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The Crystal Structure of Bisthiourea-zinc Acetate

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Bisthiourea-zinc acetate, $Zn[SC(NH_2)_2]_2(CH_3COO)_2$, is monoclinic, $P2_1/c$: $a=6{\cdot}93_8$, $b=17{\cdot}67_8$, $c=11{\cdot}79_5$ Å, $\beta=112{\cdot}6°$, $Z=4$. The structure, solved by means of three-dimensional Fourier methods, has been refined with the use of the anisotropic differential synthesis. Zn coordinates to two S atoms from two thiourea molecules (Zn–S $2{\cdot}32_6$ and $2{\cdot}26_1$ Å) and to two O atoms (Zn–O $1{\cdot}97_3$ and $1{\cdot}95_4$ Å) from two acetate groups, to form a tetrahedral arrangement. Two further oxygen atoms from the same acetate groups are involved in weaker interactions with the metal atom at $2{\cdot}99_6$ and $2{\cdot}89_1$ Å; as a consequence of these interactions the planes of the acetate ions are oriented in such a way that the Zn atom almost lies within them. There are no significant differences between corresponding bond distances and angles in the two thiourea molecules: these are much the same as in the uncoordinated thiourea.

Introduction

Thiourea adducts with acetates of divalent metals have been prepared and described by Nardelli & Chierici (1959), who showed that the bisthiourea compounds of cobalt and zinc are isostructural. A three-dimensional X-ray analysis has now been carried out to study the coordination of the thiourea molecule and carboxyl group by the metal atom in these compounds. In particular, it seemed interesting to determine the role played by the oxygen atoms in the coordination and the influence, if any, of the sulphur–metal interaction on bond distances and angles in the thiourea molecule.

Experimental

The unit-cell constants, remeasured on single-crystal rotation and Weissenberg photographs and refined by a least-squares procedure on powder diffractometer data (Cu $K\alpha$, $\lambda=1{\cdot}5418$ Å), are as follows:

$Zn[SC(NH_2)_2]_2(CH_3COO)_2$; $M=335{\cdot}7$

$a=6{\cdot}938\pm0{\cdot}003$, $b=17{\cdot}678\pm0{\cdot}006$, $c=11{\cdot}795\pm0{\cdot}006$ Å

$\beta=112°47'\pm18'$; $V=1334$ Å^3; $Z=4$; $D_x=1{\cdot}671$, $D_m=1{\cdot}61$ g.cm^{-3}

$\mu=54{\cdot}6$ cm^{-1} (Cu $K\alpha$), $F(000)=632$.

Space group: $P2_1/c$ (from systematic absences).

Two series of equi-inclination Weissenberg photographs (filtered Cu radiation, multiple film technique) were taken at room temperature about [100] with levels $h=0,1,\ldots 6$, and about [001] with levels $l=0,1,\ldots 10$. 2128 independent reflexions were observed out of a possible 2554. The intensities were measured photometrically and corrected for Lorentz, polarization and spot shape effects. The sample used to take the photographs around [100] was a prism elongated along this axis and was considered as a cylinder with a mean radius of 0·008 cm in calculating the absorption correction; the photographs around [001] were taken with a nearly spherical fragment with a mean radius of

Table 1. *Final atomic fractional coordinates* ($\times10^4$), *thermal parameters* ($\times10$ Å^2) *with e.s.d.'s and ratios* (*e.s.d.*)/(*coordinate shift*)

	x/a (σ)	y/b (σ)	z/c (σ)	B_{11} (σ)	B_{22} (σ)	B_{33} (σ)	B_{12} (σ)	B_{13} (σ)	B_{23} (σ)	$\lvert r(x)\rvert$	$\lvert r(y)\rvert$	$\lvert r(z)\rvert$
Zn	1938 (2)	1748 (0)	123 (1)	38 (1)	38 (0)	43 (1)	2 (1)	13 (1)	−1 (1)	17	1	11
S(1)	−9 (3)	894 (1)	−1387 (2)	34 (1)	34 (0)	46 (2)	2 (1)	9 (2)	−6 (1)	7	4	8
S(2)	5050 (3)	2063 (1)	54 (2)	36 (2)	45 (0)	33 (2)	−3 (1)	12 (2)	−2 (1)	8	1	∞
O(1)	−117 (10)	2580 (2)	−358 (6)	43 (5)	36 (1)	39 (5)	8 (3)	7 (6)	−4 (4)	12	3	7
O(2)	1838 (10)	3274 (3)	1204 (6)	36 (5)	45 (1)	50 (5)	5 (4)	7 (6)	−13 (4)	5	9	8
O(3)	1827 (11)	1441 (3)	1688 (8)	40 (6)	46 (1)	51 (7)	9 (5)	17 (8)	6 (5)	26	4	6
O(4)	4368 (15)	663 (3)	1952 (10)	55 (10)	50 (2)	64 (10)	18 (8)	29 (12)	13 (8)	9	11	96
N(1)	2758 (16)	448 (3)	−2239 (10)	59 (9)	44 (0)	53 (9)	13 (4)	25 (11)	8 (4)	41	14	50
N(2)	2506 (14)	−278 (2)	−712 (9)	53 (7)	39 (0)	52 (8)	10 (4)	15 (10)	4 (5)	19	∞	9
N(3)	5719 (14)	2607 (4)	2286 (9)	38 (6)	57 (2)	41 (7)	1 (6)	14 (9)	−12 (6)	29	21	5
N(4)	8481 (11)	2110 (4)	2023 (7)	31 (5)	58 (2)	46 (7)	2 (5)	9 (8)	−6 (6)	107	13	9
C(1)	1930 (12)	313 (4)	−1437 (8)	36 (6)	30 (1)	40 (7)	0 (5)	10 (8)	−4 (5)	16	2	8
C(2)	6491 (13)	2277 (3)	1573 (8)	33 (6)	39 (1)	30 (6)	1 (5)	12 (8)	−3 (5)	5	4	4
C(3)	2967 (21)	716 (6)	3481 (13)	57 (11)	66 (3)	49 (10)	1 (9)	19 (14)	5 (9)	8	6	131
C(4)	3080 (13)	944 (4)	2306 (9)	32 (6)	40 (1)	38 (7)	3 (5)	13 (8)	0 (5)	5	7	44
C(5)	−1379 (18)	3778 (5)	−68 (10)	56 (11)	41 (1)	66 (10)	17 (8)	13 (14)	−2 (8)	15	47	98
C(6)	247 (12)	3177 (3)	298 (9)	37 (7)	33 (1)	48 (8)	3 (5)	14 (9)	0 (5)	8	3	17

0·02 cm, and for this series of data the spherical absorption correction was used. The data of both zones were correlated and put on a common scale with the use of the least-squares procedure of Rollett & Sparks (1960). The absolute scale was determined first by Wilson's method, then by comparison with the calculated values.

Structure determination and refinement

The coordinates of Zn, S(1) and S(2) were found first from a three-dimensional Patterson synthesis. The next step was a three-dimensional Fourier synthesis calculated with the use of the signs of the contributions of these atoms to the structure factors ($R=35\%$); this synthesis showed all the other non-hydrogen atoms to be well resolved. Two more three-dimensional Fourier calculations followed by an F_o-F_c synthesis improved the agreement index to 13·1%. The refinement was then carried out by means of nine cycles of Booth's differential synthesis, two calculated with isotropic and seven with anisotropic thermal parameters. The final agreement indices were (R, for observed reflexions only; R' including unobserved reflexions; multiplicities not considered): $R=8{\cdot}4\%$, $R'=9{\cdot}2\%$, and the ratios between the e.s.d.'s and the shifts of the coordinates were as shown in Table 1, in which the final parameters with their e.s.d.'s (Cruickshank, 1949 & 1956) are also quoted. The B_{ij}'s were determined by the method of Nardelli & Fava (1960) using the second derivatives of the electron density in the differential synthesis.

No attempt was made to locate the hydrogen atoms directly. The hydrogen coordinates reported in Table 2, relating to the hydrogen atoms of the two thiourea molecules, were calculated assuming an sp^2 bond configuration for each nitrogen atom with a distance N–H = 1·03 Å. In Table 2 are reported also the values of the electron density found from a final F_o-F_c synthesis at the points corresponding to the assumed coordinates of the hydrogen atoms. Data for the peaks of the other atoms are given in Table 3. Observed and calculated

Table 2. *Calculated fractional coordinates and corresponding ϱ_o values for hydrogen atoms in thiourea molecules*

	x/a	y/b	z/c	ϱ_o (e.Å^{-3})
H(1)	0·4018	0·0105	−0·2268	1·0
H(2)	0·2368	0·0908	−0·2814	0·7
H(3)	0·1904	−0·0389	−0·0091	0·8
H(4)	0·3759	−0·0622	−0·0744	0·5
H(5)	0·6832	0·2725	0·3186	0·7
H(6)	0·4329	0·2738	0·1950	0·8
H(7)	0·9407	0·2265	0·2908	0·8
H(8)	0·9157	0·1883	0·1461	0·7

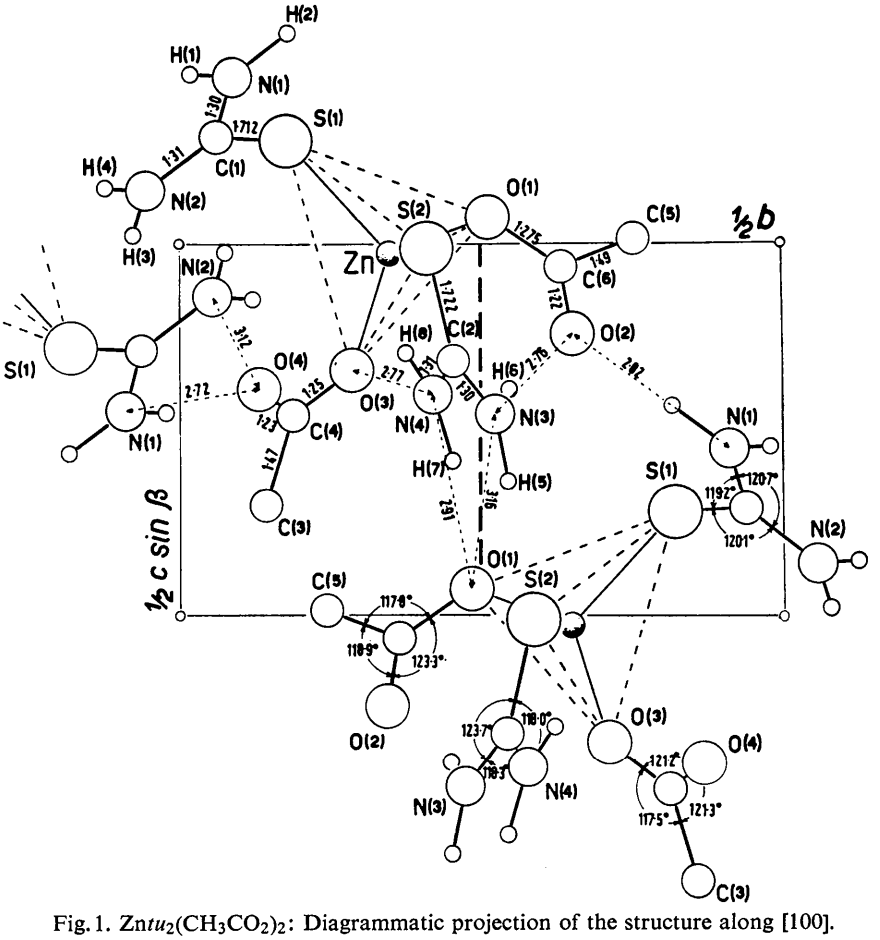

Fig. 1. $Znt{u_2}(CH_3CO_2)_2$: Diagrammatic projection of the structure along [100].

