Jones (1938) did a calculation similar to the present case (*b*), using numerical integration methods and an experimental profile for $b(x)$ which approximates closely to $(1+\kappa^2x^2)^{-2}$.

In the above analysis it is assumed that all experimental profiles have been corrected for α_1–α_2 overlap, and that influences which vary slowly with 2θ are negligible or have been taken care of.

The results from line broadening and from fringe spacing should be identical provided the specimen is not faulted and is free of strains normal to the diffracting planes. The ease with which measurements of broadening and fringe spacing can be performed, allows a quick test for strains and faults in the specimens.

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The Crystal Structure of Bis-(*N*-ethylsalicylaldiminato)copper(II)

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The structure of the complex bis-(*N*-ethylsalicylaldiminato)copper(II) of molecular formula $C_{18}H_{20}N_2O_2Cu$ has been determined with two-dimensional Weissenberg and precession data by the heavy atom method and refined with three-dimensional Weissenberg data. The crystals are monoclinic with $a=9{\cdot}824$, $b=8{\cdot}432$, $c=20{\cdot}989$ Å, $\beta=101°$. The space group is $P2_1/c$ with four molecules per unit cell. The coordination polyhedron around the copper atom is a distorted tetrahedron. The angle between the two coordination planes is 35° 52′ and the step angles between the coordination planes and the planes of the salicyl chelates are 11° 30′ and 22° 44′. No interaction is possible between copper atoms.

Introduction

The α form of bis-(*N*-methylsalicylaldiminato)copper(II), the structure of which has been determined by Lingafelter, Simmons, Morosin, Scheringer & Freiburg (1961), shows a planar arrangement of the ligand atoms about the copper atom. The space groups of the normal *N*-substituted salicylaldiminatocopper(II) complexes (Frasson & Panattoni, 1962), indicate that in the *N*-n-butyl and *N*-n-pentyl derivatives the coordination configuration of the copper atom is planar. In fact the presence of two copper atoms in a cell of space group $P2_1/c$ requires that they be at centres of symmetry. For the *N*-ethyl and *N*-n-propyl derivatives, on the basis of space group considerations alone, no information is available on the type of arrangement of ligands around the copper atom. We have now carried out the determination of the structure of bis-(*N*-ethylsalicylaldiminato)copper(II).

Experimental

The compound, of formula $C_{18}H_{20}N_2O_2Cu$, was prepared by the method of Charles (1957) as modified by Sacconi, Ciampolini, Maggio & Del Re (1960). Black crystals, which have the form of thick plates, were obtained.

The crystal data are as follows:

Molecular weight 354·9
$a=\ 9{\cdot}824\pm0{\cdot}012$ Å
$b=\ 8{\cdot}432\pm0{\cdot}012$
$c=20{\cdot}989\pm0{\cdot}026$
$\beta=101°\pm10'$
$V=1706$ Å^3
$F(000)=748$
$\varrho_m=1{\cdot}38$ g.cm^{-3}
$\varrho_{\text{calc}}=1{\cdot}40$ g.cm^{-3}
$Z=4$.

The systematic absence of reflexions $h0l$ for l odd and $0k0$ for k odd uniquely determined the space group as $P2_1/c$. The cell parameters were measured from precession photographs and the density was measured by flotation. A very small fragment (mean dimensions: 0·015 cm) was selected for intensity measurements. Equi-inclination Weissenberg photographs of $h0l$ through $h6l$ and of $0kl$ were obtained with nickel-filtered Cu $K\alpha$ radiation on a Wiebenga camera with integration in one direction only (Scatturin, Panattoni, Bardi & Bezzi, 1959). Each spot on the multiple film sets was scanned normal to the integration direction with a densitometer feeding into an amplifier and Honeywell recorder. The areas under the densitometer tracings were measured and used as relative intensities. All intensities were corrected for Lorentz and polarization factors but no correction was made for absorption or for anomalous dispersion. The atomic scattering factors used were those of Forsyth & Wells (1959). All calculations were carried out on an Olivetti Elea 6001 3K computer, with programs written by Panattoni & Frasson (1962). The corrected intensities of the various layers were put on a single relative scale, the absolute scale being established later by correlation with the calculated structure factors. A total of 1508 independent reflexions were observed.

The structure determination

The general features of the structure were deduced from two-dimensional Patterson syntheses followed by electron-density projections along [100] and [010], using phases determined by the copper atom. It was apparent that the copper atom is located at $x=0{\cdot}2815, y=0{\cdot}1140, z=0{\cdot}1630$. A series of difference syntheses on the same projections allowed the determination of the positions of the lighter atoms. The discrepancy indices R (defined as $R=\Sigma\,||F_o|-|F_c||/\Sigma\,|F_o|$, where the summation is over the observed reflections only), at this stage were $R_{0kl}=16\%$ and $R_{h0l}=14\%$. Four cycles of least-squares refinement of non-hydrogen atoms with anisotropic temperature factors reduced the R indices to $R_{0kl}=14\%$ and $R_{h0l}=12\%$.

