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The Crystal Structure of Di-imidazole-zinc (II) Dichloride

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The crystal structure of $Zn(C_3H_4N_2)_2Cl_2$ has been determined and refined from three-dimensional X-ray data. The unit cell is monoclinic with the constants $a=7{\cdot}956$, $b=11{\cdot}856$ and $c=12{\cdot}078$ Å, all $\pm 0{\cdot}005$ Å, $\beta=113°58'\pm 2'$. The space group is $P2_1/c$; there is one formula unit in the asymmetric unit and all atoms occupy general fourfold positions. The coordination of the zinc atom is tetrahedral and the bond distances are: Zn–N, 2·00 and 2·02 Å; Zn–Cl, 2·24 and 2·26 Å. Hydrogen bonds are assumed between the chlorine atoms and the imidazole nitrogen atoms that are not bonded to zinc. There are two such bonds in the structure and their lengths are 3·27 and 3·34 Å respectively.

Introduction

The investigation of the crystal structure of $[Zn(C_3H_4N_2)_2Cl_2$ was undertaken as part of a research programme initiated by Lindqvist 1962 on compounds related to enzymes. In this connection the crystal structure of carbonic anhydrase form *C*, which is a zincmetalloenzyme, is currently being investigated at this Institute (Strandberg, Tilander, Fridborg, Lindskog & Nyman, 1962); (Tilander, Strandberg & Fridborg, 1965).

For the direct study of the binding of an individual metal ion to a particular group in a protein it is necessary, however, to determine the structure of the whole protein; this is in practice a time-consuming task of uncertain outcome. In order to obtain some indirect knowledge of the nature of the interactions involved in a proposed enzyme–metal-ion–substrate complex, model compounds are being studied. The metal-ion–substrate model compounds chosen are glycylglycinocopper(II) trihydrate (Strandberg, Lindqvist & Rosenstein, 1961) and bis(bisglycylglycinatoaquozinc(II)) dihydrate (Sandmark & Lindqvist, 1966).

Since the imidazole residue of the amino acid histidine possesses a great ability for binding metal ions, the following zinc–imidazole complexes are being investigated: $Zn(C_3H_3N_2)_2$, (Strandberg, Svensson & Brändén, 1966), $Zn(C_3H_4N_2)_6Cl_2.2H_2O$, (Sandmark, personal communication) and $Zn(C_3H_4N_2)_2Cl_2$ the subject of this communication. Magnesium, cobalt, copper, nickel and silver complexes with imidazole are also being investigated.

Experimental

The crystals were obtained by slow evaporation of a cold saturated solution prepared according to Edsall, Felsenfeld, Goodman & Gurd (1954). Analyses for zinc and nitrogen confirmed the stoichiometry.

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Crystal data

The unit-cell dimensions were determined from Weissenberg photographs and confirmed and refined from powder data. The cell is monoclinic and the dimensions are:

$$a = 7{\cdot}956 \text{ Å} \pm 0{\cdot}005 \text{ Å}$$
$$b = 11{\cdot}856 \text{ Å} \pm 0{\cdot}005$$
$$c = 12{\cdot}078 \text{ Å} \pm 0{\cdot}005$$
$$\beta = 113°58' \pm 2'$$

The density was determined by the flotation method, which gave $1{\cdot}72 \pm 0{\cdot}02$ g.cm^{-3} at 21 °C. With four formula units in the unit cell the calculated density is 1·73 g.cm^{-3}.

Systematic extinctions were found for $h0l$ reflexions with l odd and for $0k0$ reflexions with k odd.

Precession photographs were taken as a check to confirm the space group $P2_1/c$. All atoms are in general fourfold positions and the centre of symmetry is situated at the origin of the unit cell.

Intensity data

The colourless crystals obtained were stable in air. The crystal selected for the Weissenberg photographs had the dimensions $0{\cdot}08 \times 0{\cdot}19 \times 0{\cdot}10$ mm^3, the longest direction being parallel to the b axis of the unit cell. The transmission factors in directions perpendicular to this axis were 54% and 47% respectively. No corrections were made for absorption. Equi-inclination Weissenberg photographs were taken with Cu $K\alpha$ radiation. The crystal was rotated around the twofold axis and reflexions in ten layer lines ($k=0$–9) were recorded. The intensities of 1465 independent X-ray reflexions were estimated visually by the multiple film technique (five films). Corrections for Lorentz and polarization factors were made in the usual way with the aid of a computer program written by the author.

Structure determination

In the space group $P2_1/c$ the symmetrical vectors lie on a Harker line $(0;2y-\frac{1}{2};\frac{1}{2})$ and a Harker section $(2x;\frac{1}{2};2z-\frac{1}{2})$. From the calculations of these the peak with the highest value was taken as the Zn–Zn vector. In a three-dimensional Patterson synthesis a generally well-resolved peak with a high value was assumed to derive from a Zn–Cl(1) vector. The quartet of unsymmetrical peaks, together with the Harker and inversion peaks calculated on this assumption, were checked and had reasonable values (Lindqvist, 1960). Of the remaining peaks, one that was well-defined was taken as a Zn–Cl(2) vector peak and with these Zn, Cl(1) and Cl(2) positions all peaks with numerical values exceeding half of a Zn–Cl vector peak were explained. An electron density map was calculated with only the zinc atom contributing to F_c. The F_o values were scaled to the values of F_c and an arbitrary B value of 3·5 Å^2 was used. The residual R for observed reflexions was 52·7%. The two chlorine positions obtained from the Patterson map were confirmed. A method suggested by Dawson (1961) and adapted to a computer by Lundberg & Olovsson (1962) was used to obtain accurate values for the atomic positions from the electron density maps.

The second electron density calculation with signs obtained by means of the known Zn, Cl(1) and Cl(2) positions gave the coordinates of the two nitrogen atoms which are coordinated to the zinc atom. The R value decreased to 37·7%. From a third calculation the remaining two nitrogen atoms were found. The R value at this point was 28%.

A trial model of plastic balls on steel rods was constructed. The balls had different colours for certain levels of electron density maxima in the Fourier syntheses. When the two imidazole rings were fitted into appropriate positions, it was clear that there was only one reasonable way of orienting each ring in order to obtain electron density maxima for the carbon atoms. No extra peak appeared.

At this stage a check was made of interatomic bond distances and angles. The arrangement around the zinc atom was shown to be tetrahedral, as expected, and the Zn–N and Zn–Cl bond lengths were reasonable.

The computer programs used for calculation of structure factors, Fourier syntheses, bond distances and bond angles were written by Liminga & Olovsson (1964) for the Swedish computers BESK and FACIT.

Refinement of parameters

The refinement of the structural parameters was carried out by least-squares methods, with the use of a computer program written by Åsbrink & Brändén (1962). The scattering functions chosen were, for Zn, that of Thomas & Umeda (1957), where account was taken of the real part of the dispersion correction, and for the other atoms those of Berghuis, Haanappel, Loopstra, MacGillavry & Veenendaal (1955). Individual isotropic temperature factors were applied and the program employed the block diagonal approximation for solving the normal equations. After five cycles of refinement the R value had decreased to 9·8% and the largest shifts were in the ten scale factors (one for each layer of reflexions). The relative weighting factor used was that proposed by Cruickshank, Pilling, Bujosa, Lovell & Truter (1961): $w=1/(a+|F_o|+c|F_o|^2)$. Between the first cycles the constants a and c were changed to obtain approximately the same mean value of $w(|F_o|-|F_c|)^2$ in all intervals of F_o's (the intervals having a magnitude of $0{\cdot}1|F_{o,\max}|$). Final values for the constants were $a=3{\cdot}0$ and $c=0{\cdot}02$. The final R value for the observed reflexions was 9·8%.

When the refinement was stopped the shifts in the parameters were less than one tenth of the standard deviations, derived from the inverse least-squares matrix. Interatomic distances and bond angles are given in Tables 2 and 3 together with approximate standard deviations, which were calculated assuming that for the atomic positions these were the same in all directions and equal to 0·0014 Å for zinc, 0·0030 Å for chlorine, 0·011 Å for nitrogen and 0·015 Å for carbon. The unobserved reflexions were not used during the refinement, but a calculation was made using the final parameters and no F_c had a value exceeding 1·5 times the threshold value for the observed structure factors. No attempt to locate the hydrogen atoms had been made. Observed and calculated structure factors are given in Table 4.

Table 1. *Final atomic parameters and their estimated standard deviations*

	x/a (Å)	$\sigma(x)$ (Å)	y/b (Å)	$\sigma(y)$ (Å)	z/c (Å)	$\sigma(z)$ (Å)	B (Å^2)	$\sigma(B)$ (Å^2)
Zn	0·2454	0·0012	0·3188	0·0014	0·2500	0·0012	3·15	0·02
Cl(1)	0·2175	0·0025	0·1398	0·0028	0·1808	0·0025	3·73	0·04
Cl(2)	0·0199	0·0025	0·3631	0·0030	0·3081	0·0025	3·85	0·04
N(1)	0·2522	0·0080	0·4148	0·0092	0·1162	0·0083	3·44	0·13
N(2)	0·2030	0·0098	0·0250	0·0106	0·4337	0·0101	4·68	0·18
N(3)	0·4894	0·0080	0·3451	0·0090	0·3911	0·0082	3·47	0·14
N(4)	0·7824	0·0105	0·3674	0·0106	0·4965	0·0105	4·90	0·18
C(1)	0·1783	0·0115	0·1104	0·0123	0·4994	0·0115	4·35	0·19
C(2)	0·3310	0·0117	0·5188	0·0130	0·1239	0·0120	4·68	0·21
C(3)	0·6978	0·0135	0·0599	0·0147	0·4881	0·0134	5·41	0·24
C(4)	0·6486	0·0113	0·3535	0·0122	0·3856	0·0114	4·31	0·20
C(5)	0·5178	0·0113	0·1527	0·0121	0·0108	0·0116	4·17	0·19
C(6)	0·7028	0·0115	0·1359	0·0128	0·0765	0·0120	4·65	0·21

Table 2. *Bond distances and angles for the tetrahedral arrangement around the zinc atom*
(See also Fig. 1)

	Distances (Å)	σ (Å)		Angle (°)	σ (°)
Zn–Cl(1)	2·258	0·003	Cl(1)–Zn–Cl(2)	111·46	0·12
Zn–Cl(2)	2·239	0·003	Cl(1)–Zn–N(1)	105·51	0·33
Zn–N(1)	1·995	0·011	Cl(1)–Zn–N(3)	111·95	0·33
Zn–N(3)	2·020	0·011	Cl(2)–Zn–N(1)	114·11	0·33
			Cl(2)–Zn–N(3)	108·48	0·33
			N(1)–Zn–N(3)	105·20	0·45

Description of the structure

The configuration of the molecule is shown in Fig. 1. The coordination around the zinc atom is tetrahedral. The average Zn–Cl bond length is 2·25 Å which is in accordance with some other determinations listed in Table 5.