(not including H atoms) structure factors are compared in Table 4.

The atomic scattering factors used throughout the calculations are those of Thomas & Umeda (1957) for Zn^{2+}, of Dawson (1960) for S and of Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955) for O, N and C.

All the calculations were performed on the Olivetti Elea 6001/S computer of the Centro di Calcolo Elettronico della Università di Parma with the programs of Nardelli, Musatti, Domiano & Andreetti (1964, 1965).

Discussion

Fig. 1 shows a diagrammatic projection of the structure along [100]. Each zinc atom coordinates to two sulphur atoms from two thiourea molecules and to two oxygen atoms from two acetate groups, forming a tetrahedral arrangement. Two more oxygen atoms from the same carboxyl groups are involved in a weaker interaction with the metal atom as shown in Fig. 2. Distances and angles in the coordination polyhedron are (the e.s.d.'s quoted in parentheses are in units of the last place):

Zn–S(1) 2·326(2) Å	Zn–S(2) 2·261(4) Å
Zn–O(1) 1·973(6)	Zn–O(3) 1·954(8)
Zn–O(2) 2·996(5)	Zn–O(4) 2·891(9)

S(1)–Zn–S(2)	114·3°(0·1°)
S(1)–Zn–O(1)	97·1 (0·2)
S(1)–Zn–O(3)	108·6 (0·2)
S(2)–Zn–O(1)	113·6 (0·2)
S(2)–Zn–O(3)	119·3 (0·3)
O(1)–Zn–O(3)	101·0 (0·3)

The two Zn–S distances are significantly different ($t_0 =$ 14·5, significance test of Cruickshank & Robertson, 1953): one is amongst the shortest hitherto observed [2·286(6) and 2·298(6) Å in tetrahedral monothiosemicarbazide-zinc chloride (Cavalca, Nardelli & Branchi, 1960)]; the other is comparable with the sum of Paul-

Table 3. *Atomic peak heights* (e.Å^{-3}), *curvatures* (e.Å^{-5}) *and e.s.d.'s*

		ϱ	$-A_{hh}$	$-A_{kk}$	$-A_{ll}$	A_{kl}	A_{hl}	A_{hk}
Zn	obs.	51·1	429	508	384	−16	117	13
	calc.	53·1	432	518	387	−16	114	13
S(1)	obs.	25·0	217	247	176	3	52	−10
	calc.	26·1	219	253	179	2	51	−10
S(2)	obs.	25·8	223	243	215	0	63	−14
	calc.	26·6	224	250	215	1	59	−15
O(1)	obs.	10·1	79	97	67	0	18	−16
	calc.	10·4	81	98	68	0	18	−17
O(2)	obs.	9·8	73	75	67	−8	18	8
	calc.	10·1	73	77	68	−8	18	8
O(3)	obs.	9·3	69	78	51	−2	16	2
	calc.	9·7	70	80	52	−2	16	2
O(4)	obs.	8·2	64	65	52	0	24	9
	calc.	8·5	65	67	53	−1	24	9
N(1)	obs.	7·2	50	57	45	−7	18	−3
	calc.	7·3	50	58	45	−7	18	−3
N(2)	obs.	7·2	51	68	42	−5	12	−5
	calc.	7·5	51	70	43	−5	12	−4
N(3)	obs.	7·8	53	50	48	1	16	−3
	calc.	8·1	53	51	49	1	15	−3
N(4)	obs.	7·6	65	50	51	−1	13	−5
	calc.	8·0	65	51	52	0	13	−5
C(1)	obs.	7·2	60	58	56	−3	17	4
	calc.	7·6	61	59	57	−3	18	4
C(2)	obs.	7·4	59	62	58	−1	20	−5
	calc.	8·0	59	63	59	−1	19	−5
C(3)	obs.	5·7	41	39	38	1	15	−3
	calc.	5·6	42	40	37	1	15	−3
C(4)	obs.	7·0	58	62	48	−2	15	5
	calc.	7·3	59	64	48	−2	15	6
C(5)	obs.	5·8	35	41	36	−5	7	2
	calc.	6·0	36	42	37	−5	8	2
C(6)	obs.	7·3	57	78	44	−3	12	4
	calc.	7·7	57	79	45	−3	12	4
	e.s.d.	0·2	1	1	1	1	1	1

Table 4. *Observed and calculated structure factors*

A minus sign for F_o means 'less than'.

h	k	l	$\lvert 10F_o \rvert$	$10F_c$
1	0	0	554	569
2	0	0	358	-289
3	0	0	702	-769
4	0	0	686	705
5	0	0	622	610
6	0	0	574	589
7	0	0	18-	-7
1	1	0	850	-1036
2	1	0	633	-712
3	1	0	660	685
4	1	0	527	493
5	1	0	50	48
6	1	0	274	-282
7	1	0	221	-174
0	2	0	670	-1179
1	2	0	8-	26
2	2	0	512	-437
3	2	0	739	764
4	2	0	17-	-4
5	2	0	179	-167
6	2	0	279	-271
7	2	0	189	173
1	3	0	728	-799
2	3	0	586	569
3	3	0	236	-202
4	3	0	17-	1
5	3	0	19-	-26
6	3	0	100	111
7	3	0	55	-69
0	4	0	9-	16
1	4	0	691	-739
2	4	0	406	336
3	4	0	153	113
4	4	0	45	55
5	4	0	236	-217
6	4	0	126	-118
7	4	0	50	-58
1	5	0	665	764
2	5	0	601	592
3	5	0	153	-140
4	5	0	495	-457
5	5	0	89	-86
6	5	0	300	268
7	5	0	176	146
0	6	0	11-	113
1	6	0	279	297
2	6	0	971	-1203
3	6	0	1056	-1160
4	6	0	110	-120
5	6	0	284	254
6	6	0	20-	34
7	6	0	258	-259
1	7	0	897	-1100
2	7	0	554	-585
3	7	0	126	122
4	7	0	565	551
5	7	0	57	63
6	7	0	316	-288
7	7	0	210	-162
0	8	0	739	-924
1	8	0	47	52
2	8	0	274	267
3	8	0	486	453
4	8	0	258	-258
5	8	0	168	-164
6	8	0	179	-158
7	8	0	80	97
1	9	0	364	354
2	9	0	68	-72
3	9	0	18-	-33
4	9	0	20-	-24
5	9	0	73	66
6	9	0	57	51
7	9	0	14-	33
0	10	0	113	103
1	10	0	16-	2
2	10	0	427	407
3	10	0	19-	27
4	10	0	236	212
5	10	0	136	-124
6	10	0	183	174
7	10	0	13-	-1
1	11	0	469	467
2	11	0	236	201
3	11	0	115	-99
4	11	0	258	-230
5	11	0	40	-45
6	11	0	17-	0
7	11	0	45	54
0	12	0	443	424
1	12	0	495	494
2	12	0	68	-73
3	12	0	206	179
4	12	0	110	112
5	12	0	416	399
6	12	0	89	90
7	12	0	50	61
1	13	0	448	-419
2	13	0	364	-356
3	13	0	179	169

h	k	l	$\lvert 10F_o \rvert$	$10F_c$
4	13	0	274	264
5	13	0	136	118
6	13	0	153	-127
0	14	0	390	-362
1	14	0	400	-359
2	14	0	385	339
3	14	0	77	69
4	14	0	45	-54
5	14	0	279	-264
6	14	0	12-	-11
1	15	0	263	226
2	15	0	110	100
3	15	0	104	-106
4	15	0	104	-106
5	15	0	16-	-8
6	15	0	69	84
0	16	0	100	-97
1	16	0	50	-40
2	16	0	20-	-40
3	16	0	100	-92
4	16	0	100	-100
5	16	0	14-	3
1	17	0	77	71
2	17	0	19-	41
3	17	0	18-	-42
4	17	0	16-	-21
5	17	0	11-	10
0	18	0	19-	-32
1	18	0	77	-63
2	18	0	200	-169
3	18	0	157	-130
4	18	0	153	-123
5	18	0	8-	-1
1	19	0	115	-102
2	19	0	84	-88
3	19	0	14-	23
4	19	0	142	128
0	20	0	173	-147
1	20	0	110	-79
2	20	0	200	178
3	20	0	142	119
1	21	0	142	114
2	21	0	121	102
0	22	0	95	99
1	22	0	142	127
0	1	1	586	1158
1	1	1	179	163
2	1	1	148	113
2	1	$\bar{1}$	469	-465
3	1	1	411	-424
3	1	$\bar{1}$	51	-55
4	1	1	311	297
4	1	$\bar{1}$	322	325
5	1	1	258	236
5	1	$\bar{1}$	305	293
6	1	1	183	179
6	1	$\bar{1}$	115	104
7	1	1	68	-64
7	1	$\bar{1}$	11-	-6
8	1	1	31-	-6
0	2	1	226	-251
1	2	1	200	-201
1	2	$\bar{1}$	1214	-1353
2	2	1	157	-131
2	2	$\bar{1}$	955	-1034
3	2	1	453	462
3	2	$\bar{1}$	126	-81
4	2	1	627	658
4	2	$\bar{1}$	300	296
5	2	1	263	264
5	2	$\bar{1}$	11-	-27
6	2	1	110	-103
6	2	$\bar{1}$	236	-223
7	2	1	30	-35
8	2	$\bar{1}$	57	-48
0	3	1	763	-783
1	3	1	486	536
1	3	$\bar{1}$	89	81
2	3	1	183	270
2	3	$\bar{1}$	206	221
3	3	1	480	509
3	3	$\bar{1}$	1061	1059
4	3	1	189	-183
4	3	$\bar{1}$	126	-126
5	3	1	110	-99
5	3	$\bar{1}$	274	-244
6	3	1	194	-192
6	3	$\bar{1}$	305	-277
7	3	1	183	174
7	3	$\bar{1}$	153	201
8	3	$\bar{1}$	77	53
0	4	1	189	239
1	4	1	934	1264
1	4	$\bar{1}$	33	39
2	4	1	347	402
2	4	$\bar{1}$	380	393
3	4	1	395	-380
3	4	$\bar{1}$	586	-557
4	4	1	242	-246
4	4	$\bar{1}$	548	-491

