10	13	23.1	18.5
-4	7	7	30.9	28.4	3	8	3	57.2	53.2	2	9	1	8.0	9.7	-4	9	12	7.4	-6.1	-4	10	13	11.1	9.4
5	7	7	10.1	11.1	-3	8	3	48.8	-42.9	-2	9	1	7.3	-6.2	-5	9	12	17.1	-16.6	-5	10	13	18.5	-15.2
0	7	8	14.7	13.7	-4	8	3	36.8	37.2	3	9	1	14.5	14.1	0	9	13	10.3	11.2	-4	10	14	11.5	-9.4
1	7	8	21.3	21.9	-5	8	3	61.0	54.4	-3	9	1	22.9	19.0	-1	9	13	16.5	16.8	-5	10	14	14.1	-13.4
-1	7	8	9.5	10.8	0	8	4	14.7	-14.5	4	9	1	11.4	-9.0	-3	9	13	25.2	-23.0	1	11	0	8.9	-8.9
2	7	8	14.1	15.6	1	8	4	42.1	-38.4	-4	9	1	20.1	18.5	-4	9	13	13.3	-12.3	2	11	0	3.7	-4.4
-2	7	8	8.2	8.6	2	8	4	9.4	12.8	5	9	1	5.2	5.9	-5	9	13	5.0	-5.4	3	11	0	16.7	-14.6
3	7	8	9.9	-5.0	3	8	4	29.8	25.3	-5	9	1	4.6	-4.5	0	9	14	6.0	6.8	4	11	0	11.4	-9.0
-3	7	8	12.7	-10.5	-3	8	4	11.2	-10.4	0	9	2	19.6	-20.2	-1	9	14	17.2	-17.8	5	11	0	10.9	8.6
4	7	8	21.5	-20.0	4	8	4	8.8	7.3	1	9	2	25.5	-25.5	-3	9	14	9.6	7.4	0	11	1	11.4	-11.1
-4	7	8	22.0	-20.0	-4	8	4	24.9	-22.7	-1	9	2	12.4	13.5	-2	9	15	8.0	9.7	1	11	1	11.8	13.1
-5	7	8	14.8	-12.0	0	8	5	36.0	-38.5	-2	9	2	31.6	-33.9	-4	9	15	9.2	-7.5	2	11	1	18.1	21.9
0	7	9	28.4	-30.4	1	8	5	9.5	11.1	3	9	2	39.4	33.7	-5	9	15	13.5	-13.0	-2	11	1	8.4	9.8
1	7	9	11.2	-12.4	2	8	5	59.6	60.0	-3	9	2	24.4	-20.7	0	10	0	29.5	-31.5	-3	11	1	7.8	7.9
-1	7	9	16.0	19.6	-2	8	5	19.6	-24.3	-4	9	2	32.1	29.3	1	10	0	14.8	-17.9	4	11	1	16.9	-13.7
-2	7	9	38.1	40.3	3	8	5	23.1	21.2	-5	9	2	27.5	24.0	2	10	0	7.8	10.8	5	11	1	9.4	-8.4
-3	7	9	10.1	-8.7	-3	8	5	17.5	-16.4	0	9	3	12.0	-12.8	3	10	0	15.8	23.4	0	11	2	24.0	-23.6
-4	7	9	4.2	4.2	4	8	5	21.1	-19.1	1	9	3	33.7	-32.8	4	10	0	10.1	-8.1	1	11	2	13.0	-14.3
5	7	9	11.1	-10.8	-4	8	5	6.7	6.9	-1	9	3	19.6	20.7	5	10	0	12.9	-9.4	-1	11	2	13.6	-15.6
-5	7	9	6.2	-6.6	5	8	5	12.4	-12.0	-2	9	3	18.1	-21.9	1	10	1	23.1	-24.1	2	11	2	7.5	-9.1
0	7	10	15.3	17.2	-5	8	5	42.9	39.5	-3	9	3	22.1	-19.3	-1	10	1	19.0	-19.3	-2	11	2	20.8	-24.5
1	7	10	9.5	12.3	0	8	6	13.7	-12.6	4	9	3	9.1	8.2	2	10	1	14.1	-18.4	3	11	2	11.2	-9.6