The Zn–Cl bond distances given by Brehler (1961) in α-$ZnCl_2$, β-$ZnCl_2$ and γ-$ZnCl_2$ are 2·34, 2·31 and 2·27 Å respectively, but these values are not quite comparable with those listed in Table 5 because in the $ZnCl_2$ modifications each chlorine atom is shared between two zinc atoms.

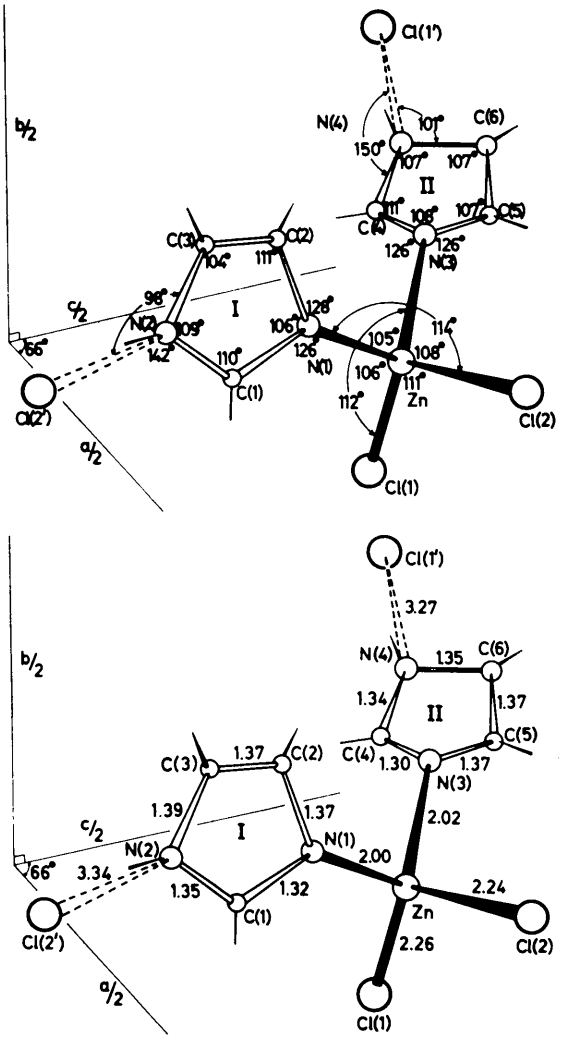


Fig. 1. Bond angles and bond distances in the asymmetric unit.

Table 3. *Bond distances and angles in the imidazole rings*
(See also Fig. 1)

	Distance		Angle
N(2)–C(1)	1·349 Å	Zn —N(1)–C(1)	126·03°
C(1)–N(1)	1·324	Zn —N(1)–C(2)	128·40
N(1)–C(2)	1·369	C(1)—N(1)–C(2)	105·58
C(2)–C(3)	1·367	Cl(2')–N(2)–C(1)	142·50
C(3)–N(2)	1·387	Cl(2')–N(2)–C(3)	97·60
N(4)–C(4)	1·340	C(1)—N(2)–C(3)	108·81
C(4)–N(3)	1·299	Zn —N(3)–C(4)	126·30
N(3)–C(5)	1·370	Zn —N(3)–C(5)	125·71
C(5)–C(6)	1·374	C(4)—N(3)–C(5)	107·77
C(6)–N(4)	1·354	Cl(1')–N(4)–C(4)	130·35
σC —C	0·021	Cl(1')–N(4)–C(6)	100·71
σC —N	0·019	C(4)—N(4)–C(6)	107·34
		N(1)—C(1)–N(2)	110·48
		N(1)—C(2)–C(3)	111·46
		N(2)—C(3)–C(2)	103·65
		N(3)—C(4)–N(4)	110·74
		N(3)—C(5)–C(6)	106·95
		N(4)—C(6)–C(5)	107·08

The average Zn–N bond length is 2·01 Å. The bond length between zinc and the nitrogen atom in the imidazole ring reported for di-(L-histidino)zinc(II) dihydrate (Kretsinger, Cotton & Bryan, 1963) is 2·04 Å, while for di(histidino)zinc(II) pentahydrate (Harding & Cole, 1963) it is 2·00 Å. For $Zn(imidazole^-)_2$ (Strandberg, Svensson & Brändén) the mean value of eight Zn–N bond lengths is 1·99 Å, no bond length differing significantly from this value. This shows that the interaction of zinc with the uncharged imidazole molecule is of the same order of strength as that with the anion, in which the negative net charge is thought to be equally distributed on the two nitrogens of the imidazole ring. The bond lengths and bond angles in the imidazole rings are shown in Fig. 1 and listed in Table 3. There are no significant differences from the values given by Donohue & Caron (1964) in their comparison of histidine compounds.

A number of planes containing different atoms were calculated using a computer program written by Dr Brändén and based on a method of least squares described by Blow (1960). The equations of the planes are given in Table 6 together with the displacements in Å from these planes for the atoms (Fig. 1).

As can be seen from Table 6, the atoms in each imidazole ring lie in a plane and the zinc atom lies