With these coordinates and anisotropic temperature factors a three-dimensional Fourier synthesis and two three-dimensional difference syntheses were made which reduced the R_{hkl} index to 15%.

A further series of non-hydrogen atoms least-squares refinement was carried out with a program written by Panattoni, Grubissich & Frasson (1965) in which are described the basis of the choice of the following weighting scheme:

$$w=\frac{1}{+0{\cdot}0044F_o^2-0{\cdot}095F_o+63{\cdot}0}$$

for reflexions with $F_o>12{\cdot}0$

$$w=\frac{N_1\Sigma' w(\Delta F)^2}{N_2\Sigma''(\Delta F)^2}$$

for reflexions with $F_o<12{\cdot}0$

N_1 = number of reflexions with $F_o<12{\cdot}0$

N_2 = number of reflexions with $F_o>12{\cdot}0$

$\Sigma''(\Delta F)^2$ = sum of $(\Delta F)^2$ of reflexions with $F_o<12{\cdot}0$

$\Sigma' w(\Delta F)^2$ = weighted sum $(\Delta F)^2$ of reflexions with $F_o>12{\cdot}0$.

At this stage the R_{hkl} value was 10·3%.

We tried to find the positions of the hydrogen atoms from three-dimensional difference syntheses. However, the calculated positions of the hydrogen atoms were not consistent with the residual maxima in the maps; accordingly, no further attempt was made to define the positions of hydrogen atoms. The values of the observed and calculated structure factors are reported in Table 8. The values of the parameters and their estimated standard deviations are given in Tables 1 and 2. Tables 3 and 4 show least-squares equations for molecular planes, the angles between these planes and the deviations of the atoms from the planes.

Discussion

The crystal consists of discrete molecules. Figs. 1 and 2 show a perspective view of the molecule and a projection of the atomic coordinates on (010). The coordination configuration about the copper atom is a distorted flattened tetrahedron. The bond lengths and angles with their e.s.d.'s are listed in Tables 5 and 6. The bond lengths of several complexes of *N*-substituted salicylaldimines are compared in Table 7 with our values. The Cu–O distances of 1·90 and 1·89 Å agree with the values found in octahedral or planar complexes, 1·90 (column 1 of Table 7), 1·88 (column 4), 1·92 (column 2) and 1·91 (column 3). They are similar also to the values found in other distorted tetrahedral complexes, 1·93 and 1·89 Å reported in columns (7) and (8) and 1·87 and 1·89 Å in 2,2′-biphenylbis-(2-iminomethylenephenolato)copper(II) (Cheeseman,

Table 1. *Coordinates* (× 10⁴) *and their e.s.d.'s* (*in parentheses*)

	x/a	*y/b*	*z/c*
Cu	2821 (1)	1144 (2)	1637 (0)

First salicylaldimine group				Second salicylaldimine group			
	x/a	*y/b*	*z/c*		*x/a*	*y/b*	*z/c*
O	2913 (8)	1026 (11)	2546 (3)	O′	2132 (8)	449 (11)	783 (3)
N	1477 (9)	2893 (13)	1536 (4)	N′	4626 (10)	142 (13)	1690 (4)
C(1)	2111 (13)	1724 (16)	2882 (5)	C(1′)	2697 (11)	−529 (17)	443 (5)
C(2)	2245 (15)	1278 (21)	3541 (5)	C(2′)	1961 (17)	−1022 (25)	−177 (7)
C(3)	1371 (15)	1964 (20)	3925 (6)	C(3′)	2522 (18)	−1989 (28)	−552 (8)
C(4)	335 (16)	3002 (20)	3669 (6)	C(4′)	3941 (24)	−2576 (27)	−369 (9)
C(5)	171 (12)	3459 (17)	3023 (6)	C(5′)	4670 (14)	−2096 (20)	231 (6)
C(6)	1041 (11)	2801 (16)	2622 (5)	C(6′)	4101 (12)	−1107 (19)	626 (5)
C(7)	837 (12)	3389 (16)	1970 (6)	C(7′)	4998 (12)	−700 (17)	1244 (6)
C(8)	1187 (18)	3737 (23)	910 (7)	C(8′)	5734 (13)	405 (19)	2303 (5)
C(9)	2433 (16)	4686 (21)	806 (7)	C(9′)	6483 (12)	1943 (16)	2261 (6)