h	k	l	$\lvert 10F_o \rvert$	$10F_c$
5	4	1	77	83
5	4	$\bar{1}$	231	-215
6	4	1	316	311
6	4	$\bar{1}$	84	61
7	4	1	100	81
7	4	$\bar{1}$	30	49
8	4	$\bar{1}$	104	-101
0	5	1	660	864
1	5	1	47	25
1	5	$\bar{1}$	1066	-1266
2	5	1	463	-493
2	5	$\bar{1}$	612	-625
3	5	1	801	-911
3	5	$\bar{1}$	945	-891
4	5	1	57	49
4	5	$\bar{1}$	68	64
5	5	1	173	-164
5	5	$\bar{1}$	35	-40
6	5	1	73	55
6	5	$\bar{1}$	153	145
7	5	1	173	-162
7	5	$\bar{1}$	347	-311
8	5	$\bar{1}$	77	-70
0	6	1	7-	-11
1	6	1	126	106
1	6	$\bar{1}$	163	90
2	6	1	210	-222
2	6	$\bar{1}$	279	267
3	6	1	10-	17
3	6	$\bar{1}$	173	188
4	6	1	153	150
4	6	$\bar{1}$	84	64
5	6	1	12-	-15
5	6	$\bar{1}$	12-	-1
6	6	1	121	-110
6	6	$\bar{1}$	77	-77
7	6	1	9-	-26
7	6	$\bar{1}$	10-	11
8	6	$\bar{1}$	84	65
0	7	1	274	-371
1	7	1	221	218
1	7	$\bar{1}$	369	400
2	7	1	686	-769
2	7	$\bar{1}$	194	-241
3	7	1	157	156
3	7	$\bar{1}$	10-	40
4	7	1	148	-138
4	7	$\bar{1}$	210	-205
5	7	1	269	258
5	7	$\bar{1}$	12-	-9
6	7	1	179	-168
6	7	$\bar{1}$	104	-93
7	7	1	8-	20
7	7	$\bar{1}$	40	43
8	7	$\bar{1}$	121	-103
0	8	1	89	114
1	8	1	539	-633
1	8	$\bar{1}$	142	-147
2	8	1	512	-560
2	8	$\bar{1}$	153	148
3	8	1	11-	-20
3	8	$\bar{1}$	231	221
4	8	1	95	97
4	8	$\bar{1}$	459	446
5	8	1	100	-81
5	8	$\bar{1}$	332	301
6	8	1	121	-112
6	8	$\bar{1}$	89	-102
7	8	1	163	-142
7	8	$\bar{1}$	50	-58
8	8	$\bar{1}$	95	79
0	9	1	289	-307
1	9	1	269	-280
1	9	$\bar{1}$	332	-338
2	9	1	486	480
2	9	$\bar{1}$	490	513
3	9	1	385	372
3	9	$\bar{1}$	226	219
4	9	1	30	44
4	9	$\bar{1}$	168	146
5	9	1	332	-310
5	9	$\bar{1}$	289	-260
6	9	1	30	33
6	9	$\bar{1}$	11-	0
7	9	1	7-	25
7	9	$\bar{1}$	9-	31
0	10	1	90	-80
1	10	1	104	124
1	10	$\bar{1}$	691	745
2	10	1	51	58
2	10	$\bar{1}$	216	214
3	10	1	332	-326
3	10	$\bar{1}$	163	-140
4	10	1	311	-283
4	10	$\bar{1}$	300	-289
5	10	1	84	-86
5	10	$\bar{1}$	45	51
6	10	1	10-	26
6	10	$\bar{1}$	269	251
7	10	1	6-	31

h	k	l	$\lvert 10F_o \rvert$	$10F_c$
7	10	$\bar{1}$	84	78
0	11	1	385	412
1	11	1	173	172
1	11	$\bar{1}$	438	441
2	11	1	11-	-21
2	11	$\bar{1}$	189	-185
3	11	1	12-	-21
3	11	$\bar{1}$	231	-231
4	11	1	12-	14
4	11	$\bar{1}$	279	262
5	11	1	274	253
5	11	$\bar{1}$	289	253
6	11	1	130	114
6	11	$\bar{1}$	95	65
7	11	1	5-	-2
7	11	$\bar{1}$	7-	11
0	12	1	236	245
1	12	1	73	-72
1	12	$\bar{1}$	300	-301
2	12	1	40	-51
2	12	$\bar{1}$	173	-167
3	12	1	104	96
3	12	$\bar{1}$	115	116
4	12	1	130	122
4	12	$\bar{1}$	104	96
5	12	1	189	168
5	12	$\bar{1}$	30	-37
6	12	1	8-	-6
6	12	$\bar{1}$	157	-154
7	12	$\bar{1}$	6-	-36
0	13	1	77	-62
1	13	1	68	-37
1	13	$\bar{1}$	279	286
2	13	1	68	63
2	13	$\bar{1}$	104	109
3	13	1	163	153
3	13	$\bar{1}$	100	96
4	13	1	12-	-11
4	13	$\bar{1}$	168	-159
5	13	1	10-	-32
5	13	$\bar{1}$	100	90
6	13	1	8-	29
6	13	$\bar{1}$	9-	-2
7	13	$\bar{1}$	95	77
0	14	1	100	96
1	14	1	89	100
1	14	$\bar{1}$	163	-155
2	14	1	142	140
2	14	$\bar{1}$	269	-261
3	14	1	12-	30
3	14	$\bar{1}$	12-	10
4	14	1	148	139
4	14	$\bar{1}$	12-	22
5	14	1	115	104
5	14	$\bar{1}$	153	-142
6	14	1	6-	6
6	14	$\bar{1}$	62	-63
0	15	1	194	-175
1	15	1	295	-287
1	15	$\bar{1}$	121	-111
2	15	1	289	269
2	15	$\bar{1}$	332	311
3	15	1	40	50
3	15	$\bar{1}$	12-	7
4	15	1	50	61
4	15	$\bar{1}$	11-	-9
5	15	1	179	-165
5	15	$\bar{1}$	173	-168
6	15	1	42	-41
6	15	$\bar{1}$	7-	4
0	16	1	80	-75
1	16	1	295	278
1	16	$\bar{1}$	168	171
2	16	1	206	195
2	16	$\bar{1}$	40	52
3	16	1	11-	10
3	16	$\bar{1}$	200	-189
4	16	1	130	-124
4	16	$\bar{1}$	173	-160
5	16	1	7-	26
5	16	$\bar{1}$	8-	-28
6	16	$\bar{1}$	5-	28
0	17	1	100	-102
1	17	1	12-	-17
1	17	$\bar{1}$	12-	-2
2	17	1	332	-309
2	17	$\bar{1}$	327	-314
3	17	1	136	-132
3	17	$\bar{1}$	121	-110
4	17	1	77	-73
4	17	$\bar{1}$	221	-199
5	17	1	51	54
5	17	$\bar{1}$	121	117
0	18	1	73	-64
1	18	1	183	-171
1	18	$\bar{1}$	104	-98
2	18	1	157	-143
2	18	$\bar{1}$	57	-50
3	18	1	9-	-17
3	18	$\bar{1}$	115	112

h	k	l	$\lvert 10F_o \rvert$	$10F_c$
4	18	1	68	71
4	18	$\bar{1}$	216	196
5	18	$\bar{1}$	40	44
0	19	1	10-	-7
1	19	1	70	-66
1	19	$\bar{1}$	60	-57
2	19	1	148	144
2	19	$\bar{1}$	168	155
3	19	1	5-	30
3	19	$\bar{1}$	9-	-4
4	19	1	5-	19
4	19	$\bar{1}$	7-	26
0	20	1	110	-93
1	20	1	51	-41
1	20	$\bar{1}$	57	60
2	20	1	62	-64
2	20	$\bar{1}$	62	70
3	20	1	47	-50
3	20	$\bar{1}$	7-	9
4	20	$\bar{1}$	5-	22
0	21	1	73	-70
1	21	1	7-	-6
1	21	$\bar{1}$	40	48
2	21	1	6-	2
2	21	$\bar{1}$	40	42
3	21	$\bar{1}$	57	60
0	22	1	6-	-26
1	22	1	62	54
1	22	$\bar{1}$	100	96
2	22	$\bar{1}$	45	51
0	0	2	744	884
1	0	2	666	657
1	0	$\bar{2}$	438	506
2	0	2	247	-246
2	0	$\bar{2}$	543	600
3	0	2	755	-772
3	0	$\bar{2}$	644	-719
4	0	2	638	611
4	0	$\bar{2}$	206	195
5	0	2	173	181
5	0	$\bar{2}$	274	265
6	0	2	189	162
6	0	$\bar{2}$	443	417
7	0	2	295	-274
0	1	2	596	-613
1	1	2	347	-388
1	1	$\bar{2}$	813	-1015
2	1	2	84	61
2	1	$\bar{2}$	775	-1027
3	1	2	633	606
3	1	$\bar{2}$	516	-476
4	1	2	654	642
4	1	$\bar{2}$	284	295
5	1	2	121	58
5	1	$\bar{2}$	189	168
6	1	2	236	-227
6	1	$\bar{2}$	274	-250
7	1	2	11-	-10
0	2	2	924	-1279
1	2	2	411	309
1	2	$\bar{2}$	512	-536
2	2	2	104	135
2	2	$\bar{2}$	559	-625
3	2	2	62	-46
3	2	$\bar{2}$	660	715
4	2	2	527	-493
4	2	$\bar{2}$	512	-477
5	2	2	14-	-24
5	2	$\bar{2}$	179	-158
6	2	2	168	-152
6	2	$\bar{2}$	385	-351
7	2	2	153	134
0	3	2	638	731
1	3	2	1098	1247
1	3	$\bar{2}$	574	606
2	3	2	84	61
2	3	$\bar{2}$	236	-275
3	3	2	289	274
3	3	$\bar{2}$	337	-350
4	3	2	13-	3
4	3	$\bar{2}$	342	-336
5	3	2	110	104
5	3	$\bar{2}$	189	-163
6	3	2	126	116
6	3	$\bar{2}$	263	-261
7	3	2	104	91
0	4	2	142	-76
1	4	2	580	573
1	4	$\bar{2}$	596	-755
2	4	2	521	514
2	4	$\bar{2}$	274	275
3	4	2	153	162
3	4	$\bar{2}$	448	438
4	4	2	126	113
4	4	$\bar{2}$	601	559
5	4	2	206	-191
5	4	$\bar{2}$	104	-93
6	4	2	115	101
6	4	$\bar{2}$	42	31
7	4	2	10-	31