-1	7	10	38.5	-41.6	1	8	6	7.7	7.9	-4	9	3	13.9	11.7	-2	10	1	22.9	-26.6	4	11	2	5.3	5.3
-2	7	10	7.3	7.3	-1	8	6	21.3	-24.4	5	9	3	24.3	24.0	3	10	1	19.6	-20.1	1	11	3	6.5	7.8
3	7	10	10.1	-11.2	2	8	6	9.0	10.4	-5	9	3	10.7	8.0	-3	10	1	13.9	-11.8	-1	11	3	5.9	-7.9
-3	7	10	28.4	24.4	-2	8	6	15.4	-16.8	0	9	4	52.5	-51.7	5	10	1	14.8	14.4	2	11	3	6.9	9.5
4	7	10	10.3	-9.2	-3	8	6	11.2	9.1	1	9	4	10.1	-11.0	-5	10	1	5.0	5.4	4	11	3	7.4	-6.4
-4	7	10	14.3	-13.5	4	8	6	12.6	-11.5	-1	9	4	9.5	11.0	0	10	2	11.4	-11.4	5	11	3	14.6	-11.9
-5	7	10	19.7	-17.3	-4	8	6	19.2	18.7	2	9	4	35.6	38.7	1	10	2	9.5	-11.5	-5	11	3	10.7	10.4
1	7	11	14.8	18.0	5	8	6	6.8	6.5	-2	9	4	22.5	-26.6	2	10	2	13.2	16.7	0	11	4	35.0	-36.7
-1	7	11	18.4	-22.6	-5	8	6	6.2	-6.6	3	9	4	14.7	14.6	-2	10	2	14.5	-20.1	1	11	4	4.7	-5.8
2	7	11	7.8	-9.5	0	8	7	17.5	-18.8	-3	9	4	43.8	-37.9	4	10	2	11.2	-10.8	-1	11	4	17.8	20.8
3	7	11	10.4	-10.5	1	8	7	29.0	29.7	4	9	4	10.9	-9.6	-4	10	2	16.3	14.2	2	11	4	8.0	11.3
-3	7	11	14.7	13.6	2	8	7	39.4	44.8	-4	9	4	8.3	7.2	5	10	2	15.7	15.2	-2	11	4	21.6	-25.4
4	7	11	10.9	-9.2	-2	8	7	8.8	-11.0	5	9	4	11.8	-10.3	0	10	3	39.9	-41.3	-3	11	4	30.7	-30.3
-4	7	11	10.6	8.9	-3	8	7	17.5	0.8	-5	9	4	30.0	29.1	1	10	3	5.9	-7.0	4	11	4	14.7	-13.7
-5	7	11	24.9	23.0	4	8	7	17.3	-16.6	0	9	5	27.3	-29.6	-1	10	3	9.5	-10.4	5	11	4	21.9	-17.5
0	7	12	38.3	46.1	-4	8	7	8.9	-6.1	1	9	5	9.5	10.9	2	10	3	8.6	9.9	-5	11	4	5.2	5.3
1	7	12	6.5	6.4	5	8	7	9.4	-8.8	-1	9	5	16.0	-19.4	-2	10	3	43.8	-46.9	-2	11	5	7.1	-7.9
-1	7	12	26.7	-31.9	-5	8	7	5.4	5.6	2	9	5	14.1	18.0	-3	10	3	17.3	-13.3	4	11	5	13.9	-11.0
2	7	12	12.4	-16.7	0	8	8	13.7	15.8	-2	9	5	8.0	9.1	-4	10	3	14.7	12.6	-4	11	5	12.9	11.4
-2	7	12	7.1	7.3	1	8	8	10.1	-10.8	3	9	5	11.2	10.2	5	10	3	9.2	-10.9	5	11	5	12.0	-11.0
3	7	12	12.2	-16.3	-1	8	8	16.0	20.1	-3	9	5	19.3	-17.3	-5	10	3	18.9	19.0	-5	11	5	3.0	3.7