Table 4. *Observed and calculated structure factors*

h	k	l	F OBS	F CALC	h	k	l	F OBS	F CALC	h	k	l	F OBS	F CALC	h	k	l	F OBS	F CALC
10	0	- 8	15.72	- 14.39	9	1	-11	8.85	8.72	3	1	-11	5.74	- 7.23	8	2	- 9	15.96	- 15.72
10	0	- 6	13.39	12.63	9	1	-10	5.80	4.80	3	1	-10	23.57	- 23.27	8	2	- 8	12.06	- 12.30
10	0	- 4	4.03	- 7.46	9	1	- 8	5.59	- 8.01	3	1	- 9	24.49	22.83	8	2	- 7	16.13	16.19
9	0	-12	5.42	- 4.20	9	1	- 6	14.72	15.29	3	1	- 8	33.77	30.00	8	2	- 6	16.60	17.38
9	0	- 8	6.97	- 9.17	9	1	- 5	5.55	5.47	3	1	- 7	75.98	- 77.16	8	2	- 5	19.03	- 17.21
9	0	- 6	6.03	- 4.46	9	1	- 4	19.16	- 16.59	3	1	- 6	71.70	- 71.80	8	2	- 4	15.58	- 16.60
9	0	- 4	17.24	13.79	9	1	- 3	4.03	2.55	3	1	- 5	31.35	32.01	8	2	- 3	6.31	6.02
9	0	- 2	15.53	- 14.30	9	1	- 2	23.49	18.80	3	1	- 4	96.37	98.39	8	2	- 2	14.86	12.93
9	0	0	13.42	11.27	9	1	- 1	10.85	- 9.48	3	1	- 3	21.47	- 19.21	8	2	- 1	26.83	- 24.25
8	0	- 8	19.53	19.81	9	1	0	17.88	- 14.54	3	1	- 2	103.28	-111.90	8	2	0	13.92	- 14.72
8	0	- 6	33.39	- 31.44	8	1	-13	4.02	- 2.44	3	1	- 1	7.86	7.08	8	2	1	21.14	18.97
8	0	- 4	38.97	37.50	8	1	-12	3.61	3.51	3	1	0	73.62	77.91	8	2	2	7.61	6.22
8	0	- 2	43.14	- 42.13	8	1	-11	3.89*	1.29	3	1	1	13.99	- 14.00	8	2	3	12.27	- 10.03
8	0	0	25.46	22.25	8	1	-10	5.09	- 4.82	3	1	2	53.90	- 49.26	7	2	-14	2.80	- 3.85
8	0	2	7.17	- 7.97	8	1	- 9	15.60	15.30	3	1	3	7.97	7.07	7	2	-13	8.95	6.78
7	0	-14	13.14	12.58	8	1	- 8	4.88*	1.71	3	1	4	4.78	2.95	7	2	-12	5.17	5.44
7	0	-12	18.61	- 16.56	8	1	- 7	15.92	- 14.07	3	1	5	23.25	- 17.50	7	2	-11	5.09	- 4.57
7	0	-10	10.75	7.55	8	1	- 6	11.30	- 8.27	3	1	6	12.99	- 11.47	7	2	- 9	17.74	15.76
7	0	- 8	6.11	- 3.84	8	1	- 5	12.75	11.36	3	1	7	17.46	15.22	7	2	- 8	6.64	8.17
7	0	- 6	8.42	- 10.99	8	1	- 2	13.47	- 11.64	3	1	8	26.64	22.80	7	2	- 7	24.39	- 24.88
7	0	- 4	11.72	9.31	8	1	1	13.97	11.47	3	1	9	20.21	- 18.22	7	2	- 5	10.35	12.00
7	0	- 2	14.49	- 10.61	7	1	-14	6.88	- 8.16	3	1	10	19.46	- 19.17	7	2	- 3	24.66	24.26
7	0	0	21.94	- 19.15	7	1	-13	5.17	5.55	3	1	11	4.78	4.34	7	2	- 1	14.64	- 12.97
7	0	2	11.77	12.36	7	1	-12	7.39	7.93	2	1	-14	9.81	10.51	7	2	0	4.86	4.77
6	0	-14	21.99	18.80	7	1	-11	17.11	- 17.85	2	1	-13	4.55	- 4.28	7	2	1	7.75	8.16
6	0	-12	17.72	- 16.94	7	1	-10	13.77	- 13.70	2	1	-12	17.74	- 17.90	7	2	5	8.05	- 6.93
6	0	-10	38.63	32.89	7	1	- 9	11.89	11.05	2	1	-11	5.22	- 3.03	6	2	-14	7.59	- 7.53
6	0	- 8	30.19	- 26.03	7	1	- 8	27.24	23.10	2	1	-10	11.02	12.37	6	2	-13	20.17	18.68
6	0	- 6	37.41	35.30	7	1	- 7	30.27	- 30.97	2	1	- 9	17.39	16.06	6	2	-12	12.63	12.57
6	0	- 4	40.60	- 41.11	7	1	- 6	52.01	- 46.80	2	1	- 8	15.57	14.75	6	2	-11	36.36	- 35.39
6	0	- 2	51.41	49.97	7	1	- 5	11.67	8.32	2	1	- 7	9.20	6.82	6	2	-10	19.08	- 17.47
6	0	0	14.94	- 13.73	7	1	- 4	48.38	45.78	2	1	- 6	23.13	- 22.24	6	2	- 9	56.05	54.89
6	0	2	22.21	22.97	7	1	- 3	9.50	- 6.89	2	1	- 5	6.17	- 4.93	6	2	- 8	20.22	19.06
6	0	4	20.05	- 17.28	7	1	- 2	27.24	- 25.44	2	1	- 4	54.15	57.20	6	2	- 7	23.58	- 21.45
6	0	6	19.44	19.34	7	1	0	17.96	18.53	2	1	- 3	26.63	24.35	6	2	- 6	21.08	- 23.44
5	0	- 8	26.67	- 25.27	7	1	1	8.81	- 7.40	2	1	- 2	68.95	- 73.21	6	2	- 5	13.22	14.84
5	0	- 6	23.78	24.16	7	1	2	11.92	- 9.79	2	1	- 1	61.93	66.15	6	2	- 4	23.38	20.92
5	0	- 4	23.28	17.79	7	1	3	6.38	5.83	2	1	0	51.88	- 58.80	6	2	- 3	9.55	10.81
5	0	- 2	44.60	- 41.93	7	1	5	10.97	- 8.66	2	1	1	30.55	30.04	6	2	- 2	29.89	- 29.88
5	0	0	36.33	34.96	6	1	-14	15.02	12.32	2	1	2	65.03	69.38	6	2	- 1	5.95	4.66
5	0	2	25.35	- 22.84	6	1	-13	5.05	- 3.25	2	1	3	13.85	- 16.71	6	2	0	18.80	20.08
5	0	4	11.94	10.18	6	1	-12	17.71	- 17.62	2	1	4	40.99	- 38.26	6	2	1	10.99	- 12.19
5	0	6	14.77	12.78	6	1	- 8	21.80	24.29	2	1	5	7.91	- 5.62	6	2	2	11.03	- 11.65
5	0	8	13.80	- 13.98	6	1	- 6	15.83	- 11.19	2	1	6	8.41	6.43	6	2	3	33.27	32.66
4	0	-14	20.91	- 20.73	6	1	- 5	6.38	- 5.10	2	1	9	12.19	10.56	6	2	4	16.56	16.44
4	0	-12	14.81	16.01	6	1	- 4	6.69	4.37	2	1	10	13.10	- 14.23	6	2	5	27.58	- 29.09
4	0	-10	12.75	15.02	6	1	- 1	6.89	7.75	2	1	12	7.39	7.28	6	2	6	8.27	- 8.30
4	0	- 8	19.72	19.04	6	1	0	26.57	- 26.71	1	1	-14	21.22	20.74	6	2	7	18.92	18.81
4	0	- 6	52.08	- 49.93	6	1	2	30.57	28.59	1	1	-13	10.33	- 9.58	5	2	-15	3.88	- 4.51