h	k	l	$\lvert 10F_o \rvert$	$10F_c$
0	5	2	501	555
1	5	2	960	1176
1	5	$\bar{2}$	47	63
2	5	2	73	68
2	5	$\bar{2}$	385	428
3	5	2	400	-384
3	5	$\bar{2}$	258	-261
4	5	2	14-	-17
4	5	$\bar{2}$	390	-372
5	5	2	242	224
5	5	$\bar{2}$	126	-117
6	5	2	269	250
6	5	$\bar{2}$	14-	2
7	5	2	104	96
0	6	2	902	1229
1	6	2	433	-460
1	6	$\bar{2}$	242	268
2	6	2	559	-562
2	6	$\bar{2}$	311	-314
3	6	2	264	-277
3	6	$\bar{2}$	539	-547
4	6	2	194	164
4	6	$\bar{2}$	12-	-28
5	6	2	337	315
5	6	$\bar{2}$	194	175
6	6	2	40	44
6	6	$\bar{2}$	200	200
7	6	2	100	-86
0	7	2	506	-552
1	7	2	824	-956
1	7	$\bar{2}$	9-	-75
2	7	2	691	-711
2	7	$\bar{2}$	459	-477
3	7	2	104	106
3	7	$\bar{2}$	263	260
4	7	2	14-	31
4	7	$\bar{2}$	543	544
5	7	2	95	-78
5	7	$\bar{2}$	364	382
6	7	2	284	-270
6	7	$\bar{2}$	126	-121
7	7	2	231	-181
0	8	2	422	-485
1	8	2	148	152
1	8	$\bar{2}$	10-	-14
2	8	2	142	157
2	8	$\bar{2}$	194	208
3	8	2	475	468
3	8	$\bar{2}$	416	437
4	8	2	231	-219
4	8	$\bar{2}$	13-	-18
5	8	2	148	-145
5	8	$\bar{2}$	247	-230
6	8	2	62	-63
6	8	$\bar{2}$	206	-201
7	8	2	183	140
0	9	2	157	-191
1	9	2	210	202
1	9	$\bar{2}$	543	575
2	9	2	279	274
2	9	$\bar{2}$	539	576
3	9	2	453	-429
3	9	$\bar{2}$	13-	47
4	9	2	274	-250
4	9	$\bar{2}$	14-	-1
5	9	2	115	-111
5	9	$\bar{2}$	35	39
6	9	2	77	80
6	9	$\bar{2}$	247	235
7	9	2	7-	-34
0	10	2	210	243
1	10	2	353	-353
1	10	$\bar{2}$	433	-450
2	10	2	200	198
2	10	$\bar{2}$	62	46
3	10	2	200	-191
3	10	$\bar{2}$	295	-309
4	10	2	14-	32
4	10	$\bar{2}$	221	208
5	10	2	121	-114
5	10	$\bar{2}$	110	-98
6	10	2	11-	7
6	10	$\bar{2}$	13-	-21
0	11	2	35	41
1	11	2	200	195
1	11	$\bar{2}$	279	288
2	11	2	40	54
2	11	$\bar{2}$	194	191
3	11	2	258	-243
3	11	$\bar{2}$	68	83
4	11	2	200	-180
4	11	$\bar{2}$	100	-96
5	11	2	73	64
5	11	$\bar{2}$	115	-104
6	11	2	10-	30
6	11	$\bar{2}$	42	42
0	12	2	179	186
1	12	2	210	209
1	12	$\bar{2}$	633	638
2	12	2	512	-506

h	k	l	$\lvert 10F_o \rvert$	$10F_c$
2	12	$\bar{2}$	305	-306
3	12	2	14-	-5
3	12	$\bar{2}$	136	-132
4	12	2	14-	17
4	12	$\bar{2}$	173	-176
5	12	2	263	247
5	12	$\bar{2}$	322	313
6	12	2	31	-31
6	12	$\bar{2}$	77	69
0	13	2	121	121
1	13	2	206	-202
1	13	$\bar{2}$	490	-497
2	13	2	50	59
2	13	$\bar{2}$	486	-479
3	13	2	210	196
3	13	$\bar{2}$	68	-60
4	13	2	353	334
4	13	$\bar{2}$	269	260
5	13	2	69	79
5	13	$\bar{2}$	100	-84
6	13	2	30	-35
6	13	$\bar{2}$	210	-204
0	14	2	358	-353
1	14	2	295	-283
1	14	$\bar{2}$	337	-339
2	14	2	274	255
2	14	$\bar{2}$	258	243
3	14	2	142	126
3	14	$\bar{2}$	153	137
4	14	2	40	49
4	14	$\bar{2}$	14-	-7
5	14	2	258	-245
5	14	$\bar{2}$	247	-230
6	14	2	5-	-28
6	14	$\bar{2}$	47	-51
0	15	2	104	109
1	15	2	332	306
1	15	$\bar{2}$	14-	38
2	15	2	210	196
2	15	$\bar{2}$	30	-39
3	15	2	14-	-14
3	15	$\bar{2}$	221	-192
4	15	2	40	-42
4	15	$\bar{2}$	269	-244
5	15	2	115	106
5	15	$\bar{2}$	115	-83
6	15	$\bar{2}$	42	35
0	16	2	179	164
1	16	2	115	101
1	16	$\bar{2}$	274	271
2	16	2	89	-83
2	16	$\bar{2}$	40	-44
3	16	2	13-	26
3	16	$\bar{2}$	40	42
4	16	2	42	49
4	16	$\bar{2}$	13-	-22
5	16	2	68	65
5	16	$\bar{2}$	89	85
6	16	$\bar{2}$	89	77
0	17	2	14-	13
1	17	2	14-	30
1	17	$\bar{2}$	50	42
2	17	2	13-	16
2	17	$\bar{2}$	100	90
3	17	2	12-	28
3	17	$\bar{2}$	13-	19
4	17	2	73	-75
4	17	$\bar{2}$	35	-40
5	17	$\bar{2}$	9-	-25
6	17	$\bar{2}$	4-	-2
0	18	2	84	90
1	18	2	13-	17
1	18	$\bar{2}$	115	113
2	18	2	121	-119
2	18	$\bar{2}$	68	-69
3	18	2	68	-61
3	18	$\bar{2}$	168	-153
4	18	2	7-	30
4	18	$\bar{2}$	77	-71
5	18	$\bar{2}$	84	83
0	19	2	168	-155
1	19	2	295	-268
1	19	$\bar{2}$	100	-87
2	19	2	163	-146
2	19	$\bar{2}$	11-	-19
3	19	2	9-	21
3	19	$\bar{2}$	168	151
4	19	2	5-	24
4	19	$\bar{2}$	153	148
0	20	2	168	-158
1	20	2	136	-120
1	20	$\bar{2}$	110	-98
2	20	2	200	185
2	20	$\bar{2}$	163	143
3	20	2	84	65
3	20	$\bar{2}$	68	58
4	20	2	6-	26
0	21	2	9-	-25
1	21	2	68	57
1	21	$\bar{2}$	148	132

Table 4 (*cont.*)