-3	7	12	20.3	18.2	-2	8	8	8.4	-9.3	-4	9	5	10.3	-10.0	0	10	4	15.8	-17.6	0	11	6	8.2	-7.0
-5	7	12	23.9	-23.2	-3	8	8	20.6	-17.9	0	9	6	19.6	-20.2	2	10	4	7.5	8.5	-1	11	6	16.5	19.2
0	7	13	13.1	14.9	4	8	8	7.4	7.2	1	9	6	8.9	9.3	-3	10	4	18.1	-15.9	-3	11	6	13.5	-10.5
1	7	13	8.2	-10.3	-4	8	8	8.0	-8.5	-1	9	6	10.1	12.6	-5	10	4	8.8	6.3	4	11	6	10.5	-9.4
-1	7	13	4.7	5.8	0	8	9	22.4	25.3	2	9	6	24.4	28.5	0	10	5	23.0	-23.1	-4	11	6	9.7	-8.8
2	7	13	18.5	-20.1	1	8	9	32.0	30.5	-2	9	6	10.7	-12.8	-1	10	5	37.3	37.7	-5	11	6	19.5	-16.1
-5	7	13	20.5	19.6	-3	8	9	21.8	20.0	-3	9	6	15.8	-12.8	2	10	5	13.5	17.8	0	11	7	15.8	16.4
0	7	14	19.6	28.7	4	8	9	7.4	-6.8	4	9	6	16.5	-16.3	-2	10	5	10.9	-13.0	-1	11	7	7.7	8.0
-1	7	14	26.7	-30.5	5	8	9	15.1	-13.9	-4	9	6	17.4	-14.3	-3	10	5	32.0	-28.8	-2	11	7	9.7	-12.2
2	7	14	20.6	-23.3	-5	8	9	33.0	-29.6	5	9	6	8.6	-7.4	4	10	5	19.4	-17.0	-3	11	7	9.4	-8.5
-3	7	14	24.7	24.6	0	8	10	9.8	-11.3	-5	9	6	10.9	8.7	5	10	5	15.3	-12.9	4	11	7	10.1	-7.3
-5	7	14	19.1	-17.4	1	8	10	13.0	14.7	0	9	7	12.0	12.9	1	10	6	13.0	15.5	-4	11	7	20.0	17.4
-1	7	15	4.1	-4.8	-1	8	10	5.3	-4.7	1	9	7	17.2	18.5	-1	10	6	12.4	-13.6	-5	11	7	19.7	14.1
-2	7	15	6.5	-7.6	2	8	10	8.4	11.0	-1	9	7	5.9	-6.9	2	10	6	7.5	9.3	0	11	8	7.7	-8.7
-3	7	15	18.8	18.5	-2	8	10	11.6	14.4	2	9	7	6.9	-7.4	-2	10	6	12.0	-15.3	1	11	8	13.6	-14.1
-4	7	15	8.8	8.2	-3	8	10	12.4	-8.8	-2	9	7	23.5	-29.7	-3	10	6	17.0	-16.7	-1	11	8	4.7	5.8
-5	7	15	8.6	-7.4	-4	8	10	6.7	-5.6	-3	9	7	27.7	-25.9	-4	10	6	9.5	8.2	-2	11	8	6.7	7.2
-1	7	16	11.2	-11.3	5	8	10	4.6	-5.3	4	9	7	12.7	12.0	-5	10	6	12.0	10.7	-3	11	8	10.4	-8.2
-2	7	16	11.6	-13.3	-5	8	10	11.4	-11.3	-4	9	7	13.9	-11.9	0	10	7	9.8	-10.7	-4	11	8	6.0	-4.4
-3	7	16	9.2	-9.3	0	8	11	35.0	42.5	5	9	7	9.2	7.0	1	10	7	5.3	-5.9	0	11	9	4.9	4.1
-5	7	16	12.9	10.5	1	8	11	6.5	6.3	-5	9	7	12.2	11.2	-1	10	7	11.2	12.2	-1	11	9	14.2	14.7
-1	7	17	6.5	7.1	-1	8	11	13.6	-14.7	0	9	8	10.9	-10.6	-2	10	7	8.6	10.8	2	11	9	7.5	-9.0