4	0	- 4	99.16	109.00	6	1	3	17.83	- 14.79	1	1	-12	25.88	- 24.38	5	2	-13	8.88	10.77
4	0	- 2	84.51	- 85.27	6	1	4	12.19	- 12.40	1	1	-11	9.49	8.84	5	2	-11	17.19	- 15.10
4	0	0	124.20	136.60	6	1	6	4.00	- 4.17	1	1	-10	31.04	30.93	5	2	- 9	6.08	5.57
4	0	2	55.15	- 51.62	6	1	7	4.34	- 4.32	1	1	- 9	33.63	- 35.18	5	2	- 8	7.00	- 7.75
4	0	4	15.05	11.81	5	1	-15	6.78	6.94	1	1	- 8	27.66	- 24.44	5	2	- 7	9.86	10.45
4	0	8	10.95	9.15	5	1	-14	25.58	23.11	1	1	- 7	41.65	39.00	5	2	- 6	9.67	- 9.10
4	0	10	15.31	- 11.76	5	1	-13	18.22	- 16.10	1	1	- 6	5.99*	2.53	5	2	- 5	35.50	- 37.87
3	0	-12	33.35	- 33.19	5	1	-12	13.88	- 12.59	1	1	- 5	9.75	6.50	5	2	- 4	4.09	- 4.55
3	0	-10	13.42	11.11	5	1	-11	12.67	13.18	1	1	- 4	39.77	- 33.94	5	2	- 3	41.43	36.24
3	0	- 8	22.27	- 23.00	5	1	-10	17.53	17.12	1	1	- 3	24.89	- 26.21	5	2	- 2	13.77	13.75
3	0	- 6	12.89	- 16.41	5	1	- 9	15.78	- 15.36	1	1	- 2	111.11	144.85	5	2	- 1	9.02	- 9.03
3	0	- 4	22.36	24.20	5	1	- 8	17.96	- 17.08	1	1	- 1	39.55	- 43.29	5	2	0	6.13	- 5.69
3	0	- 2	76.49	- 76.77	5	1	- 7	27.30	28.53	1	1	0	97.25	-119.09	5	2	2	9.60	8.46
3	0	0	9.24	- 8.23	5	1	- 6	28.96	26.56	1	1	1	20.74	19.96	5	2	3	13.67	11.38
3	0	2	7.47	7.45	5	1	- 5	14.88	12.57	1	1	2	96.11	127.26	5	2	4	5.31	- 3.91
3	0	4	49.64	- 48.12	5	1	- 4	28.79	- 29.98	1	1	3	52.26	- 53.27	5	2	9	3.09	3.62
2	0	-14	18.14	18.37	5	1	- 3	8.44	- 9.65	1	1	4	71.39	- 76.72	4	2	-15	5.38	6.08
2	0	-12	33.88	- 32.58	5	1	- 2	73.62	69.19	1	1	5	49.10	51.88	4	2	-14	8.24	9.30
2	0	-10	32.55	29.36	5	1	- 1	26.11	- 23.37	1	1	6	50.21	55.29	4	2	-13	12.58	- 12.79
2	0	- 8	50.18	- 49.49	5	1	0	57.27	- 62.59	1	1	7	47.07	- 44.49	4	2	-12	14.03	- 14.83
2	0	- 6	57.80	66.69	5	1	1	26.27	24.02	1	1	8	19.03	- 16.52	4	2	-11	8.03	8.32
2	0	- 4	83.41	- 85.89	5	1	2	49.29	45.80	1	1	9	17.66	16.13	4	2	-10	14.03	14.08
2	0	- 2	13.95	16.72	5	1	3	29.35	- 28.11	1	1	10	14.58	14.73	4	2	- 9	33.32	- 36.41
2	0	0	126.79	-158.53	5	1	4	13.46	- 13.85	1	1	12	14.49	- 12.86	4	2	- 8	24.41	- 23.48
2	0	2	60.82	54.48	5	1	5	26.02	25.77	0	1	2	9.95	10.61	4	2	- 7	30.22	32.26
2	0	4	49.33	- 45.44	5	1	6	21.30	21.07	0	1	3	54.35	- 60.26	4	2	- 6	28.68	30.00
2	0	6	34.33	32.44	5	1	7	10.27	- 9.65	0	1	4	5.08*	- 0.06	4	2	- 5	62.51	- 62.87
2	0	8	34.32	- 37.35	5	1	8	11.74	- 9.66	0	1	5	40.71	45.60	4	2	- 4	35.00	- 35.55
2	0	10	31.89	30.44	4	1	-15	4.74	5.02	0	1	6	5.42	- 3.20	4	2	- 3	14.02	10.50
2	0	12	22.78	- 18.96	4	1	-13	5.13	- 6.13	0	1	7	14.81	- 13.34	4	2	- 2	65.90	62.81
1	0	-12	16.86	15.48	4	1	-12	6.63	5.86	0	1	8	10.91	- 11.37	4	2	- 1	63.35	- 67.74
1	0	-10	8.36	10.01	4	1	-11	13.36	14.04	0	1	9	10.53	- 9.11	4	2	0	43.49	- 42.64
1	0	- 8	30.08	- 28.48	4	1	- 9	9.92*	2.81	0	1	10	8.10	8.52	4	2	1	41.55	41.68
1	0	- 6	12.72	10.38	4	1	- 8	9.24	8.17	0	1	11	15.77	16.06	4	2	2	25.16	22.26
1	0	- 4	29.14	- 26.64	4	1	- 7	25.36	- 24.79	0	1	13	7.52	- 6.89	4	2	3	50.29	- 52.86
1	0	- 2	8.41	- 6.30	4	1	- 6	16.13	- 14.96	10	2	- 7	5.11	- 5.87	4	2	4	28.61	- 25.99
1	0	0	15.36	16.25	4	1	- 5	46.29	41.48	10	2	- 6	7.44	- 8.27	4	2	5	14.08	11.66
1	0	2	99.57	-122.01	4	1	- 3	29.80	- 32.00	10	2	- 5	3.80	- 2.93	4	2	6	11.03	11.21
1	0	4	72.44	70.18	4	1	- 1	11.50	- 12.76	9	2	-11	4.20	- 2.50	4	2	7	26.71	- 25.78
1	0	6	31.08	32.84	4	1	0	26.72	24.40	9	2	-10	6.24*	0.36	4	2	8	10.75	- 11.20
1	0	8	37.72	- 37.83	4	1	1	40.74	37.74	9	2	- 8	4.70*	- 1.20	4	2	9	3.70	3.39
1	0	12	12.27	- 10.94	4	1	2	8.63	- 6.52	9	2	- 7	12.35	12.74	4	2	10	7.69	7.52
0	0	-14	17.05	- 18.66	4	1	3	7.20	- 7.25	9	2	- 5	14.61	- 13.02	3	2	-10	4.63	- 5.81
0	0	-12	23.44	21.91	4	1	4	6.78	- 6.32	9	2	- 4	3.67	- 4.45	3	2	- 9	12.03	8.57
0	0	- 8	31.11	30.80	4	1	5	18.77	16.75	9	2	- 3	8.20	6.14	3	2	- 8	17.33	18.25
0	0	- 6	12.74	- 12.73	4	1	7	9.44	7.92	9	2	- 2	7.16	6.38	3	2	- 7	39.60	- 40.60
0	0	- 4	67.19	67.06	4	1	8	6.14	- 3.30	9	2	0	2.69	- 1.92	3	2	- 6	19.21	18.33
0	0	- 2	52.96	- 62.67	4	1	9	8.00	- 8.29	8	2	-13	7.05	- 8.91	3	2	- 5	42.04	42.63
10	1	- 8	8.94	7.30	3	1	-14	14.22	- 14.13	8	2	-12	8.05	- 8.21	3	2	- 4	3.89	- 3.07
10	1	- 6	3.94*	- 1.75	3	1	-13	5.31	3.66	8	2	-11	4.23	7.91	3	2	- 3	10.67	8.30
10	1	- 4	4.36	- 3.66	3	1	-12	10.10	9.26	8	2	-10	5.61	5.66	3	2	- 2	4.05	2.93