h	k	l	$10F_o$	$10F_c$
2	21	2	6-	-8
2	21	3	115	105
3	21	2	6-	16
0	22	2	6-	-8
1	22	2	5-	28
1	22	3	84	72
0	1	3	385	-401
1	1	3	226	-180
1	1	3	548	-633
2	1	3	453	-442
2	1	3	554	-452
3	1	3	342	-321
3	1	3	448	-448
4	1	3	50	-54
4	1	3	10-	20
5	1	3	62	-58
6	1	3	168	-161
0	1	3	40	-45
6	1	3	12-	-27
7	1	3	115	-111
0	2	3	210	288
1	2	3	385	-388
1	2	3	766	-896
2	2	3	206	-211
2	2	3	670	-878
3	2	3	374	360
3	2	3	148	130
4	2	3	300	284
4	2	3	295	283
5	2	3	194	180
5	2	3	153	133
6	2	3	40	-44
6	2	3	332	-293
7	2	3	8-	6
0	3	3	707	-845
1	3	3	433	400
1	3	3	279	246
2	3	3	411	420
2	3	3	194	260
3	3	3	618	604
3	3	3	929	1027
4	3	3	311	-291
4	3	3	136	-136
5	3	3	173	-166
5	3	3	236	-219
6	3	3	84	-92
6	3	3	247	-213
7	3	3	153	150
0	4	3	100	111
1	4	3	801	843
1	4	3	866	1137
2	4	3	654	650
2	4	3	7-	105
3	4	3	183	-184
3	4	3	353	-355
4	4	3	406	-375
4	4	3	722	-732
5	4	3	35	-38
5	4	3	300	-285
6	4	3	226	218
6	4	3	168	158
7	4	3	95	88
0	5	3	960	1161
1	5	3	77	-73
1	5	3	50	65
2	5	3	179	149
2	5	3	279	264
3	5	3	443	-420
3	5	3	592	-630
4	5	3	380	353
4	5	3	443	435
5	5	3	194	187
5	5	3	148	136
6	5	3	226	226
6	5	3	279	260
7	5	3	68	-68
0	6	3	258	-266
1	6	3	100	-116
1	6	3	342	-353
2	6	3	40	-52
2	6	3	316	-346
3	6	3	11-	17
3	6	3	327	327
4	6	3	73	-66
4	6	3	284	280
5	6	3	126	132
5	6	3	157	137
6	6	3	50	-52
6	**6**	**3**	**168**	**-137**
7	6	3	6-	-24
0	7	3	68	93
1	7	3	448	455
1	7	3	316	344
2	7	3	148	123
2	7	3	173	-153
3	7	3	279	261
3	7	3	569	562
4	7	3	62	-43
4	7	3	110	-113
5	7	3	210	190
5	7	3	347	346
6	7	3	10-	7
6	7	3	13-	-18
7	7	3	100	86
0	8	3	284	-306
1	8	3	153	-168
1	8	3	100	93
2	8	3	11-	10
2	8	3	231	-244
3	8	3	30	-38
3	8	3	179	199
4	8	3	73	61
4	8	3	374	375
5	8	3	40	-43
5	8	3	12-	-33
6	8	3	68	-65
6	8	3	13-	-8
0	9	3	475	-537
1	9	3	390	-389
1	9	3	596	-666
2	9	3	400	367
2	9	3	601	638
3	9	3	50	61
3	9	3	242	251
4	9	3	89	99
4	9	3	89	53
5	9	3	258	-241
5	9	3	390	-369
6	9	3	110	-108
6	9	3	179	-154
0	10	3	284	-274
1	10	3	469	463
1	10	3	533	566
2	10	3	194	176
2	10	3	548	547
3	10	3	406	-419
3	10	3	221	-202
4	10	3	411	-403
4	10	3	274	-268
5	10	3	35	-39
5	10	3	13-	-5
6	10	3	121	126
6	10	3	206	202
0	11	3	411	442
1	11	3	12-	20
1	11	3	11-	13
2	11	3	586	-585
2	11	3	633	-638
3	11	3	438	-437
3	11	3	501	-511
4	11	3	50	-52
4	11	3	300	-307
5	11	3	110	114
5	11	3	183	189
6	11	3	7-	-12
6	11	3	115	109
0	12	3	90	72
1	12	3	148	-132
1	12	3	258	-284
2	12	3	77	-71
2	12	3	300	-294
3	12	3	173	167
3	12	3	84	-74
4	12	3	221	210
4	12	3	274	270
5	12	3	10-	22
5	12	3	12-	-4
6	12	3	6-	-6
6	12	3	126	-127
0	13	3	206	-195
1	13	3	12-	40
1	13	3	12-	-11
2	13	3	163	-159
2	13	3	50	-71
3	13	3	12-	11
3	13	3	13-	-16
4	13	3	104	-106
4	13	3	89	-94
5	13	3	30	-37
5	13	3	77	-76
6	13	3	65	-75
6	13	3	77	-66
0	14	3	64	58
1	14	3	13-	-33
1	14	3	163	-149
2	14	3	30	36
2	14	3	13-	-12
3	14	3	45	52
3	**14**	**3**	**77**	**-61**
4	14	3	84	87
4	14	3	12-	-8
5	14	3	8-	2
5	14	3	11-	15
6	14	3	100	-99
0	15	3	13-	-18
1	15	3	121	-125
1	15	3	13-	-18
2	15	3	274	269
2	15	3	289	278
3	15	3	210	199
3	15	3	247	228
4	15	3	100	96
4	15	3	183	172
5	15	3	95	-94
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3	6	5	242	-233
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3	13	5	9-	-35
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Table 4 (*cont.*)

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3	15	5	73	62
4	15	5	6-	-2
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5	15	5	68	-68
6	15	5	47	-54
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2	16	5	9-	10
2	16	5	258	245
3	16	5	142	-137
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4	16	5	121	-127
4	16	5	153	-147
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1	17	5	50	48
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2	17	5	183	-184
2	17	5	163	-160
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1	18	5	110	-120
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3	18	5	84	83
3	18	5	100	-93
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5	18	5	35	30
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3	19	5	7-	23
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2	20	5	57	-55
3	20	5	95	-87
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1	11	6	216	225
2	11	6	9-	27
3	11	6	57	55
3	11	6	8-	13
4	11	6	30	37
4	11	6	89	-93
5	11	6	104	-116
5	11	6	4-	5
6	11	6	42	48
7	11	6	42	54
0	12	6	110	89
1	12	6	168	131
1	12	6	436	428
2	12	6	200	-210
2	12	6	183	-193
3	12	6	84	95
3	12	6	9-	19
4	12	6	6-	25
4	12	6	9-	16
5	12	6	279	275
6	12	6	8-	8
7	12	6	47	65
0	13	6	168	-167
1	13	6	350	-303
1	13	6	104	-114
2	13	6	77	-80
2	13	6	226	-218
3	13	6	7-	11
3	13	6	163	168
4	13	6	57	58
4	13	6	316	315
5	13	6	115	120
6	13	6	42	-48
7	13	6	51	-46
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1	14	6	295	-303
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2	14	6	25	34
3	14	6	6-	24
3	14	6	77	83
4	14	6	4-	-7
4	14	6	62	65
5	14	6	183	-187
6	14	6	95	-97
0	15	6	110	-113
1	15	6	8-	22
1	15	6	189	184
2	15	6	31	-44
2	15	6	121	122
3	15	6	68	-86
3	15	6	57	69
4	15	6	8-	-24
5	15	6	7-	-14
6	15	6	148	132
0	16	6	6-	18
1	16	6	8-	-1
1	16	6	8-	23
2	16	6	104	-116
2	16	6	110	-108
3	16	6	20	-38
3	16	6	8-	-16
4	16	6	7-	-29
5	16	6	36	36
6	16	6	31	-29
0	17	6	7-	-6
1	17	6	7-	13
1	17	6	84	-64
2	17	6	25	33
2	17	6	51	50
3	17	6	3-	-5
3	17	6	7-	15
4	17	6	6-	-21
5	17	6	5-	-22
0	18	6	42	50
1	18	6	6-	-23
1	18	6	7-	-2
2	18	6	73	-71
2	18	6	77	-84
3	18	6	36	-43
4	18	6	73	-60
5	18	6	4-	21
0	19	6	5-	16
1	19	6	36	-34
1	19	6	104	-105
2	19	6	95	-98
3	19	6	5-	-18
4	19	6	4-	27
0	20	6	62	-73
1	20	6	2-	8
1	20	6	84	-84
2	20	6	100	101
3	20	6	62	68
1	21	6	1-	-9