Table 4 (*cont.*)

H	K	L	FO	FC
-2	11	9	3.1	3.8
-3	11	9	6.6	-7.2
-5	11	9	8.2	5.5
-2	11	10	23.3	22.3
-3	11	10	19.6	16.5
-4	11	10	24.5	-21.4
-5	11	10	16.5	-13.1
0	11	11	6.5	7.7
-2	11	12	9.4	11.2
-3	11	12	26.2	24.3
-4	11	12	8.3	6.5
-5	11	12	24.3	-18.3
0	12	0	10.3	-10.0
1	12	0	7.1	7.4
2	12	0	17.7	17.6
4	12	0	11.8	-10.2
5	12	0	9.0	-7.5
1	12	2	16.0	15.5
2	12	2	10.9	11.5
-2	12	2	14.3	17.7
4	12	2	10.1	-8.8
5	12	2	3.4	-19.2
-5	12	2	4.4	5.2
0	12	3	14.2	-16.9
1	12	3	17.8	-16.8
2	12	3	5.6	4.6
-2	12	3	19.9	-20.6
3	12	3	19.6	15.7
-3	12	3	16.0	-14.2
-4	12	3	15.4	12.1
-5	12	3	19.9	15.4
0	12	4	9.8	9.4
1	12	4	5.9	6.8
2	12	4	10.5	6.7
-3	12	4	13.9	9.3
4	12	4	10.1	-17.6
-4	12	4	8.2	6.3
-5	12	4	12.2	9.7
0	12	5	7.1	-8.8
1	12	5	4.1	5.9
-1	12	5	8.9	8.4
-3	12	5	10.7	-8.7
-4	12	5	9.8	-8.1
-5	12	5	7.0	6.4
0	12	6	12.6	13.7
-1	12	6	10.7	10.1
-2	12	6	8.2	-9.5
-4	12	6	19.0	16.3
-5	12	6	11.1	8.3
-1	12	7	4.1	-4.5
-4	12	7	4.5	4.8
-5	12	7	5.2	-3.8
0	12	8	5.4	5.8
-1	12	8	13.6	13.8
-2	12	8	4.4	-5.0
-3	12	8	9.2	-5.6
-4	12	8	15.2	14.1
-5	12	8	11.8	10.0
-1	12	9	7.7	8.3
-2	12	9	5.4	5.1
1	13	0	11.2	11.8
2	13	0	6.1	7.1
0	13	1	11.4	-10.0
2	13	1	9.2	10.1
-2	13	1	14.7	15.9
3	13	1	9.9	8.3
-3	13	1	6.1	5.6
0	13	4	9.3	-10.2
-3	13	4	12.9	-11.5
0	13	5	7.1	7.6