Table 4 (*cont.*)

h	k	l	F OBS	F CALC	h	k	l	F OBS	F CALC	h	k	l	F OBS	F CALC	h	k	l	F OBS	F CALC
3	2	- 1	61.45	- 59.48	7	3	2	9.69	10.08	2	3	- 2	45.87	- 55.51	5	4	- 6	26.69	- 29.75
3	2	0	11.24	13.16	7	3	3	16.91	- 17.23	2	3	- 1	29.79	29.07	5	4	- 5	4.70	7.04
3	2	1	27.07	24.20	7	3	4	14.03	- 14.21	2	3	0	47.60	- 41.05	5	4	- 4	13.75	- 9.83
3	2	3	31.22	- 30.60	7	3	5	12.97	11.91	2	3	2	34.12	29.41	5	4	- 3	24.63	- 23.79
3	2	5	4.09	- 2.95	6	3	-14	6.36	5.92	2	3	3	7.31	- 4.55	5	4	- 2	27.08	23.77
3	2	7	22.03	24.73	6	3	-12	10.91	- 9.31	2	3	4	25.38	- 26.22	5	4	- 1	10.36	11.45
3	2	8	6.56	6.92	6	3	-11	5.14	- 4.01	2	3	5	7.75	- 6.47	5	4	0	25.77	- 25.20
3	2	9	17.55	- 19.83	6	3	-10	4.95	- 7.35	2	3	6	4.53	- 2.58	5	4	2	18.21	20.11
3	2	11	6.80	7.06	6	3	- 9	5.97	- 4.02	2	3	7	8.78	10.11	5	4	3	4.89	- 6.03
2	2	-14	10.39	- 9.56	6	3	- 8	16.55	18.55	2	3	9	15.80	- 13.07	5	4	4	4.88	- 4.35
2	2	-13	13.39	13.64	6	3	- 6	10.38	- 10.33	2	3	10	10.14	- 9.33	5	4	5	10.25	- 8.85
2	2	-12	16.86	16.87	6	3	- 5	16.53	17.86	2	3	12	5.36	5.15	5	4	6	18.67	- 17.91
2	2	-11	27.07	- 28.36	6	3	- 4	7.78	6.88	1	3	-13	15.42	14.09	5	4	8	9.06	9.01
2	2	-10	23.11	- 25.73	6	3	- 2	8.67	- 11.72	1	3	-11	33.46	- 36.06	4	4	-14	3.00	4.71
2	2	- 9	76.98	76.53	6	3	- 1	13.46	- 11.82	1	3	-10	6.78	- 6.55	4	4	-13	15.46	14.90
2	2	- 8	20.72	20.89	6	3	0	15.64	- 15.18	1	3	- 9	50.21	51.26	4	4	-11	27.11	- 27.44
2	2	- 7	63.15	- 67.76	6	3	1	7.08	- 8.96	1	3	- 8	21.75	23.57	4	4	-10	30.77	- 30.96
2	2	- 6	34.36	- 34.56	6	3	2	14.85	14.00	1	3	- 7	39.24	- 39.02	4	4	- 9	28.30	27.88
2	2	- 5	74.42	74.04	6	3	3	13.46	12.36	1	3	- 6	34.55	- 38.11	4	4	- 8	14.38	11.47
2	2	- 4	47.33	46.69	6	3	5	4.22	- 5.02	1	3	- 5	53.87	55.43	4	4	- 7	40.38	- 40.18
2	2	- 3	10.24	7.57	6	3	6	5.61	- 5.09	1	3	- 4	52.99	53.55	4	4	- 5	50.21	55.22
2	2	- 2	90.14	-102.47	6	3	7	3.78	3.93	1	3	- 3	24.22	- 23.28	4	4	- 4	27.08	- 25.94
2	2	- 1	21.49	- 26.16	5	3	-15	10.38	- 14.10	1	3	- 2	3.34	- 3.88	4	4	- 3	54.17	- 56.62
2	2	0	8.14	7.30	5	3	-14	5.67	4.02	1	3	- 1	64.34	72.62	4	4	- 2	54.13	57.21
2	2	1	22.74	18.40	5	3	-13	22.32	21.57	1	3	0	3.52	- 1.82	4	4	- 1	34.85	31.21
2	2	2	53.63	- 50.31	5	3	-12	11.78	12.21	1	3	1	21.29	- 22.66	4	4	0	59.17	- 59.70
2	2	3	87.68	72.24	5	3	-11	23.77	- 25.79	1	3	2	10.05	9.22	4	4	1	55.96	- 55.58
2	2	4	46.32	47.14	5	3	-10	11.16	- 11.28	1	3	3	84.16	88.47	4	4	3	45.63	40.66
2	2	5	50.15	- 51.29	5	3	- 9	45.79	48.81	1	3	4	21.97	19.21	4	4	4	9.08	9.37
2	2	6	25.14	- 24.33	5	3	- 8	23.71	21.03	1	3	5	119.44	-115.32	4	4	5	33.93	- 30.76
2	2	7	66.81	64.16	5	3	- 7	27.65	- 31.03	1	3	6	7.52	- 5.16	4	4	6	20.27	- 20.05
2	2	8	16.46	15.76	5	3	- 6	16.19	- 17.31	1	3	7	65.87	67.03	4	4	7	19.96	18.45
2	2	9	35.29	- 36.91	5	3	- 5	7.83	8.51	1	3	8	17.61	15.60	4	4	9	12.60	- 11.80
2	2	10	15.19	- 15.22	5	3	- 4	27.07	25.01	1	3	9	17.30	- 14.86	3	4	-14	5.06	- 4.94
2	2	11	8.94	10.69	5	3	- 3	8.89	- 7.23	1	3	10	12.89	- 12.25	3	4	-13	3.70	3.69
2	2	12	11.27	9.58	5	3	- 2	4.25*	- 0.76	1	3	11	18.14	16.64	3	4	-12	19.39	18.49
1	2	-13	6.36	7.26	5	3	- 1	48.15	48.28	1	3	12	5.00	6.18	3	4	-11	7.95	6.23
1	2	-12	4.55	2.55	5	3	0	5.34	- 5.80	0	3	3	67.68	61.68	3	4	-10	11.58	- 10.30
1	2	-11	13.86	- 13.18	5	3	1	49.24	- 46.29	0	3	5	30.19	- 30.81	3	4	- 8	32.41	31.05
1	2	-10	7.86	10.16	5	3	2	4.19*	1.14	0	3	6	12.13	11.48	3	4	- 7	18.74	17.55
1	2	- 9	30.75	35.16	5	3	3	43.74	43.71	0	3	7	9.99	8.14	3	4	- 6	34.40	35.27
1	2	- 7	17.64	- 18.94	5	3	4	19.47	17.72	0	3	11	17.02	- 19.27	3	4	- 5	4.77	- 6.27
1	2	- 6	23.02	- 22.61	5	3	5	41.88	- 38.65	0	3	13	9.56	9.93	3	4	- 4	18.60	- 21.17
1	2	- 5	49.63	- 49.16	5	3	6	4.78	- 3.71	9	4	-10	7.41	- 7.25	3	4	- 3	8.86	8.83
1	2	- 4	5.42	- 4.04	5	3	7	26.63	24.58	9	4	- 9	4.88	6.81	3	4	- 2	54.26	55.78
1	2	- 3	96.43	103.95	5	3	8	4.47	3.94	9	4	- 8	8.27	9.68	3	4	0	5.91	5.68
1	2	- 2	23.30	22.99	4	3	-15	4.92	- 5.07	9	4	- 7	4.44	- 5.22	3	4	1	17.13	- 14.17
1	2	- 1	20.00	19.81	4	3	-13	12.13	10.33	9	4	- 4	11.52	- 9.11	3	4	2	9.63	- 8.22
1	2	1	73.07	70.56	4	3	-12	5.16	4.28	9	4	- 3	6.02	- 5.08	3	4	3	17.72	18.22
1	2	2	15.99	12.53	4	3	-11	16.75	- 19.03	9	4	- 2	11.60	11.07	3	4	4	27.43	25.47
1	2	3	20.47	23.47	4	3	-10	5.38	4.95	9	4	- 1	3.48	3.19	3	4	5	8.49	10.78
1	2	5	27.85	- 27.83	4	3	- 9	18.02	- 18.25	8	4	-12	11.42	10.79	3	4	7	10.24	- 10.12
1	2	6	10.08	7.34	4	3	- 7	36.51	38.19	8	4	-11	13.91	- 15.44	3	4	8	8.85	10.37
1	2	7	29.22	30.89	4	3	- 6	12.33	- 9.86	8	4	-10	15.74	- 14.11	3	4	10	6.41	4.52
1	2	9	8.86	9.01	4	3	- 5	55.95	- 55.07	8	4	- 9	15.91	17.03	3	4	11	3.97	- 3.78
1	2	10	8.16	- 7.28	4	3	- 3	4.92	3.56	8	4	- 7	14.96	- 15.99	2	4	-14	4.91	- 4.70
1	2	13	5.95	4.55	4	3	- 2	25.65	23.20	8	4	- 6	15.21	15.52	2	4	-13	16.82	- 14.68
0	2	2	93.20	93.27	4	3	- 1	21.32	- 21.15	8	4	- 5	19.72	18.61	2	4	-12	13.28	13.30
0	2	3	67.02	- 58.99	4	3	0	16.69	18.10	8	4	- 4	15.46	- 13.61	2	4	-11	34.38	31.89
0	2	4	59.21	- 54.86	4	3	1	38.85	- 38.32	8	4	- 3	18.00	- 19.28	2	4	-10	4.88	- 3.33
0	2	5	31.97	35.52	4	3	3	25.30	25.36	8	4	- 2	17.25	18.09	2	4	- 9	42.54	- 43.85
0	2	6	27.18	27.27	4	3	4	4.81	- 4.78	8	4	- 1	19.82	17.15	2	4	- 8	8.55	8.27
0	2	7	61.71	- 61.89	4	3	5	13.99	- 12.08	8	4	0	9.91	- 9.14	2	4	- 7	44.87	47.42
0	2	8	21.21	- 18.79	4	3	6	8.05	9.70	8	4	1	17.78	- 14.51	2	4	- 5	67.68	- 73.22
0	2	9	24.88	23.35	4	3	7	10.30	- 10.76	8	4	2	5.44	- 4.25	2	4	- 4	8.66	7.69
0	2	10	13.06	13.91	4	3	9	10.27	11.36	7	4	-12	16.69	13.27	2	4	- 3	59.12	66.89
0	2	12	13.17	- 13.39	3	3	-13	4.31	- 4.72	7	4	-11	5.38	5.18	2	4	- 2	14.50	- 15.61
0	2	13	5.69	5.60	3	3	-12	15.86	- 16.76	7	4	- 9	9.78	- 10.45	2	4	- 1	18.21	- 14.66
9	3	-11	10.78	- 11.95	3	3	-11	32.30	32.80	7	4	- 8	5.72	3.60	2	4	0	16.97	12.83
9	3	-10	9.72	- 9.17	3	3	-10	12.17	10.67	7	4	- 7	11.53	11.23	2	4	1	61.07	60.80
9	3	- 9	10.16	12.95	3	3	- 9	53.60	- 49.88	7	4	- 6	13.97	14.76	2	4	2	10.38	12.87
9	3	- 8	8.24	6.35	3	3	- 8	17.33	- 16.21	7	4	- 5	4.47	- 4.14	2	4	3	58.53	- 57.27
9	3	- 7	4.52	- 6.61	3	3	- 7	70.22	79.58	7	4	- 4	10.61	- 10.04	2	4	4	12.85	11.34
9	3	- 6	3.86	- 3.67	3	3	- 5	80.72	- 80.74	7	4	- 2	11.56	11.63	2	4	5	60.20	60.40
9	3	- 5	10.83	- 9.94	3	3	- 4	8.94	- 8.03	7	4	0	8.45	7.36	2	4	6	6.45	4.09
9	3	- 1	13.46	13.62	3	3	- 3	59.53	63.93	7	4	2	7.86	- 9.01	2	4	7	31.90	- 30.54
8	3	-13	3.88	4.51	3	3	- 2	9.38	- 9.34	7	4	4	4.27	4.55	2	4	8	6.64	9.46
8	3	- 9	19.52	- 19.86	3	3	- 1	35.80	- 33.27	7	4	5	3.78	4.91	2	4	9	31.10	29.86
8	3	- 7	18.14	15.88	3	3	0	7.31	- 4.88	6	4	-14	4.80	- 5.09	2	4	10	7.88	- 8.88
8	3	- 6	4.74	- 3.78	3	3	1	39.85	36.76	6	4	-13	14.30	- 13.99	2	4	11	17.99	- 15.28
8	3	- 5	19.08	- 18.97	3	3	2	22.93	21.63	6	4	-11	31.24	32.13	2	4	12	6.58	6.83
8	3	- 3	5.05	2.89	3	3	3	24.35	- 20.02	6	4	-10	9.10	- 6.51	1	4	-14	3.97	3.35
8	3	- 1	7.20	8.12	3	3	4	50.13	- 44.61	6	4	- 9	32.71	- 32.23	1	4	-13	3.61	- 3.10
8	3	0	3.77*	- 1.83	3	3	5	54.35	46.01	6	4	- 7	26.54	23.29	1	4	-12	7.13	- 5.89
8	3	1	12.69	- 10.28	3	3	6	16.16	16.40	6	4	- 6	6.80	- 8.39	1	4	- 9	9.47	- 8.79
7	3	-14	2.38	3.27	3	3	7	34.97	- 36.66	6	4	- 5	28.71	- 26.77	1	4	- 8	13.58	16.43
7	3	-13	13.74	- 12.84	3	3	8	4.88	- 5.14	6	4	- 4	4.72	- 5.19	1	4	- 6	35.57	- 35.80
7	3	-12	13.30	- 12.14	3	3	9	18.57	21.64	6	4	- 3	36.16	37.51	1	4	- 5	7.34	7.00
7	3	-11	24.13	25.28	3	3	10	3.47	2.54	6	4	- 2	12.97	- 17.12	1	4	- 4	9.22	9.89
7	3	-10	7.55	8.29	3	3	11	14.11	- 13.39	6	4	- 1	13.13	- 11.57	1	4	- 3	36.58	- 40.91
7	3	- 9	28.35	- 30.62	2	3	-14	4.69	5.78	6	4	1	20.96	23.49	1	4	- 2	11.06	11.08
7	3	- 8	4.52	- 3.40	2	3	-12	13.96	- 11.57	6	4	2	6.30	5.72	1	4	- 1	5.31	5.65
7	3	- 7	41.15	41.55	2	3	-10	4.75	3.07	6	4	3	27.83	- 26.92	1	4	0	24.77	- 27.76
7	3	- 6	7.08	- 6.39	2	3	- 9	11.94	- 9.63	6	4	5	22.53	24.74	1	4	1	3.95	3.34
7	3	- 5	28.47	- 25.59	2	3	- 8	7.92	10.16	6	4	6	3.95	- 3.88	1	4	2	68.89	70.01
7	3	- 3	22.71	18.71	2	3	- 7	11.39	- 12.43	6	4	7	9.66	- 10.67	1	4	3	7.42	- 6.95
7	3	- 2	5.41	6.22	2	3	- 6	12.81	- 13.85	5	4	-14	5.99	5.19	1	4	4	31.22	- 30.29
7	3	- 1	4.97	- 4.18	2	3	- 5	4.19	- 4.47	5	4	-13	8.05	- 7.51	1	4	5	9.83	- 6.50
7	3	0	8.75	- 6.86	2	3	- 4	33.46	35.40	5	4	-10	12.11	- 11.90	1	4	6	13.66	- 14.13
7	3	1	22.11	21.26	2	3	- 3	12.46	15.82	5	4	- 8	9.99	9.56	1	4	7	11.27	- 13.67