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1	1	7	36	47
1	1	7	506	472
2	1	7	95	89
2	1	7	353	326
3	1	7	10-	-20
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4	1	7	77	-80
5	1	7	145	145
5	1	7	347	336
6	1	7	289	290
7	1	7	443	-443
1	2	7	322	-296
2	2	7	210	-221
2	2	7	145	-156
3	2	7	665	-664
3	2	7	289	278
4	2	7	226	-220
4	2	7	168	158
5	2	7	416	423
6	2	7	47	-43
7	2	7	380	357
0	3	7	110	-92
1	3	7	612	-582
1	3	7	358	331
2	3	7	142	-142
2	3	7	263	256
3	3	7	142	-139
3	3	7	559	556
4	3	7	300	-295
4	3	7	57	57
5	3	7	73	-79
5	3	7	9-	-27
6	3	7	322	-297
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1	4	7	374	345
1	4	7	364	358
2	4	7	42	-56
2	4	7	486	497
3	4	7	327	-320
3	4	7	179	179
4	4	7	115	-112
4	4	7	226	-191
5	4	7	6-	16
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6	4	7	68	-62
7	4	7	342	342
1	5	7	475	-482
2	5	7	269	-279
2	5	7	183	-195
3	5	7	7-	-29
3	5	7	236	-225
4	5	7	654	-672
4	5	7	68	73
5	5	7	66	-75
5	5	7	62	-63
6	5	7	210	-185
6	5	7	173	158
0	6	7	183	-191
1	6	7	9-	17
1	6	7	163	-171
2	6	7	104	-114
2	6	7	173	-176
3	6	7	110	107
3	6	7	126	123
4	6	7	36	32
4	6	7	153	142
5	6	7	6-	20
5	6	7	10-	20
6	6	7	84	-70
0	7	7	168	-154
1	7	7	9-	-36
1	7	7	231	230
2	7	7	374	-351
2	7	7	300	-298
3	7	7	10-	-11
3	7	7	77	-84
4	7	7	95	-100
4	7	7	316	-303
5	7	7	47	48
5	7	7	10-	-32
6	7	7	62	-73
7	7	7	126	117
0	8	7	89	-81
1	8	7	279	-283
1	8	7	274	-265
2	8	7	168	168
2	8	7	327	-311
3	8	7	157	158
3	8	7	84	-64
4	8	7	89	97
4	8	7	142	158
5	8	7	31	-33
5	8	7	89	89
6	8	7	89	-91
7	8	7	153	-141
0	9	7	9-	-14
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1	9	7	543	-536
2	9	7	327	321
2	9	7	289	260
3	9	7	100	95
3	9	7	305	312
4	9	7	7-	-22
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5	9	7	89	-106
5	9	7	148	-130
6	9	7	68	-67
7	9	7	30	-36
0	10	7	115	101
1	10	7	126	126
1	10	7	89	78
2	10	7	62	-65
2	10	7	168	211
3	10	7	142	-143
3	10	7	104	114
4	10	7	62	-65
4	10	7	194	-192
5	10	7	168	-170
6	10	7	130	125
7	10	7	89	93
1	11	7	236	232
1	11	7	136	131
2	11	7	360	361
2	11	7	84	-86
3	11	7	10-	22
3	11	7	8-	8
4	11	7	89	-92
4	11	7	157	159
5	11	7	10-	17
5	11	7	179	173
6	11	7	142	147
7	11	7	57	51
1	12	7	77	72
1	12	7	148	-154
2	12	7	206	-193
2	12	7	47	43
3	12	7	95	-106
3	12	7	110	112
4	12	7	62	-65
4	12	7	51	53
5	12	7	104	105
6	12	7	89	-86
7	12	7	77	-67
1	13	7	51	43
1	13	7	77	90
2	13	7	100	99
2	13	7	8-	-5
3	13	7	77	63
3	13	7	77	84
4	13	7	142	149
4	13	7	4-	-3
5	13	7	42	-45
5	13	7	73	63
6	13	7	7-	-3
7	13	7	73	-76
1	14	7	110	-106
1	14	7	62	56
2	14	7	8-	-31
2	14	7	68	-54
3	14	7	6-	27
3	14	7	73	72
4	14	7	95	81
5	14	7	73	68
6	14	7	6-	22
0	15	7	142	-134
1	15	7	84	-82
2	15	7	236	-200
2	15	7	115	119
3	15	7	9-	-19
3	15	7	62	57
4	15	7	126	121
5	15	7	189	-182
6	15	7	100	-88
0	16	7	68	64
1	16	7	89	85
1	16	7	51	47
2	16	7	6-	-5
2	16	7	189	180
3	16	7	8-	5
4	16	7	84	-87
5	16	7	62	-61
6	16	7	42	45
0	17	7	7-	-18
1	17	7	57	-59
1	17	7	51	68
2	17	7	206	-198
2	17	7	210	-198
3	17	7	115	-107
4	17	7	163	-161
5	17	7	42	44
6	17	7	62	-61
1	18	7	62	-69
1	18	7	57	-54
2	18	7	89	-95
3	18	7	51	46
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0	19	7	31	-31
1	19	7	77	-83
2	19	7	42	44
3	19	7	5-	-9
4	19	7	36	52
5	20	7	3-	-8
6	20	7	3-	-8
0	0	8	660	666
1	0	8	395	311
2	0	8	142	-155
3	0	8	183	-159
4	0	8	486	-485
5	0	8	289	285
6	0	8	51	39
7	0	8	62	53
0	1	8	226	218
1	1	8	490	482
2	1	8	104	-95
3	1	8	247	-216
4	1	8	459	-454
5	1	8	9-	-23
6	1	8	559	-539
7	1	8	269	265
0	2	8	121	119
1	2	8	179	-160
2	2	8	231	228
3	2	8	427	391
4	2	8	157	-155
5	2	8	25	26
6	2	8	9-	-12
7	2	8	142	-126
0	3	8	179	175
1	3	8	9-	27
2	3	8	51	52
3	3	8	73	79
4	3	8	142	127
5	3	8	89	82
6	3	8	57	-40
7	3	8	7-	15
0	4	8	210	-193
1	4	8	4-	-21
2	4	8	47	-39
3	4	8	95	-88
4	4	8	136	-139
5	4	8	163	-169
6	4	8	327	-322
7	4	8	157	141
0	5	8	7-	15
1	5	8	68	-71
2	5	8	157	148
3	5	8	31	-37
4	5	8	353	-340
5	5	8	89	87
6	5	8	258	-237
7	5	8	9-	11
0	6	8	183	171
1	6	8	236	-217
2	6	8	274	262
3	6	8	269	-254
4	6	8	194	-202
5	6	8	153	-161
6	6	8	559	-573
7	6	8	7-	-3
0	7	8	179	-150
1	7	8	95	92
2	7	8	148	132
3	7	8	47	-43
4	7	8	374	-373
5	7	8	433	-429
6	7	8	183	-199
7	7	8	236	-225
0	8	8	194	-200
1	8	8	73	74
2	8	8	179	193
3	8	8	25	44
4	8	8	506	506
5	8	8	231	215
6	8	8	57	-53
7	8	8	42	-40
0	9	8	295	-294
1	9	8	9-	32
2	9	8	189	-189
3	9	8	126	117
4	9	8	8-	3
5	9	8	57	65
6	9	8	316	315
7	9	8	121	-115
0	10	8	126	-131
1	10	8	142	129
2	10	8	77	67
3	10	8	95	79
4	10	8	134	-126
5	10	8	89	100
6	10	8	5-	-26
7	10	8	136	-126
0	11	8	231	226
1	11	8	121	-103
2	11	8	95	106
3	11	8	231	229
4	11	8	7-	-16
5	11	8	9-	-15
6	11	8	134	102
7	11	8	179	171
0	12	8	73	-73
1	12	8	142	141
2	12	8	31	-48
3	12	8	9-	15
4	12	8	77	83
5	12	8	48	-52
6	12	8	157	159
7	12	8	51	-54
0	13	8	253	243
1	13	8	57	-60
2	13	8	62	59
3	13	8	17	17
4	13	8	9-	17
5	13	8	121	-110
6	13	8	7-	10
7	13	8	42	62
0	14	8	148	149
1	14	8	153	156
2	14	8	284	273
3	14	8	157	-159
4	14	8	100	-93
5	14	8	30	36
6	14	8	57	54
7	14	8	126	-126
0	15	8	284	266
1	15	8	148	141
2	15	8	100	105
3	15	8	30	39
4	15	8	194	-189
5	15	8	231	-217
6	15	8	7-	23
7	15	8	279	-261
0	16	8	153	150
1	16	8	57	-50
2	16	8	134	101
3	16	8	73	63
4	16	8	115	-111
5	16	8	126	-137
6	16	8	7-	-12
7	16	8	200	-202
0	17	8	148	150
1	17	8	200	184
2	17	8	51	54
3	17	8	153	141
4	17	8	134	104
5	17	8	236	-218
6	17	8	62	-58
7	17	8	95	100
0	18	8	104	111
1	18	8	8-	3
2	18	8	5-	24
3	18	8	121	115
4	18	8	84	-64
5	18	8	153	-148
6	18	8	57	-58
7	18	8	47	43
0	19	8	7-	-22
1	19	8	47	-42
2	19	8	57	53
3	19	8	84	-86
4	19	8	110	-96
5	19	8	73	-70
6	19	8	57	-61
7	19	8	5-	0
0	20	8	2-	-1
1	20	8	6-	14
2	20	8	4-	10
3	20	8	57	64
4	20	8	42	34
5	20	8	6-	7