Table 5. *Comparison of peak heights* (e.Å^{-3}) *and curvatures* (e.Å^{-5}) *from differential synthesis*

		ϱ	$-A_{hh}$	$-A_{kk}$	$-A_{ll}$	A_{hk}	A_{hl}	A_{kl}
Cu	obs.	54·0	442	462	531	−10	199	−13
	calc.	55·1	454	470	542	−12	205	−13
S(1)	obs.	28·7	247	231	293	−17	114	2
	calc.	29·1	251	237	300	−16	116	3
S(2)	obs.	30·9	262	274	312	−7	117	3
	calc.	31·2	266	275	317	−7	120	2
S(3)	obs.	27·0	219	252	275	−21	130	−4
	calc.	27·4	223	252	277	−21	126	−5
S(4)	obs.	32·1	286	279	349	−3	132	−2
	calc.	33·4	300	292	361	−3	137	−2
N(1)	obs.	9·6	76	72	83	0	29	−5
	calc.	9·7	78	73	85	1	31	−4
N(2)	obs.	10·9	86	92	102	−2	36	−8
	calc.	10·8	86	92	105	−2	38	−8
C(1)	obs.	8·0	60	58	75	7	20	−9
	calc.	8·2	62	60	78	7	22	−9
C(2)	obs.	6·6	53	42	48	−6	18	−2
	calc.	6·5	50	41	47	−7	18	−1
C(3)	obs.	7·1	49	42	61	1	19	−7
	calc.	7·3	53	46	65	2	21	−7
C(4)	obs.	5·9	40	41	41	−3	17	1
	calc.	5·7	38	39	40	−3	16	1
C(5)	obs.	5·6	33	28	44	−1	11	1
	calc.	5·6	35	30	45	−1	13	1
C(6)	obs.	8·5	65	70	82	8	27	−5
	calc.	8·6	68	70	85	7	30	−6
C(7)	obs.	7·4	58	50	58	2	26	−6
	calc.	7·3	59	50	58	2	26	−6
C(8)	obs.	7·4	55	55	59	−2	22	−2
	calc.	7·4	55	57	59	−2	23	−2
C(9)	obs.	6·2	37	34	59	−1	22	0
	calc.	6·1	38	36	59	−1	22	1
C(10)	obs.	5·5	32	37	30	1	14	1
	calc.	5·2	31	35	30	3	13	1

$\sigma(\varrho) = 0{\cdot}18$ e.Å^{-3}

$\sigma(A_{hh}) = 1{\cdot}94$ $\sigma(A_{kk}) = 2{\cdot}56$ $\sigma(A_{ll}) = 2{\cdot}06$ e.Å^{-5}

$\sigma(A_{hk}) = 1{\cdot}16$ $\sigma(A_{hl}) = 1{\cdot}38$ $\sigma(A_{kl}) = 1{\cdot}28$ e.Å^{-5} .

Calculations

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

Intensity corrections and structure factors were calculated using programs of V. Scatturin and co-workers. D. van der Helm's general Fourier synthesis for the Fourier syntheses, 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 copper diethyldithiocarbamate, as seen down the line which makes an angle of 90° with the b axis and $60° - (\beta - 90°) = 36°8'$ with the c axis, is given in Fig. 1. The asymmetric unit is chosen so as to contain one molecule. However, each pair of centrosymmetrically related copper atoms, at the rather short distance of 3·59 Å, share sulphur atoms, thus forming a type of bimolecular unit.

The bond lengths and angles, with their e.s.d.'s (Cruickshank & Robertson, 1953), are listed in Tables 6 and 7, respectively, and are also shown in Fig. 2. All the relevant bond, interaction and contact distances and angles in the copper coordination sphere are reported in Table 8, including, for the sake of completeness, some of the values already given in Tables 6 and 7.

The results of the calculation of a number of significant least-squares planes are presented in Table 9.

Table 6. *Bond lengths with standard deviations*

Cu–S(1)	2·317 Å	(0·002)
Cu–S(2)	2·297	(0·002)
Cu–S(3)	2·301	(0·002)
Cu–S(4)	2·339	(0·002)
S(1)–C(1)	1·711	(0·008)
S(2)–C(1)	1·713	(0·008)
S(3)–C(6)	1·708	(0·007)
S(4)–C(6)	1·736	(0·007)
C(1)–N(1)	1·35	(0·010)
C(6)–N(2)	1·33	(0·008)
N(1)–C(2)	1·47	(0·012)
N(1)–C(3)	1·47	(0·011)
N(2)–C(7)	1·46	(0·010)
N(2)–C(8)	1·48	(0·010)
C(2)–C(4)	1·52	(0·016)
C(3)–C(5)	1·52	(0·017)
C(7)–C(9)	1·53	(0·015)
C(8)–C(10)	1·51	(0·017)