Table 4 (*cont.*)

h	k	l	F OBS	F CALC
1	4	8	21.53	22.81
1	4	10	14.50	- 14.28
1	4	12	7.60	7.02
0	4	2	27.18	28.71
0	4	3	65.31	58.85
0	4	4	21.32	- 17.89
0	4	5	62.56	- 63.27
0	4	6	38.46	- 35.14
0	4	7	43.93	46.11
0	4	8	10.99	10.29
0	4	9	28.54	- 29.44
0	4	10	20.22	- 22.41
0	4	11	18.24	17.34
0	4	12	8.77	- 6.99
0	4	13	10.19	- 11.17
9	5	- 9	12.58	- 12.15
9	5	- 7	11.52	10.53
9	5	- 6	5.80	- 8.18
9	5	- 5	16.24	- 17.05
9	5	- 4	10.44	10.36
9	5	- 3	10.13	11.44
9	5	- 2	12.89	- 14.04
9	5	- 1	8.53	- 9.82
8	5	-10	6.30	4.90
8	5	- 6	4.11	3.36
8	5	- 5	6.16	- 7.29
8	5	- 3	5.72	- 6.17
8	5	- 2	17.17	14.66
8	5	- 1	12.02	9.97
8	5	1	6.83	- 6.25
7	5	-13	9.78	11.08
7	5	-12	5.52	- 4.50
7	5	-11	16.44	- 14.21
7	5	- 9	9.81	9.73
7	5	- 8	10.14	- 7.61
7	5	- 7	9.06	- 8.44
7	5	- 6	30.58	32.79
7	5	- 5	21.61	23.48
7	5	- 4	31.22	- 34.96
7	5	- 3	24.04	- 23.71
7	5	- 2	13.60	15.56
7	5	- 1	23.46	21.83
7	5	0	4.56	- 3.63
7	5	1	13.47	- 13.65
7	5	3	15.08	14.80
6	5	-14	10.72	- 11.19
6	5	-12	14.42	12.77
6	5	- 9	5.95	- 5.93
6	5	- 8	23.43	- 24.74
6	5	- 7	6.02	6.50
6	5	- 6	21.49	18.97
6	5	- 5	4.97	4.54
6	5	- 4	11.77	- 13.46
6	5	- 3	11.60	14.74
6	5	- 2	9.69	- 10.07
6	5	0	16.47	18.00
6	5	2	23.88	- 24.76
6	5	4	8.74	10.14
6	5	5	4.17	3.70
5	5	-14	12.55	- 13.88
5	5	-13	9.95	- 10.48
5	5	-12	10.56	9.10
5	5	-11	17.21	16.94
5	5	- 9	16.99	- 17.41
5	5	- 7	30.54	27.35
5	5	- 6	4.31	- 4.28
5	5	- 5	45.59	- 44.94
5	5	- 4	15.80	15.79
5	5	- 3	43.82	46.95
5	5	- 2	42.98	- 45.83
5	5	- 1	29.99	- 29.88
5	5	0	32.41	33.52
5	5	1	15.69	16.32
5	5	2	27.68	- 27.02
5	5	3	19.02	19.37
5	5	4	6.45	7.95
5	5	5	15.19	13.16
5	5	6	9.14	- 9.33
5	5	7	10.60	- 7.48
4	5	-13	3.99	4.70
4	5	-11	6.36	- 7.72
4	5	-10	9.92	8.68
4	5	- 9	4.78	5.29
4	5	- 8	6.86	- 5.08
4	5	- 7	14.35	12.71
4	5	- 6	5.22	3.41
4	5	- 5	23.30	- 19.60
4	5	- 4	6.89	7.57
4	5	- 3	12.16	- 10.05
4	5	- 2	23.25	20.21
4	5	- 1	11.53	7.99
4	5	0	4.31	- 2.46
4	5	1	14.16	- 11.30
4	5	2	10.22	7.63
4	5	3	10.35	10.82
4	5	4	11.22	10.71
4	5	5	11.35	- 12.54
4	5	8	9.85	6.86
4	5	9	5.94	4.53
3	5	-14	6.20	5.98
3	5	-12	5.33	- 3.83
3	5	-11	23.49	- 21.57
3	5	- 9	15.33	14.75
3	5	- 8	14.21	- 11.26
3	5	- 7	24.54	- 23.80
3	5	- 6	34.85	35.55
3	5	- 5	36.82	33.53
3	5	- 4	67.64	- 69.58
3	5	- 3	58.10	- 56.12
3	5	- 2	64.75	65.73
3	5	- 1	45.34	40.57
3	5	0	33.41	- 31.17
3	5	1	58.45	- 51.42
3	5	2	21.41	18.80
3	5	3	54.23	52.60
3	5	4	5.97	5.76
2	5	-14	10.50	- 9.95
2	5	-12	16.30	15.01
2	5	-10	17.97	- 15.74
2	5	- 9	7.00	- 8.12
2	5	- 8	12.99	- 13.73
2	5	- 7	7.27	- 4.46
2	5	- 6	32.16	32.01
2	5	- 5	7.02	- 8.69
2	5	- 4	43.52	- 45.58
2	5	- 3	14.16	15.05
2	5	- 2	37.91	38.40
2	5	- 1	8.85	5.52
2	5	0	18.30	20.41
2	5	2	66.65	- 65.73
2	5	3	6.53*	- 2.54
2	5	4	26.71	26.93
2	5	6	14.63	- 15.05
2	5	10	17.19	15.65
2	5	11	3.38*	- 1.46
1	5	-13	11.50	- 10.46
1	5	-12	18.13	17.05
1	5	-11	13.86	13.47
1	5	-10	10.94	- 13.71
1	5	- 9	20.28	- 22.75
1	5	- 8	9.88	7.32
1	5	- 7	37.91	34.41
1	5	- 6	32.33	30.93
1	5	- 5	41.96	45.92
1	5	- 4	18.82	14.01
1	5	- 3	75.64	83.55
1	5	- 2	60.07	- 73.66
1	5	- 1	52.20	- 63.93
1	5	0	45.63	50.89
1	5	1	44.71	52.38
1	5	2	67.07	- 71.62
1	5	3	52.26	- 52.22
1	5	4	50.07	54.14
1	5	5	24.19	20.17
1	5	6	17.66	- 18.10
1	5	7	22.94	- 16.78
1	5	8	4.58*	1.45
1	5	9	25.64	22.60
1	5	10	5.63	- 4.97
1	5	11	17.39	- 16.56
1	5	12	7.28	6.19
0	5	-10	13.60	10.01
0	5	- 9	12.58	10.12
0	5	- 8	17.82	- 14.96
0	5	- 7	13.19	12.74
0	5	- 6	13.69	- 12.82
0	5	- 5	13.30	- 11.48
0	5	- 4	10.00	- 8.47
0	5	- 3	24.04	23.15
9	6	- 5	6.59	5.56
9	6	- 4	5.52	5.80
9	6	- 2	5.28	- 8.15
8	6	-11	6.70	6.31
8	6	-10	4.45	- 4.18
8	6	- 9	7.13	- 6.19
8	6	- 8	9.30	12.72
8	6	- 7	10.31	10.80
8	6	- 6	12.75	- 13.40
8	6	- 5	6.77	- 9.38
8	6	- 4	21.38	25.44
8	6	- 3	8.72	8.26
8	6	- 2	17.69	- 18.53
8	6	0	13.09	12.95
8	6	1	4.45	2.50
7	6	-12	5.84	- 5.86
7	6	-11	4.53	2.46
7	6	-10	5.56	3.90
7	6	- 9	11.41	- 9.70
7	6	- 8	8.94	- 6.84
7	6	- 7	8.77	7.47
7	6	- 6	7.02	- 7.87
7	6	- 3	17.55	- 20.69
7	6	- 1	10.80	10.71
7	6	0	11.31	- 12.39
7	6	1	10.03	- 11.48
6	6	-12	12.39	- 13.48
6	6	-11	7.61	6.76
6	6	-10	21.94	21.69
6	6	- 9	8.47	- 8.92
6	6	- 8	13.27	- 12.11
6	6	- 7	16.80	- 17.59
6	6	- 6	17.99	16.86
6	6	- 5	23.89	22.18
6	6	- 4	37.19	- 36.16
6	6	- 3	34.06	- 33.98
6	6	- 2	28.47	28.68
6	6	- 1	37.11	36.91
6	6	0	9.58	- 9.28
6	6	1	16.24	- 16.25
5	6	-13	10.39	13.34
5	6	-11	7.44	9.38
5	6	-10	10.95	- 8.88
5	6	- 9	8.70	- 10.03
5	6	- 8	9.69	- 7.18
5	6	- 7	17.89	14.42
5	6	- 6	19.69	17.69
5	6	- 5	21.88	- 15.45
5	6	- 3	27.38	- 26.74
5	6	- 2	6.31	7.27
5	6	- 1	14.11	11.34
5	6	0	12.28	9.36
5	6	1	6.03	- 3.54
4	6	-14	19.69	- 15.52
4	6	-13	9.00	6.52
4	6	-12	9.13	- 11.39
4	6	-11	9.06	- 9.49
4	6	-10	12.34	14.59
4	6	- 9	13.61	15.08
4	6	- 8	8.03	- 5.95
4	6	- 7	13.47	- 11.03
4	6	- 6	12.17	10.18
4	6	- 5	24.74	25.58
4	6	- 4	30.64	- 30.52
4	6	- 3	6.25	- 4.34
4	6	- 2	56.07	59.44
4	6	- 1	32.42	29.68
4	6	0	40.17	- 43.17
4	6	1	29.50	- 26.16
3	6	-13	48.27	50.14
3	6	-12	14.16	9.75
3	6	-11	32.05	- 31.39
3	6	- 9	6.50	- 4.44
3	6	- 8	24.33	19.63
3	6	- 7	17.89	16.34
3	6	- 6	5.27	- 7.65
3	6	- 5	6.44	7.46
3	6	- 4	9.59	11.89
3	6	- 3	5.78	6.52
3	6	- 2	9.98	- 9.49
3	6	- 1	10.52	7.09
3	6	0	13.64	9.78
3	6	1	9.42	- 8.88
3	6	2	26.13	22.76
3	6	3	11.30	- 10.89
3	6	4	18.58	- 15.45
3	6	5	14.75	11.16
3	6	6	7.59	- 6.48
3	6	7	35.36	35.92
2	6	-13	8.63	7.67
2	6	-12	16.53	- 17.31
2	6	-10	28.14	27.19
2	6	- 9	14.84	- 13.92
2	6	- 8	14.22	- 11.68
2	6	- 7	4.94	- 3.55
2	6	- 6	38.11	43.96
2	6	- 5	7.05	5.57
2	6	- 4	47.17	- 47.45
2	6	- 2	67.71	- 69.50
2	6	- 1	50.91	50.45
2	6	0	81.61	87.91
2	6	1	32.96	- 32.08
2	6	2	50.02	- 53.62
2	6	3	54.72	54.41
2	6	4	21.94	21.52
2	6	5	30.22	- 31.87
2	6	6	6.64	- 4.98
2	6	7	21.99	22.63
2	6	8	9.73	- 8.03
2	6	10	10.67	- 12.87
2	6	11	20.53	20.78
1	6	-11	6.44	6.38
1	6	-10	5.58	7.98
1	6	- 9	7.16	- 5.48
1	6	- 8	28.83	- 30.18
1	6	- 6	11.99	- 11.65
1	6	- 5	7.81	8.52
1	6	- 4	15.72	18.35
1	6	- 3	13.36	- 11.94
1	6	- 2	49.91	- 52.45
1	6	1	20.31	- 20.14
1	6	2	26.06	- 30.32
1	6	3	23.30	- 22.29
1	6	4	25.38	- 22.70
1	6	5	28.38	26.37
1	6	7	11.75	7.95
0	6	-13	26.86	- 25.66
0	6	-11	18.24	- 16.46
0	6	- 9	15.63	- 13.96
0	6	- 8	14.64	12.40
0	6	- 7	13.84	12.04
0	6	- 6	29.91	- 26.81
0	6	- 5	22.61	- 20.96
0	6	- 4	37.08	34.24
0	6	- 3	38.49	37.53
0	6	- 2	58.47	- 63.01
0	6	- 1	13.47	14.63
8	7	- 9	11.92	- 11.69
8	7	- 7	7.00	4.72
8	7	- 5	7.22	- 7.61
8	7	- 1	3.70	4.22
7	7	0	8.05	13.56
7	7	-12	7.58	- 8.79
7	7	-11	11.67	- 13.65
7	7	-10	17.00	17.02
7	7	- 8	9.56	- 7.80
7	7	- 7	12.92	- 12.94
7	7	- 6	19.33	22.15
7	7	- 4	6.47	6.37
7	7	- 3	13.87	- 13.49
7	7	- 2	16.01	- 16.04
7	7	- 1	18.61	18.69
7	7	0	5.86	6.62
7	7	1	12.00	- 16.12
7	7	2	6.42	- 5.39
6	7	- 8	10.51	9.40
6	7	- 6	6.06	- 10.23
6	7	- 4	10.81	9.54
6	7	- 1	4.75	- 5.67
5	7	-13	10.39	- 12.65
5	7	-12	5.28	4.59
5	7	-11	20.87	22.65
5	7	-10	28.22	- 30.74
5	7	- 8	10.67	- 7.69
5	7	- 7	26.65	26.09
5	7	- 6	27.79	24.67
5	7	- 5	31.39	- 34.98
5	7	- 4	26.83	- 27.75
5	7	- 3	27.64	28.74
5	7	- 2	6.19	4.31
5	7	- 1	25.95	- 27.80
5	7	0	18.36	18.10
5	7	2	15.51	- 16.77
5	7	3	19.53	- 18.41
5	7	4	15.94	13.93
5	7	5	14.94	15.40
5	7	6	7.19	- 10.60
4	7	-13	12.86	16.72
4	7	-11	17.90	15.12
4	7	- 9	6.81	3.89
4	7	- 8	19.97	- 18.07
4	7	- 7	33.75	30.07
4	7	- 5	8.20	- 6.35
4	7	- 4	20.36	- 18.05
4	7	- 3	12.25	- 8.30
4	7	- 2	5.06*	2.15
4	7	- 1	12.05	9.22
4	7	0	44.20	40.59
4	7	1	20.67	- 21.29
4	7	3	10.73	10.20
4	7	5	6.48	7.12
4	7	7	6.89	- 8.89
3	7	-13	13.72	17.78
3	7	-12	32.83	- 28.19
3	7	-10	21.83	21.78
3	7	- 8	25.12	- 27.07
3	7	- 7	32.06	- 32.32
3	7	- 6	11.09	11.47
3	7	- 5	48.12	42.35
3	7	- 4	4.53	3.85
3	7	- 3	47.57	- 35.73
3	7	- 2	37.17	- 31.39
3	7	- 1	51.92	42.00
3	7	0	30.93	28.81
3	7	1	48.12	- 39.17
3	7	2	13.47	- 11.37
3	7	3	39.06	36.44
3	7	4		

Table 4 (*cont.*)