Table 4 (*cont.*)

h	k	l	$10F_o$	$10F_c$
4	17	$\bar{7}$	47	-27
5	17	$\bar{8}$	4-	4
0	18	$\bar{8}$	4-	-3
1	18	$\bar{8}$	31	31
2	18	$\bar{8}$	73	-72
3	18	$\bar{8}$	100	-105
4	18	$\bar{8}$	77	-70
1	19	$\bar{8}$	3-	0
2	19	$\bar{8}$	52	-55
3	19	$\bar{8}$	57	58
1	0	9	26-	0
0	1	9	153	140
1	1	9	126	-113
1	1	9	51	37
2	1	9	40	-42
2	1	9	4-	-7
3	1	9	31	31
3	1	9	189	-141
4	1	9	30	38
4	1	9	136	130
5	1	9	77	-76
6	1	9	95	77
0	2	9	7-	-2
1	2	9	62	-50
1	2	9	427	-345
2	2	9	157	152
2	2	9	342	-301
3	2	9	189	188
3	2	9	153	-115
4	2	9	62	63
4	2	9	62	-50
5	2	9	73	-62
6	2	9	51	-51
0	3	9	274	-249
1	3	9	221	186
1	3	9	148	-127
2	3	9	104	99
2	3	9	173	-144
3	3	9	104	100
3	3	9	395	373
4	3	9	173	-165
4	3	9	77	58
5	3	9	8-	17
6	3	9	242	-216
0	4	9	322	303
1	4	9	130	120
1	4	9	57	33
2	4	9	104	97
2	4	9	110	89
3	4	9	77	-75
3	4	9	121	109
4	4	9	5-	-7
4	4	9	380	-371
5	4	9	289	-276
6	4	9	95	63
0	5	9	258	231
1	5	9	110	-93
1	5	9	73	69
2	5	9	8-	-9
2	5	9	216	202
3	5	9	168	-161
3	5	9	422	-399
4	5	9	136	135
4	5	9	8-	-8
5	5	9	8-	2
5	5	$\bar{9}$	216	185
0	6	9	8-	-10
1	6	9	77	-64
1	6	9	168	-161
2	6	9	47	-52
2	6	9	84	91
3	6	9	31	24
3	6	9	130	122
4	6	9	4-	-26
4	6	9	121	110
5	6	9	8-	-25
6	6	9	8-	-11
0	7	9	216	-197
1	7	9	84	66
1	7	9	77	71
2	7	9	42	-43
2	7	9	142	-131
3	7	9	68	69
3	7	9	206	183
4	7	9	62	-60
4	7	9	231	-224
5	7	9	173	166
6	7	9	121	-98
0	8	9	84	-77
1	8	9	173	-169
1	8	9	136	139
2	8	9	104	-116
2	8	9	42	-32
3	8	9	6-	17
3	8	9	73	84
4	8	9	3-	13
4	8	9	121	114
5	8	9	130	125
6	8	9	62	47
0	9	9	100	-105
1	9	9	8-	1
1	9	9	221	-196
2	9	9	148	155
2	9	9	148	126
3	9	9	42	-44
3	9	9	95	85
4	9	9	130	135
5	9	9	115	-118
6	9	9	57	-62
0	10	9	36	47
1	10	9	62	73
1	10	9	130	126
2	10	9	100	-104
2	10	9	433	411
3	10	9	173	-170
3	10	9	126	117
4	10	9	100	-87
5	10	9	57	-54
6	10	9	100	94
0	11	9	183	175
1	11	9	62	-78
1	11	9	142	140
2	11	9	110	-109
2	11	9	104	-105
3	11	9	4-	-15
3	11	9	183	-175
4	11	9	126	-118
5	11	9	104	94
6	11	9	126	117
0	12	9	8-	30
1	12	9	7-	-2
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2	12	9	6-	-19
2	12	9	168	-165
3	12	9	103	114
3	12	9	68	-52
4	12	9	8-	19
5	12	9	7-	-13
6	12	9	104	-91
0	13	9	57	-61
1	13	9	51	53
1	13	9	84	75
2	13	9	5-	-9
2	13	9	68	46
3	13	9	62	61
4	13	9	7-	-3
5	13	9	7-	-1
6	13	9	5-	-19
0	14	9	32	36
1	14	9	6-	-1
2	14	9	84	-89
2	14	9	89	87
3	14	9	68	-62
3	14	9	57	-59
4	14	9	57	-54
5	14	9	6-	-7
6	14	9	4-	-28
0	15	9	6-	16
1	15	9	51	-39
1	15	9	130	-129
2	15	9	100	91
3	15	9	6-	22
4	15	9	110	-100
5	15	9	95	-83
0	16	9	84	86
1	16	9	142	139
1	16	9	31	31
2	16	9	73	81
3	16	9	6-	-8
4	16	9	104	-92
5	16	9	126	-103
0	17	9	3-	9
1	17	9	148	138
2	17	9	84	-70
3	17	9	77	-65
4	17	9	89	-80
1	18	9	2-	4
2	18	9	51	-71
3	18	9	3-	10
0	0	10	189	152
1	0	10	342	-305
2	0	10	5-	18
3	0	10	130	-127
4	0	10	126	101
5	0	10	221	-209
6	0	10	748	-677
1	1	10	5-	-19
2	1	10	89	-113
3	1	10	179	-172
4	1	10	51	-47
5	1	10	253	-209
6	1	10	173	-141
1	1	10	179	169
2	1	10	231	-196
4	1	$\bar{10}$	194	153
5	1	$\bar{10}$	73	-77
6	1	$\bar{10}$	77	-103
0	2	10	264	-241
1	2	10	130	100
2	2	$\bar{10}$	95	-89
2	2	$\bar{10}$	73	69
2	2	$\bar{10}$	104	-84
3	2	10	121	113
3	2	$\bar{10}$	400	354
4	2	$\bar{10}$	121	-109
5	2	$\bar{10}$	68	51
2	2	$\bar{10}$	295	-261
0	3	10	168	154
1	3	$\bar{10}$	77	86
1	3	$\bar{10}$	89	70
2	3	$\bar{10}$	57	40
2	3	$\bar{10}$	68	-73
3	3	$\bar{10}$	62	-56
3	3	$\bar{10}$	5-	26
4	3	$\bar{10}$	57	-52
5	3	$\bar{10}$	157	-144
6	3	$\bar{10}$	30	32
0	4	10	31	-7
1	4	10	25	28
1	4	$\bar{10}$	121	-100
2	4	$\bar{10}$	100	102
2	4	$\bar{10}$	173	147
3	4	$\bar{10}$	4-	6
4	4	$\bar{10}$	5-	9
4	4	$\bar{10}$	189	167
5	4	$\bar{10}$	110	-100
6	4	$\bar{10}$	77	62
0	5	10	206	199
1	5	10	216	195
1	5	$\bar{10}$	6-	-21
2	5	10	47	31
2	5	$\bar{10}$	226	219
3	5	$\bar{10}$	57	-61
3	5	$\bar{10}$	148	-124
4	5	$\bar{10}$	242	-218
5	5	$\bar{10}$	200	-171
6	5	$\bar{10}$	6-	-7
0	6	10	263	260
1	6	10	6-	-11
1	6	$\bar{10}$	284	266
2	6	10	89	-89
2	6	$\bar{10}$	47	52
3	6	10	31	32
3	6	$\bar{10}$	57	-47
4	6	$\bar{10}$	100	-98
5	6	$\bar{10}$	221	183
6	6	$\bar{10}$	247	234
0	7	10	189	-179
1	7	10	247	-234
1	7	$\bar{10}$	51	45
2	7	10	77	-85
2	7	$\bar{10}$	104	-95
3	7	10	95	91
3	7	$\bar{10}$	6-	-11
4	7	$\bar{10}$	221	192
5	7	$\bar{10}$	247	222
6	7	$\bar{10}$	110	93
0	8	10	206	-206
1	8	10	142	132
1	8	$\bar{10}$	84	-71
2	8	$\bar{10}$	62	64
2	8	$\bar{10}$	100	-94
3	8	$\bar{10}$	57	63
3	8	$\bar{10}$	253	228
4	8	$\bar{10}$	68	78
5	8	$\bar{10}$	57	-60
6	8	$\bar{10}$	194	-176
0	9	10	142	139
1	9	10	25	30
2	9	10	73	53
2	9	10	5-	-28
2	9	$\bar{10}$	231	209
3	9	10	77	-89
3	9	$\bar{10}$	77	74
4	9	$\bar{10}$	163	-148
5	9	$\bar{10}$	6-	-12
6	9	$\bar{10}$	5-	17
0	10	10	57	60
1	10	10	142	-136
1	10	$\bar{10}$	77	-69
2	10	10	51	40
2	10	$\bar{10}$	6-	8
3	10	$\bar{10}$	179	-167
4	10	$\bar{10}$	42	32
5	10	$\bar{10}$	89	-89
6	10	$\bar{10}$	25	19
0	11	10	6-	22
1	11	10	84	82
1	11	$\bar{10}$	84	80
2	11	10	31	-41
2	11	$\bar{10}$	206	185
3	11	$\bar{10}$	95	86
4	11	$\bar{10}$	84	-72
5	11	$\bar{10}$	51	-60
6	11	$\bar{10}$	62	50
0	12	10	51	-58
1	12	10	62	-53
1	12	$\bar{10}$	173	165
2	12	10	189	-185
2	12	$\bar{10}$	148	-134
3	12	$\bar{10}$	126	-127
4	12	$\bar{10}$	179	-160
5	12	$\bar{10}$	110	103
6	12	$\bar{10}$	4-	-6
0	13	10	77	-77
1	13	10	89	-84
1	13	$\bar{10}$	126	-98
2	13	$\bar{10}$	253	-235
3	13	$\bar{10}$	62	-59
4	13	$\bar{10}$	51	55
5	13	$\bar{10}$	104	92
0	14	10	4-	11
1	14	10	36	31
1	14	$\bar{10}$	168	-157
2	14	$\bar{10}$	57	56
3	14	$\bar{10}$	51	55
4	14	$\bar{10}$	142	131
5	14	$\bar{10}$	73	-64
0	15	10	95	85
1	15	$\bar{10}$	4-	-8
2	15	$\bar{10}$	62	56
3	15	$\bar{10}$	4-	-9
4	15	$\bar{10}$	110	-89
5	15	$\bar{10}$	126	-107
1	16	$\bar{10}$	57	55
2	16	$\bar{10}$	20	28
3	16	$\bar{10}$	3-	25
3	17	$\bar{10}$	2-	10
0	1	11	10-	-10
1	1	11	130	-116
2	1	11	51	-50
0	2	11	84	-98
1	2	11	115	-93
2	2	11	68	-62
3	3	11	258	-241
1	3	11	89	73
2	3	11	51	39
6	3	$\bar{11}$	210	-203
0	4	11	126	131
1	4	11	142	126
2	4	11	7-	5
4	4	$\bar{11}$	173	-158
5	4	$\bar{11}$	60	-63
6	4	$\bar{11}$	40	45
0	5	11	322	292
1	5	11	89	-76
2	5	11	77	77
3	5	$\bar{11}$	226	-177
4	5	$\bar{11}$	153	142
5	5	$\bar{11}$	9-	11
6	5	$\bar{11}$	279	250
0	6	11	45	-52
1	6	11	9-	14
2	6	$\bar{11}$	6-	-2
3	6	$\bar{11}$	173	-153
4	6	$\bar{11}$	10-	13
5	6	$\bar{11}$	40	33
6	6	$\bar{11}$	7-	9
0	7	11	10-	-37
1	7	11	126	111
2	7	$\bar{11}$	77	-69
3	7	$\bar{11}$	104	107
4	7	$\bar{11}$	9-	-25
5	7	$\bar{11}$	148	125
6	7	$\bar{11}$	30	-31
0	8	11	9-	-6
1	8	11	50	-43
2	8	$\bar{11}$	40	46
3	8	$\bar{11}$	126	-117
4	8	$\bar{11}$	10-	4
5	8	$\bar{11}$	9-	11
6	8	$\bar{11}$	84	71
0	9	11	45	-33
1	9	11	157	131
2	9	$\bar{11}$	9-	22
3	9	$\bar{11}$	40	47
4	9	$\bar{11}$	194	164
5	9	$\bar{11}$	142	-126
6	9	$\bar{11}$	68	-58
0	10	11	84	78
1	10	11	95	83
2	10	$\bar{11}$	189	162
3	10	$\bar{11}$	30	28
4	10	$\bar{11}$	121	-111
5	10	$\bar{11}$	68	-74
6	10	$\bar{11}$	62	60
0	11	11	7-	-4
1	11	11	51	-50
2	11	$\bar{11}$	84	-76
3	11	$\bar{11}$	206	-186
4	11	$\bar{11}$	157	-144
5	11	$\bar{11}$	6-	14
6	11	$\bar{11}$	5-	12
0	12	11	73	-71
1	12	11	4-	-17
2	12	$\bar{11}$	100	-88
3	12	$\bar{11}$	8-	-27
4	12	$\bar{11}$	40	41
5	12	$\bar{11}$	4-	11
6	12	$\bar{11}$	6-	-18
0	13	11	5-	-21
2	13	$\bar{11}$	100	-79
3	13	$\bar{11}$	7-	39
5	13	$\bar{11}$	5-	10
2	12	$\bar{11}$	100	-88
3	12	$\bar{11}$	8-	-27
4	12	$\bar{11}$	40	41
6	12	$\bar{11}$	4-	11
0	13	11	5-	-21
2	13	$\bar{11}$	100	-79
3	13	$\bar{11}$	7-	39
5	13	$\bar{11}$	5-	10
7	13	$\bar{11}$	7-	7
0	14	11	3-	7
1	14	$\bar{11}$	41	47
2	14	$\bar{11}$	6-	-18
3	14	$\bar{11}$	6-	21
0	0	12	153	124
1	0	12	295	-266
2	0	12	95	-81
0	1	12	163	-150
1	1	12	142	-105
2	1	12	40	-43
0	2	12	95	-110
1	2	12	130	114
2	2	12	5-	-21
3	2	12	55	-62
1	3	12	8-	-35
2	3	12	4-	-14
0	4	12	9-	6
1	4	12	77	-70
2	4	12	95	81
0	5	12	68	73
1	5	$\bar{12}$	77	67
2	5	$\bar{12}$	6-	14
0	6	12	121	104
0	8	12	55	-51
1	8	12	93	81
5	8	$\bar{12}$	7-	6
6	8	$\bar{12}$	100	-85
0	9	12	110	113
5	9	$\bar{12}$	62	-82
0	10	12	30	30
5	10	$\bar{12}$	90	-82
0	1	13	95	90
1	1	13	50	-40
2	1	13	148	-144
1	2	13	126	-97
0	3	13	110	-118
1	3	13	104	85
0	4	13	73	72
1	4	13	4-	-2
0	5	13	95	109
0	6	13	40	-45
0	7	13	52	-50
0	8	13	4-	-1

ing's covalent radii (2·35 Å) and with the values found in other zinc compounds [*e.g.* 2·35(1) Å in bisthiourea-zinc chloride (Kunchur & Truter, 1958*b*), 2·331(3), 2·355(3) and 2·383(2) Å in zinc diethyldithiocarbamate (Bonamico, Mazzone, Vaciago & Zambonelli, 1965)]. By contrast, the difference between Zn–O(1) and Zn–O(3) ($t_o = 1·9$) is not significant; these distances are just a little shorter than the sum of Pauling's covalent radii (2·05 Å) but agree well with the values usually found in tetrahedral zinc complexes [*e.g.* 1·962(7) Å in bisdipivaloylmethanido-zinc (Cotton & Wood, 1964)].