Table 7. *Bond angles with standard deviations*

S(1)–Cu–S(2)	77° 19′	(9′)
S(1)–Cu–S(3)	101 29	(10)
S(2)–Cu–S(4)	102 16	(9)
S(3)–Cu–S(4)	76 27	(9)
Cu–S(1)–C(1)	83 43	(28)
Cu–S(2)–C(1)	84 18	(27)
Cu–S(3)–C(6)	86 10	(25)
Cu–S(4)–C(6)	84 22	(24)
S(1)–C(1)–S(2)	114° 36′	(40′)
S(1)–C(1)–N(1)	122 21	(47)
S(2)–C(1)–N(1)	123 2	(47)
S(3)–C(6)–S(4)	112 56	(35)
S(3)–C(6)–N(2)	124 22	(41)
S(4)–C(6)–N(2)	122 41	(40)
C(1)–N(1)–C(2)	120 59	(55)
C(1)–N(1)–C(3)	121 31	(54)
C(2)–N(1)–C(3)	117 28	(59)
C(6)–N(2)–C(7)	121 1	(47)
C(6)–N(2)–C(8)	122 0	(47)
C(7)–N(2)–C(8)	116 56	(50)
N(1)–C(2)–C(4)	110 27	(1° 10′)
N(1)–C(3)–C(5)	111 32	(1 13)
N(2)–C(7)–C(9)	111 52	(1 4)
N(2)–C(8)–C(10)	111 44	(1 8)

Table 8 *Distances and angles in the copper coordination sphere*

Cu–S(1)	2·317 Å	S(1)–Cu–S(2)	77° 19′
Cu–S(2)	2·297	S(1)–Cu–S(3)	101 29
Cu–S(3)	2·301	S(2)–Cu–S(4)	102 16
Cu–S(4)	2·339	S(3)–Cu–S(4)	76 27
Cu–S(4′)	2·851	S(4′)–Cu–S(1)	94 34
Cu–Cu′	3·588	S(4′)–Cu–S(2)	97 46
S(1)–S(3)	3·576	S(4′)–Cu–S(3)	100 22
S(2)–S(1)	2·882	S(4′)–Cu–S(4)	93 6
S(3)–S(4)	2·871	S(1)–Cu–S(4)	172 17
S(4)–S(2)	3·610	S(2)–Cu–S(3)	161 50
S(4′)–S(1)	3·815	S(2)–S(1)–S(3)	88 40
S(4′)–S(2)	3·896	S(4)–S(2)–S(1)	90 39
S(4′)–S(3)	3·974	S(1)–S(3)–S(4)	91 31
S(4′)–S(4)	3·784	S(3)–S(4)–S(2)	88 11
Cu–C(2″)	3·784	C(2″)–H(2″)*b*–Cu	142 32
Cu–H(2″)*b*	2·859	H(2″)*b*–Cu–S(4′)	178 32

Table 9. *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	693	−507	188	1606	S(1) S(2) S(3) S(4)
II	−559	19	984	0	Cu Cu′ S(1) S(1′) S(4) S(4′)
III	743	−573	15	1210	Cu S(1) S(2) C(1) N(1) C(2) C(3)
IV	751	−568	5	1207	C(1) N(1) C(2) C(3)
V	595	−428	381	1358	Cu S(3) S(4) C(6) N(2) C(7) C(8)
VI	558	−438	418	1274	C(6) N(2) C(7) C(8)

Deviations from planes (10^{-3} Å)

	I	II	III	IV	V	VI
Cu	−259	9	23	—	39	—
Cu′	—	−9	—	—	—	—
S(1)	−104	−4	−7	—	—	—
S(1′)	—	4	—	—	—	—
S(2)	103	—	−32	—	—	—
S(3)	104	—	—	—	−74	—
S(4)	−103	−4	—	—	22	—
S(4′)	—	4	—	—	—	—
C(1)	—	—	−3	−3	—	—
N(1)	—	—	11	8	—	—
C(2)	—	—	−11	−2	—	—
C(3)	—	—	17	−2	—	—
C(6)	—	—	—	—	−16	−2
N(2)	—	—	—	—	8	5
C(7)	—	—	—	—	66	−2
C(8)	—	—	—	—	−44	−2