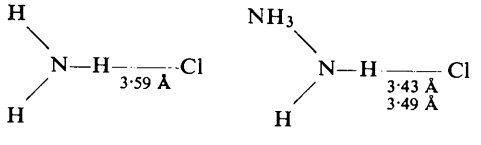
h	k	l	F OBS	F CALC	h	k	l	F OBS	F CALC	h	k	l	F OBS	F CALC	h	k	l	F OBS	F CALC
3	7	6	24.72	- 27.29	5	8	- 6	22.40	22.90	1	8	-11	8.30	- 6.48	4	9	- 0	10.49	7.10
3	7	8	11.83	15.83	5	8	- 3	21.89	19.79	1	8	- 8	7.95	- 8.17	4	9	1	7.15*	2.89
3	7	10	4.58	- 9.36	5	8	- 2	10.91	- 8.27	1	8	- 7	14.72	- 16.08	4	9	4	8.64	- 9.66
2	7	- 6	13.47	12.21	5	8	- 1	5.09*	- 2.32	1	8	- 6	16.37	15.33	3	9	-12	11.79	- 14.97
2	7	- 3	7.06*	0.91	5	8	0	17.55	15.75	1	8	- 5	19.48	- 12.56	3	9	-11	13.69	13.80
2	7	- 2	15.36	15.37	5	8	3	4.87	7.08	1	8	- 4	14.30	- 11.60	3	9	-10	13.33	14.00
2	7	- 1	5.16*	- 1.13	4	8	-12	14.31	- 16.96	1	8	- 3	34.82	31.53	3	9	- 9	12.21	- 10.10
2	7	0	6.06	- 5.40	4	8	-11	6.20	6.93	1	8	- 2	5.06	- 4.59	3	9	- 8	29.58	- 27.03
2	7	1	16.11	- 10.11	4	8	-10	27.04	32.82	1	8	1	5.30*	- 1.18	3	9	- 7	19.27	18.52
2	7	2	17.09	- 12.82	4	8	- 9	7.16	- 5.53	1	8	2	18.26	- 17.62	3	9	- 6	21.35	16.96
1	7	-12	9.81	- 12.49	4	8	- 8	40.14	- 41.09	1	8	3	8.92	8.01	3	9	- 5	15.77	- 14.42
1	7	-11	5.33	6.25	4	8	- 7	11.39	11.01	1	8	4	20.89	20.94	3	9	- 4	5.78	5.15
1	7	-10	23.33	25.61	4	8	- 6	30.81	28.92	1	8	5	10.61	- 8.59	3	9	- 3	33.30	27.76
1	7	- 9	11.01	- 10.27	4	8	- 5	9.94	- 8.72	1	8	6	11.03	10.38	3	9	- 2	4.89*	1.89
1	7	- 8	22.48	- 24.05	4	8	- 4	13.33	- 12.76	1	8	7	5.61	4.18	3	9	- 1	16.04	- 11.81
1	7	- 6	49.71	45.02	4	8	- 3	9.69	9.88	1	8	8	13.28	- 13.52	3	9	0	22.82	- 21.34
1	7	- 5	21.70	19.15	4	8	- 2	11.70	9.26	1	8	10	8.89	9.57	3	9	1	34.80	28.55
1	7	- 4	59.70	- 54.01	4	8	- 1	9.31	- 8.61	0	8	-12	5.84	- 8.60	3	9	2	31.58	29.18
1	7	- 3	34.81	- 33.21	4	8	0	14.64	- 11.33	0	8	-10	21.67	26.09	3	9	3	14.76	- 13.79
1	7	- 2	49.32	59.40	4	8	1	10.67	7.77	0	8	- 9	8.89	- 4.87	3	9	4	37.86	- 36.95
1	7	- 1	19.97	25.68	4	8	2	26.92	23.96	0	8	- 8	34.48	- 38.31	3	9	5	16.65	18.70
1	7	0	30.33	- 41.57	4	8	3	16.80	- 14.78	0	8	- 7	16.08	14.44	3	9	6	24.18	24.52
1	7	1	34.29	- 36.05	4	8	4	22.65	- 26.39	0	8	- 6	49.46	47.08	3	9	7	5.31	- 8.36
1	7	2	39.07	37.19	4	8	5	10.87	7.55	0	8	- 5	14.72	- 10.50	3	9	8	11.52	- 13.36
1	7	3	22.29	- 20.78	4	8	6	26.23	29.55	0	8	- 4	38.07	- 36.23	2	9	-12	8.21	- 8.52
1	7	4	46.14	- 39.00	4	8	7	5.34	- 4.25	0	8	- 3	25.37	21.14	2	9	-10	11.93	10.73
1	7	5	31.31	29.28	4	8	8	11.22	- 18.15	0	8	- 2	29.00	28.15	2	9	- 7	7.49	- 6.26
1	7	6	46.11	40.81	3	8	-12	10.37	- 10.01	7	9	-10	8.27	11.35	2	9	- 6	23.92	- 22.44
1	7	7	20.48	- 16.27	3	8	-10	11.33	7.71	7	9	- 9	4.19	- 5.65	2	9	- 4	42.39	41.75
1	7	8	18.50	- 15.21	3	8	- 9	12.67	9.78	7	9	- 8	7.78	- 9.75	2	9	2	23.57	20.72
1	7	10	20.23	19.32	3	8	- 8	9.58	- 8.91	7	9	- 7	10.22	10.08	2	9	3	6.92	- 5.47
0	7	-11	15.72	17.60	3	8	- 7	16.62	- 11.96	7	9	- 5	9.85	- 10.01	2	9	4	19.84	- 18.73
0	7	- 9	6.02*	1.66	3	8	- 6	21.25	- 19.88	7	9	- 4	6.25	5.00	2	9	6	13.57	11.82
0	7	- 7	5.84*	- 2.10	3	8	- 5	8.80	5.17	7	9	- 3	10.80	10.05	2	9	8	6.80	5.13
0	7	- 6	8.86	8.70	3	8	- 4	14.17	12.59	7	9	- 2	8.91	9.64	2	9	9	3.74	- 2.76
0	7	- 5	38.03	32.46	3	8	- 2	24.00	- 23.91	7	9	- 1	7.91	- 6.45	1	9	-11	5.49	- 8.52
0	7	- 4	14.78	- 12.28	3	8	- 1	9.53	- 7.69	7	9	0	10.05	- 14.13	1	9	-10	8.27	- 7.46
0	7	- 3	39.82	- 36.59	3	8	0	5.48	5.26	7	9	1	7.94	10.88	1	9	- 9	16.34	16.78
0	7	- 2	20.42	- 20.14	3	8	1	19.26	14.89	6	9	- 8	15.51	20.36	1	9	- 8	39.02	36.40
8	8	- 8	10.91	- 14.44	3	8	2	6.62	- 7.86	6	9	- 7	6.49	- 6.06	1	9	- 7	17.01	- 14.34
8	8	- 6	6.75	9.35	3	8	3	22.01	- 13.89	6	9	- 6	14.26	- 15.49	1	9	- 6	51.26	- 49.52
8	8	- 1	5.69	- 7.11	3	8	4	21.84	- 18.55	6	9	- 4	12.71	13.88	1	9	- 5	25.26	21.93
7	8	- 9	6.73	6.04	3	8	7	12.83	13.96	6	9	- 1	9.08*	- 3.73	1	9	- 4	32.37	31.81
7	8	- 7	14.31	- 12.29	2	8	-12	8.08	7.57	6	9	0	12.35	- 12.61	1	9	- 3	29.92	- 30.23
7	8	- 6	17.55	- 16.25	2	8	-11	14.30	- 13.56	6	9	2	10.40	11.76	1	9	- 2	11.60	- 14.15
7	8	- 4	7.95	8.89	2	8	-10	16.73	- 17.81	5	9	-12	6.66	10.45	1	9	- 1	22.49	28.65
7	8	- 3	5.47	6.42	2	8	- 9	21.29	20.56	5	9	-11	6.77	- 8.13	1	9	0	20.21	22.33
7	8	- 2	7.00	- 7.76	2	8	- 8	29.62	26.80	5	9	-10	15.30	- 15.72	1	9	1	15.98	- 16.65
7	8	- 1	5.66	- 4.70	2	8	- 7	16.70	- 16.03	5	9	- 9	12.24	14.62	1	9	2	9.61	- 5.63
7	8	0	4.81*	- 1.47	2	8	- 6	33.17	- 29.47	5	9	- 8	24.14	28.10	1	9	3	21.53	19.66
7	8	1	4.34	4.40	2	8	- 5	13.97	13.31	5	9	- 7	17.34	- 16.69	1	9	4	14.79	7.65
6	8	-12	8.39	10.05	2	8	- 4	39.43	38.03	5	9	- 6	31.51	- 30.22	1	9	5	28.04	- 24.06
6	8	-11	13.45	- 16.15	2	8	- 3	15.58	- 14.58	5	9	- 5	9.79	12.02	1	9	6	19.57	- 15.21
6	8	-10	11.17	- 12.21	2	8	- 2	45.84	- 49.73	5	9	- 4	16.18	15.46	1	9	7	17.21	13.00
6	8	- 9	15.48	15.59	2	8	- 1	25.83	- 25.07	5	9	- 3	17.48	- 17.13	1	9	8	28.25	29.04
6	8	- 8	19.39	20.47	2	8	0	36.84	35.76	5	9	- 2	6.13	- 5.51	1	9	9	10.49	- 8.90
6	8	- 6	21.86	- 20.10	2	8	1	21.08	15.26	5	9	- 1	13.46	16.37	1	9	10	9.27	- 12.62
6	8	- 4	19.23	19.38	2	8	2	43.14	- 42.64	5	9	0	5.35	4.78	0	9	-10	8.79	- 7.44
6	8	- 2	18.47	- 18.75	2	8	3	21.44	21.34	5	9	1	12.44	- 13.83	0	9	- 9	7.71	- 4.32
6	8	0	21.62	25.71	2	8	4	31.79	31.68	5	9	2	6.86	- 5.77	0	9	- 8	12.10	9.00
6	8	2	15.81	- 19.73	2	8	5	23.87	- 23.46	5	9	3	6.69	7.20	0	9	- 7	6.80	- 3.57
6	8	3	8.08	11.05	2	8	6	28.06	- 27.29	5	9	4	16.12	15.55	0	9	- 6	10.60	5.97
6	8	4	7.87	11.27	2	8	7	10.61	11.35	5	9	5	9.91	- 10.14	0	9	- 5	9.64	5.03
6	8	5	7.16	- 12.21	2	8	8	15.65	14.77	5	9	6	5.75	- 8.13	0	9	- 4	8.82*	- 3.74
5	8	-11	5.41	- 5.92	2	8	9	12.56	- 13.20	4	9	- 4	15.51	- 12.32	0	9	- 3	8.11*	1.44
5	8	-10	5.47	8.58	2	8	10	6.70	- 7.52	4	9	- 2	6.63*	- 2.95	0	9	- 2	12.10	- 14.35
5	8	- 8	9.36	- 8.62						4	9	- 1	7.97	- 5.68					

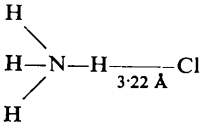
Table 5. Zn–Cl *bond lengths*

Compound	Distance	Reference
$Na_2ZnCl_4 \cdot 3H_2O$	2·26 Å	Brehler (1960)
$Zn[SC(NH_2)_2NHNH_2]Cl_2$	2·24	Cavalca, Nardelli & Branchi (1960)
$(NH_4)_3ZnCl_5$	2·25	Klug & Alexander (1944)

0·060 Å from plane 3 and 0·043 Å from plane 6. The sum of the bond angles around N(1) is 360·01° and around N(3) 359·78°; the differences from 360·00 are well within the standard deviations for the bond angles.