The O(2) and O(4) atoms, belonging to the second coordination sphere of Zn, lie on the O(1)O(3)S(2) and O(3)S(1)S(2) faces of the coordination tetrahedron, respectively. Similar behaviour is observed in other cases: in zinc salicylate dihydrate (Klug, Alexander & Sumner, 1958) a zinc atom, tetrahedrally surrounded by four oxygen atoms at 2·03 and 2·06 Å, shows two weaker interactions with oxygen atoms at 2·52 Å; in dihistidino-zinc pentahydrate (Harding & Cole, 1963) a zinc atom, tetrahedrally coordinated by four nitrogen atoms, is weakly bonded to two more

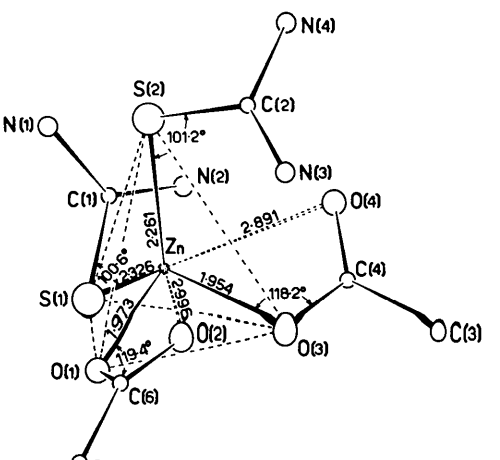

Fig. 2. Clinographic projection of a coordination polyhedron.

oxygen atoms at 2·912 Å; and in di-L-histidinozinc dihydrate (Kretsinger, Cotton & Bryan, 1963), as in the previous case, there are two more oxygen atoms at 2·79 Å from Zn. Both these long interactions are

important in determining the orientation of the acetic groups.

The two thiourea molecules are planar, their least-squares planes being:*

S(1)C(1)N(1)N(2):
$0{\cdot}4545x' + 0{\cdot}5720y' + 0{\cdot}6828z' = 0{\cdot}1583$

S(2)C(2)N(3)N(4):
$0{\cdot}3384x' + 0{\cdot}8984y' - 0{\cdot}2799z' = 4{\cdot}4709$

These two molecules are not significantly different as far as bond distances and angles are concerned. Neither are they significantly different from uncoordinated thiourea (Kunchur & Truter, 1958*a*, K. & T.), and so it appears that in the present case coordination does not influence the dimensions of the ligand molecule:

				K. & T.
S(1)–C(1)	1·712(9) Å	S(2)–C(2)	1·722(9) Å	1·707(12)
C(1)–N(1)	1·305(14)	C(2)–N(3)	1·297(13)	1·311(12)
C(1)–N(2)	1·311(10)	C(2)–N(4)	1·307(13)	

N(1)–C(1)–N(2)	120·7°(0·8°)	115·6°(1·1°)
N(3)–C(2)–N(4)	118·3 (0·8)	
S(1)–C(1)–N(1)	119·2 (0·6)	122·2 (0·6)
S(2)–C(2)–N(4)	118·0 (0·7)	
S(1)–C(1)–N(2)	120·1 (0·7)	
S(2)–C(2)–N(3)	123·7 (0·8)	

Both thiourea molecules are tilted with respect to the Zn–S bonds by the same angles: Zn–S(1)–C(1) 100·6°(0·3°), Zn–S(2)–C(2) 101·2°(0·3°). These angles are less than the tetrahedral value for the bonds involving sulphur in thiourea, as observed in other tetrahedral thiourea–metal complexes: *e.g.* 113° in bis-thiourea-cadmium chloride (Nardelli, Cavalca & Braibanti, 1957), 108·6° in bisthiourea-zinc chloride (Kunchur & Truter, 1958*b*), 105°, 105°, 108°, 113° in tristhiourea-copper(I) chloride (Okaya & Knobler, 1964).

The two acetic ions are also planar, their least-squares planes being:

O(1)O(2)C(5)C(6)
$0{\cdot}6906x' + 0{\cdot}4243y' - 0{\cdot}5857z' = 2{\cdot}2176$

O(3)O(4)C(3)C(4)
$0{\cdot}5045x' + 0{\cdot}7212y' + 0{\cdot}4747z' = 2{\cdot}9782$

There are no significant differences between corresponding bonds and angles:

C(3)–C(4)	1·474(17) Å	C(5)–C(6)	1·487(13) Å
C(4)–O(4)	1·228(14)	C(6)–O(2)	1·215(11)
C(4)–O(3)	1·252(11)	C(6)–O(1)	1·275(8)

O(3)–C(4)–O(4)	121·2°(0·9°)
O(1)–C(6)–O(2)	123·3 (0·7)
C(3)–C(4)–O(4)	121·3 (0·9)
C(5)–C(6)–O(2)	118·9 (0·7)
C(3)–C(4)–O(3)	117·5 (0·9)
C(5)–C(6)–O(1)	117·8 (0·8)

In both these two ions the C–O bond, involving the oxygen atom more closely linked to the metal atom, is longer than that involving the oxygen atom belonging to the second coordination sphere. Consequently, there is an asymmetry of the carboxyl group, which is also observed in the free acids (Nardelli, Fava & Giraldi, 1962) and in several metal compounds; *e.g.* 1·275(14) and 1·226(15) Å, 1·291(15) and 1·243(15) Å in bisglycino-copper(II) monohydrate (Freeman, Snow, Nitta & Tomita, 1964), 1·311(11) and 1·206(12) Å in glycylglycylglycinocopper(II) chloride sesquihydrate (Freeman, Robinson & Schoone, 1964), 1·28(1) and 1·23(1) Å in sodium glycylglycylglycinocuprate(II) monohydrate (Freeman, Schoone & Sime, 1965).

The orientations of the planes of the two acetate ions are determined by the interactions Zn–O(1), Zn–O(2) and Zn–O(3), Zn–O(4) and by the trigonal character of the bonds formed by the oxygen atoms and implied by the shortest contacts: Zn–O(1)–C(6) 119·4°(0·6°), Zn–O(3)–C(4) 118·2°(0·7°). It follows that the Zn atom lies near to the two acetate planes: the distances are 0·095 Å from the O(1)O(2)C(5)C(6) plane and 0·036 Å from the O(3)O(4)C(3)C(4) plane. The longer is this distance, the weaker is the long-range Zn–O interaction.

The following N···O distances must be considered as hydrogen bonds (the corresponding H–N–O angles are quoted in square brackets; the e.s.d.'s are all 0·01 Å):

N(1)–H(2)···O(2^{vi})	2·82 Å	[4·7°]
N(1)–H(1)···O(4″)	2·72	[14·1]
N(3)–H(6)···O(2)	2·76	[11·3]
N(4)–H(7)···O(1^{vii})	2·91	[18·7]
N(4)–H(8)···O(3″)	2·77	[29·0]

The packing in the crystal and the orientation of the thiourea molecules are determined by these interactions. Other distances less than 3·5 Å are as follows:

S(1)–O(1)	3·23 Å	O(3)–C(6)	3·45 Å
S(1)–O(3)	3·48	O(3)–N(2^{iv})	3·45
S(2)–O(4)	3·49	O(4)–N(2)	3·34
O(1)–N(4′)	3·41	O(4)–N(2‴)	3·12
O(1)–N(3^{viii})	3·16	O(4)–C(2)	3·32
O(1)–O(3)	3·03	O(4)–C(1‴)	3·34
O(1)–C(2^{viii})	3·48	N(3)–C(4)	3·47
O(2)–O(3)	3·29	N(4)–C(6″)	3·34
O(3)–N(3)	3·25		

′ $x-1,y,z$ — v $x-1,\frac{1}{2}-y,z+\frac{1}{2}$
″ $x+1,y,z$ — vi $x,\frac{1}{2}-y,z-\frac{1}{2}$
‴ $1-x,\bar{y},\bar{z}$ — vii $x+1,\frac{1}{2}-y,z+\frac{1}{2}$
iv $\bar{x},\bar{y},z$ — viii $x-1,\frac{1}{2}-y,z-\frac{1}{2}$

* Transformation matrix from monoclinic x,y,z to orthogonal x',y',z' coordinates:

$$\begin{pmatrix} 1 & 0 & \cos\beta \\ 0 & 1 & 0 \\ 0 & 0 & \sin\beta \end{pmatrix}$$

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Expectation Value of the Bijvoet Ratio*

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The theoretical expressions for the expectation values of the Bijvoet difference and the Bijvoet ratio have been derived for a non-centrosymmetric crystal in which the anomalous scatterers are all of the same type. The dependence of the expectation value of the Bijvoet ratio on the number and the strength of the anomalous scatterers in the unit cell is discussed and this is used to obtain the best conditions for accurate measurement of the Bijvoet differences of a fairly large percentage of reflexions.

1. Introduction

The increasing importance of the anomalous dispersion method in crystal structure analysis necessitates a theoretical study of the measurability of Bijvoet differences. One approach to this would be a study of the statistical distribution of Bijvoet differences, ΔI. The distribution of Bijvoet differences in a normalized form, *viz.* $x=|\Delta I|/4[\langle I_Q\rangle\langle I_P''\rangle]^{\frac{1}{2}}$ (where P and Q refer to the anomalous and normal scatterers respectively) has already been worked out (Parthasarathy & Srinivasan, 1964). However, the distribution of ΔI normalized by the local mean intensity, $\langle I_N\rangle$ (where $N=P+Q$) rather than by the factor $4[\langle I_Q\rangle\langle I_P''\rangle]^{\frac{1}{2}}$ is probably more useful. The distribution of this quantity Δ $(=|\Delta I|/\langle I_N\rangle)$ can easily be obtained from the known distribution of x, since we have in the usual notation

$$\Delta=\frac{|\Delta I|}{\langle I_N\rangle}=\frac{|\Delta I|}{4[\langle I_Q\rangle\langle I_P''\rangle]^{\frac{1}{2}}}\times\frac{4[\langle I_Q\rangle\langle I_P''\rangle]^{\frac{1}{2}}}{\langle I_N\rangle}=4k\sigma_1\sigma_2 x \quad (1)$$

where $k=f_P''/f_P'$, the ratio of the imaginary to the total real part of the atomic scattering factor of the anomalous scatterer and σ_1^2 and σ_2^2 are the fractional contribution to the mean intensity by the P- and the Q-atoms respectively.

A better normalization factor would be the mean intensity I of the Bijvoet pair of reflexions, *i.e.* $I=\frac{1}{2}[I(\mathbf{H})+I(\bar{\mathbf{H}})]$. The normalized Bijvoet difference $|\Delta I|/I$ (denoted by δ) is called the Bijvoet ratio in this paper. The distribution function of δ is difficult to cal-

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