The geometry of the coordination of copper is closely related to a tetragonal pyramid, copper having coordination number five with normal bonds to four sulphur atoms, and a fifth, long bond (2·85 Å) to a sulphur atom of the centrosymmetrically related molecule (Fig. 1 and Table 8). The four sulphur atoms S(1), S(2), S(3) and S(4) lie roughly in a plane, with the copper atom at 0·26 Å from it (Table 9), the fifth, long bond from the copper, Cu–S(4′), being approximately perpendicular to this plane. The rather high deviation values of the four atoms S(1), S(2), S(3), S(4) from the best plane through them are due to the fact that angle S(1)–Cu–S(4) is 172°17′, whereas angle S(2)–Cu–S(3) is 161°50′. It appears that the same copper–sulphur interaction which makes it possible for copper to be five-coordinated, and the strain in the four-membered ring, revealed by the valence angles around the copper atom, are responsible for the distortions from a regular square-pyramidal coordination. It is noteworthy that Cu, S(1), S(4) and the centrosymmetrically related atoms Cu′, S(1′) and S(4′) all lie in a plane within less than ±0·01 Å.

Thus, at first sight, copper diethyldithiocarbamate belongs to the growing class of structures containing five-coordinated copper(II). This classification seems even more appropriate since copper(II) with coordination number five in a tetragonal-pyramidal environment has been found in the closely related copper complex quoted in the introduction, copper di-n-propyldithiocarbamate (Pignedoli & Peyronel, 1962). Barclay & Kennard (1961) listed the compounds of this class, pointing out that the tetragonal–pyramidal arrangement of ligands (with and without association of the complexes into bimolecular units) has become as characteristic of copper(II) as are its more common (Orgel & Dunitz, 1957) square-planar, distorted octahedral and tetrahedral configurations. Besides the compound dealt with in this paper and the already mentioned copper di-n-propyldithiocarbamate, one should now also add to the list of Barclay & Kennard, *N,N′*-ethylenebis(acetylacetoneiminato)copper(II) (Hall, Rae & Waters, 1962), the *β* form of anhydrous copper 8-hydroxyquinolinate (Kanamaru, Ogawa & Nitta, 1963; Bevan, Graddon & McConnell, 1963; Palenik, 1964), sodium glycylglycylglycino cuprate(II) monohydrate (Freeman, Schoone & Sime, 1965), in all of which the complexes are associated into bimolecular units; and copper(II) monoglycylglycine trihydrate (Strandberg, Lindqvist & Rosenstein, 1961), copper glutamate dihydrate (Gramaccioli, 1963*a*, *b*), and glycylglycylglycino copper(II) chloride sesquihydrate (Freeman, Robinson & Schoone, 1964), in which there is no such association.

However, in the last two compounds listed above, it is possible that the five-coordination of copper is simply due to steric hindrance. This could be a result of the presence of a carboxylic oxygen atom (at 2·59 Å in the first case and at 2·817 Å in the second) near the sixth octahedral position, and, although the Cu···O direction does not seem to correspond to a possible bond, the location of the oxygen atom could effectively prevent the approach of any sixth ligand to the copper atom.

It appears advisable, therefore, to take a closer look at the reported cases of five-coordinated copper. In fact, our results show that the shortest intermolecular copper contact is to a carbon atom at 3·78 Å in the region of the sixth octahedral position [C(2″) in Fig. 1]. As a result, one of the hydrogen atoms linked to this carbon atom [H(2″)*b* in Fig. 1] is at 2·86 Å from the copper atom and almost exactly in the sixth octahedral position [H(2″)*b*–Cu–S(4′) angle in Fig. 1 being 178°32′].