The packing of the molecules is shown in Fig. 2. The interatomic distances N(2)–H---Cl(2′) and N(4)–H---Cl(1′) are 3·27 and 3·34 Å respectively (Fig. 1), and they can be compared with those given by Olovsson (1960):





Hydrogen bonds are assumed between the pseudo-acid imino hydrogen atoms of the imidazole rings [N(2) and N(4)] and the chlorine atoms. If the hydrogen atoms lie in the planes of the imidazole rings the angles H–N(2)---Cl(2′) and H–N(4)---Cl(1′) are 27°31′ and 8°48′ respectively. The differences in the isotropic temperature factors for the nitrogen atoms are also significant (Table 1). The value for N(2) is 1·2 Å² higher than that for N(1) and the value for N(4) is 1·4 Å²

Table 6. *Distances (Å) from the atoms to different least-squares planes*

A figure in parenthesis means that the position for that atom is not used when the plane equation is calculated

Plane number		N(1)	C(1)	C(2)	C(3)	N(2)	Zn	N(3)	C(4)	C(5)	C(6)	N(4)	Cl(2')	Cl(1')
	Standard deviation	0·011	0·015	0·015	0·015	0·011	0·0014	0·011	0·015	0·015	0·015	0·011	0·0030	0·0030
1		−0·001	0·000	0·000	(0·041)	(0·045)	0·000						(1·555)	
2		−0·009	−0·016	−0·014	0·011	0·014	0·014						(1·592)	
3		0·009	−0·008	−0·006	0·001	0·004	(0·060)						(1·543)	
4							−0·008	0·031	−0·011	−0·010	(−0·003)	(−0·007)		(−0·548)
5							−0·010	0·032	−0·008	−0·009	0·000	−0·003		(−0·538)
6							(−0·043)	0·018	−0·014	−0·015	0·007	0·003		(−0·500)
7		(−0·988)	(−0·580)	(−0·610)	0·000	0·000	(−1·958)						0·000	
8							(0·690)	(0·312)	(0·216)	(0·229)	0·000	0·000		0·000

1: $-0{\cdot}89505X+0{\cdot}43619Y-0{\cdot}09284Z+0{\cdot}74241=0$.
2: $-0{\cdot}89844X+0{\cdot}43101Y-0{\cdot}08388Z+0{\cdot}73097=0$.
3: $-0{\cdot}90293X+0{\cdot}42346Y-0{\cdot}07351Z+0{\cdot}68184=0$.
4: $-0{\cdot}11298X+0{\cdot}99019Y-0{\cdot}08216Z+3{\cdot}44264=0$.
5: $-0{\cdot}11134X+0{\cdot}99041Y-0{\cdot}08178Z+3{\cdot}44743=0$.
6: $-0{\cdot}10515X+0{\cdot}99169Y-0{\cdot}07412Z+3{\cdot}51142=0$.
7: $0{\cdot}94619X-0{\cdot}12542Y-0{\cdot}29832Z+1{\cdot}34796=0$.
8: $0{\cdot}00097X-0{\cdot}99907Y-0{\cdot}04315Z-4{\cdot}58460=0$.

higher than that for N(3). These differences can be explained as due to the strength of the bonds Zn–N(1) and Zn–N(3) in comparison with the hydrogen bonds formed by the imino hydrogen atoms on N(2) and N(4).

The hydrogen bond system and the van der Waals forces are such that the crystal is essentially a three-dimensional network. Data on intermolecular distances short enough to be classed as van der Waals contacts are given in Table 7.

Table 7. *Intermolecular distances shorter than* 4·00 Å

A, B etc. refer to Fig. 2

$Cl(1)_A$–$Cl(2)_A$	3·72	$N(1)_A$–$N(2)_F$	3·66
$Cl(1)_A$–$Cl(2)_B$	3·81	$N(1)_A$–$N(3)_A$	3·19
$Cl(1)_A$–$N(1)_A$	3·39	$N(1)_A$–$C(1)_F$	3·90
$Cl(1)_A$–$N(2)_B$	3·39	$N(1)_A$–$C(4)_A$	3·57
$Cl(1)_A$–$N(3)_A$	3·55	$N(2)_A$–$C(1)_F$	3·80
$Cl(1)_A$–$N(4)_C$	3·88	$N(2)_A$–$C(3)_I$	3·74
$Cl(1)_A$–$C(1)_B$	3·99	$N(3)_A$–$C(2)_A$	3·60
$Cl(1)_A$–$C(1)_A$	3·62	$N(3)_A$–$C(3)_E$	3·74
$Cl(1)_A$–$C(2)_E$	3·69	$N(3)_A$–$C(5)_G$	3·84
$Cl(1)_A$–$C(4)_C$	3·74	$N(3)_A$–$C(6)_G$	3·86
$Cl(1)_A$–$C(5)_D$	3·73	$N(4)_A$–$C(3)_E$	3·70
$Cl(1)_A$–$C(6)_K$	3·76	$C(1)_A$–$C(1)_F$	3·86
$Cl(2)_A$–$N(1)_A$	3·56	$C(1)_A$–$C(2)_F$	3·86
$Cl(2)_A$–$N(3)_A$	3·46	$C(1)_A$–$C(3)_F$	3·82
$Cl(2)_A$–$N(4)_H$	3·50	$C(1)_A$–$C(5)_D$	3·86
$Cl(2)_A$–$N(4)_G$	3·90	$C(2)_A$–$C(4)_A$	3·71
$Cl(2)_A$–$C(1)_B$	3·68	$C(2)_A$–$C(4)_C$	3·98
$Cl(2)_A$–$C(3)_F$	3·78	$C(2)_A$–$C(6)_G$	3·99
$Cl(2)_A$–$C(4)_H$	3·44	$C(3)_A$–$C(3)_I$	3·57
$Cl(2)_A$–$C(5)_A$	3·72	$C(3)_A$–$C(4)_C$	3·66
$Cl(2)_A$–$C(6)_K$	3·96	$C(3)_A$–$C(5)_C$	3·75
$Cl(2)_A$–$C(6)_G$	3·84	$C(3)_A$–$C(6)_C$	3·76
		$C(5)_A$–$C(5)_G$	3·63
		$C(5)_A$–$C(6)_G$	3·79

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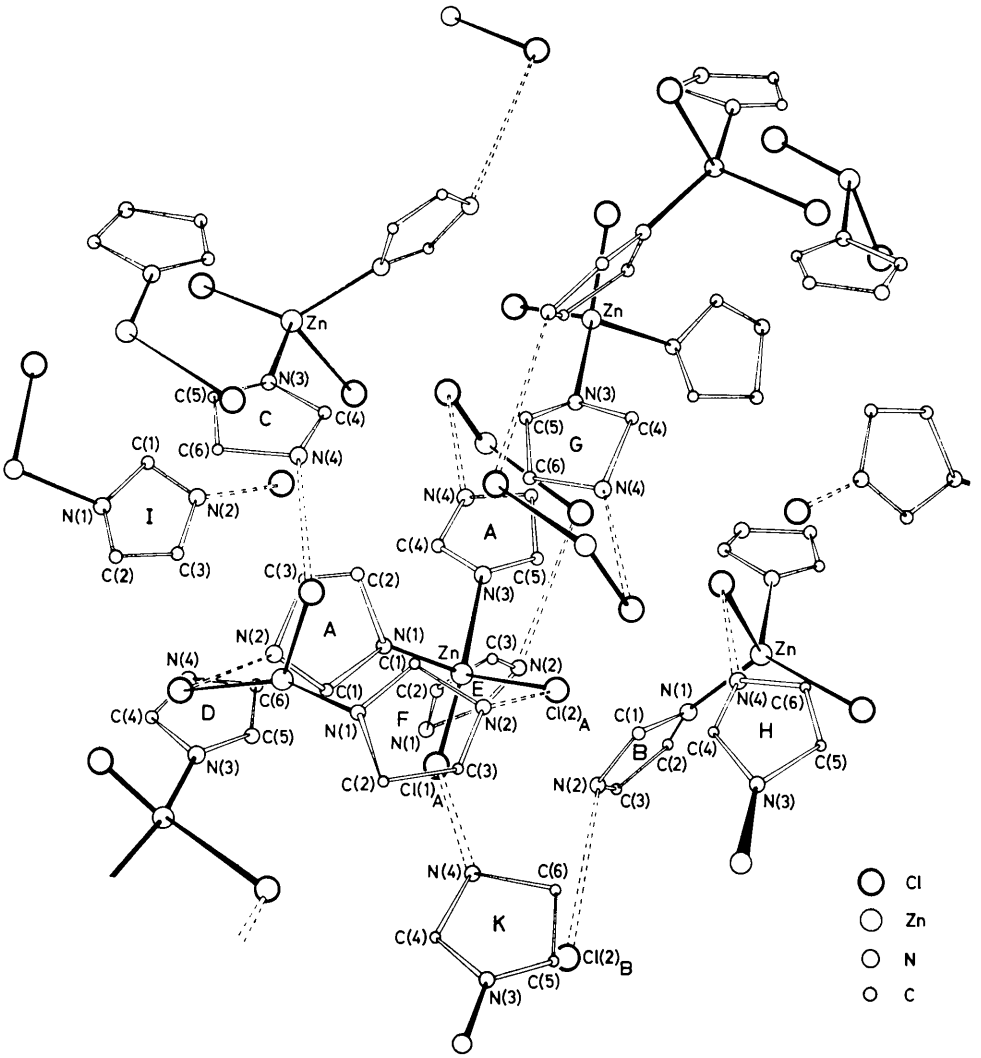

Fig. 2. Part of the structure showing van der Waals contacts between asymmetric units.

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