Similar copper contacts in the region of the sixth octahedral position had been reported for copper dimethylglyoxime (Frasson, Bardi & Bezzi, 1959; a carbon atom at 3·76 Å), *N,N′*-disalicylidene-propane-1,2-diaminecopper monohydrate (Llewellyn & Waters, 1960; an oxygen atom at 3·81 Å) and *N,N′*-disalicylidene-ethylenediaminecopper (Hall & Waters, 1960; a carbon atom at 3·84 Å), but the importance of this fact does not seem to have been noticed.*

The following is now open to discussion: whether in the reported cases of copper contacts in the region of the sixth octahedral position, or at least in some of them, it is correct to speak of five-coordinated copper with steric hindrance in the sixth position, or, whether one should think of a weak interaction as a sort of sixth 'bond', with copper approximately in the centre of a geometrically and energetically distorted octahedron. The importance of weak, long-distance interactions is becoming increasingly more noticeable, as for instance in the case of square-planar, four-coordinated, diamagnetic sulphur complexes of nickel, where a correlation between the length of the contact distance in the d_{z^2} direction of nickel and the bond distance of the four ligands has been suggested (Bonamico, Dessy, Mariani, Vaciago & Zambonelli, 1965).

As a final remark on the coordination of copper in the present compound it is worth noticing that the bimolecular unit does not seem to be present in solution: copper diethyldithiocarbamate is known to have a normal molecular weight in benzene and in chloroform (Thorn & Ludwig, 1962).

Each of the two ligand molecules is planar, except for the terminal CH_3 groups. The two planes intersect at the copper atom making an angle of about 164°. 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 the copper–sulphur or sulphur

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* Other compounds where a hydrogen atom is also found to occupy the sixth octahedral coordination site have, however, been recently reported: dichlorotris(triphenylphosphine)ruthenium(II), with a Ru–H distance of 2·59 Å (Ibers, 1965) and diiodo(dimethylphenylphosphine)palladium(II), with a Pd–H distance of 2·8 Å (Bailey, Jenkins, Mason & Shaw, 1965).

–carbon bond lengths[*]. On the other hand, the slight increase in the length of Cu–S(4) and S(4)–C(6) bonds, with respect to the other copper–sulphur and sulphur–carbon bonds in the molecule, is, in our opinion, due to the fact that S(4) is the sulphur atom involved in the formation of the bimolecular unit.

As in the case of the nickel compound (Bonamico, Dessy, Mariani, Vaciago and Zambonelli, 1965; paper I of this series) our present results on the co-planarity 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[†].

The crystal data and the structure analysis of nickel and copper diethyldithiocarbamates confirm the early finding of Livio Cambi (1936) that the stable forms, crystallized at room temperature of Ni(II) and Cu(II) salts of *N*,*N*-disubstituted dithiocarbamic acid are not isomorphous. Our data, however, do not throw much light on the supposed isomorphism of these same salts at high temperatures (Malatesta, 1937).

It has been stated in the introduction that the striking similarity in the crystal parameters of copper and zinc diethyldithiocarbamates could indicate that these compounds were isostructural. However, our results on the coordination geometry of the copper compound do not seem to be applicable to the case of the zinc complex and no detailed discussion is possible because no structural investigation of a zinc coordination compound of dithiocarbamic acid has been carried out hitherto. For this reason the structure of zinc diethyldithiocarbamate has been investigated in our laboratory and will be discussed in the third paper of this series.

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[*] Cu(II)–S bond lengths range from $2{\cdot}32_1$ to $2{\cdot}33_5$ in copper di-n-propyldithiocarbamate (Pignedoli & Peyronel, 1962), but these values are not very suitable for comparison with our results because (i) they have been determined by two-dimensional methods, and (ii) they refer to a similar case of a four-membered ring. However, Cu(II)–S bond lengths can be compared, all various effects taken into account, with the Cu(I)–S bond lengths known from reliable sources (Truter & Rutherford, 1962, and other references quoted therein; Okaya & Knobler, 1964). Our values for S–C bond lengths 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.

[†] 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 $p=0{\cdot}54$ and $p=0{\cdot}65$ respectively.