Hall & Waters, 1963). The Cu–N bond lengths of 1·96 and 1·95 Å are slightly different from the values reported for the methyl and phenyl derivatives, owing perhaps to the different steric effects of the substituents. In fact the C(8)–O′ distances in the methyl and phenyl derivatives are 2·76–2·78 Å, while in the present case they are 2·95 Å, and the sum of the van der Waals radii (Pauling, 1960) for intermolecular contacts CH_3–O and CH_2–O is 3·40 Å and for C–O contact with aromatic carbon is 3·10 Å. The fact that our C(8)–O′ distances are 0·2 Å greater than those in the two other derivatives results from the non-planar coordination and consequently from the smaller repulsive effect between the substituent and the oxygen atom.

Table 2. *Anisotropic temperature factors* (× 10^2) *and their e.s.d.'s*

Anisotropic thermal factors are of the form: $\exp\,[-\frac{1}{4}\sum_{i=l}^{3}\sum_{j=l}^{3} B_{ij}h_ih_ja_i^*a_j^*]$.

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Cu	232 (6)	304 (9)	264 (6)	51 (8)	27 (4)	−9 (8)
O	332 (38)	281 (52)	266 (27)	202 (39)	101 (29)	43 (38)
O′	234 (37)	357 (58)	284 (36)	87 (35)	67 (29)	130 (35)
N	211 (39)	250 (28)	225 (41)	22 (41)	131 (32)	6 (41)
N′	233 (45)	179 (63)	266 (46)	63 (41)	25 (36)	−79 (42)
C(1)	287 (59)	225 (80)	184 (44)	−12 (49)	15 (40)	−33 (44)
C(2)	471 (68)	351 (89)	230 (61)	−190 (67)	−23 (52)	18 (61)
C(3)	453 (73)	446 (93)	225 (58)	−149 (65)	87 (50)	−27 (57)
C(4)	481 (79)	523 (91)	329 (68)	−219 (68)	165 (58)	−174 (63)
C(5)	233 (55)	335 (87)	361 (60)	−58 (49)	29 (44)	−58 (54)
C(6)	186 (47)	156 (69)	386 (61)	−57 (44)	134 (42)	−88 (51)
C(7)	146 (46)	233 (80)	460 (66)	21 (43)	76 (44)	−15 (51)
C(8)	451 (69)	234 (94)	322 (68)	147 (65)	89 (54)	93 (63)
C(9)	720 (115)	665 (139)	437 (92)	−238 (96)	37 (81)	276 (87)
C(1′)	179 (45)	308 (81)	224 (51)	−19 (47)	74 (38)	−47 (49)
C(2′)	278 (55)	326 (83)	259 (54)	14 (56)	13 (42)	−85 (58)
C(3′)	309 (64)	486 (96)	329 (62)	47 (64)	−53 (49)	−27 (63)
C(4′)	509 (78)	409 (102)	375 (69)	32 (66)	169 (58)	11 (64)
C(5′)	350 (70)	368 (90)	376 (66)	71 (65)	107 (53)	−8 (62)
C(6′)	285 (57)	280 (81)	302 (54)	−10 (59)	119 (43)	−28 (57)
C(7′)	298 (53)	270 (89)	352 (62)	66 (50)	125 (46)	−49 (55)
C(8′)	254 (63)	465 (83)	294 (57)	111 (61)	−57 (46)	−45 (60)
C(9′)	467 (96)	810 (116)	381 (78)	−166 (82)	−49 (67)	−55 (75)

Table 3. *Least-squares planes*

Coefficients of least-squares plane equations.

$$A(x')+B(y')+C(z')=1$$

	A	B	C
Chelate ring plane I (α) [O, N, C(1), C(6), C(7)]	0·1996	0·2346	0·0816
Chelate ring plane II (β) [O′, N′, C(1′), C(6′), C(7′)]	1·0819	1·9128	−0·9849
Benzene plane I (γ) [C(1), C(2), C(3), C(4), C(5), C(6)]	0·1932	0·2414	0·0801
Benzene plane II (δ) [C(1′), C(2′), C(3′), C(4′), C(5′), C(6′)]	1·2803	2·2319	−1·2482
Coordination plane I (ε) [Cu, O, N]	0·2765	0·2465	0·0536
Coordination plane II (η) [Cu, O′, N′]	0·8602	1·6829	−0·7169

$$x'=x-z\sin(\beta-90°)$$
$$y'=y$$
$$z'=z\cos(\beta-90°)$$

Angles between the least-squares planes

	β	γ	δ	ε	η
α	40°30′	2°30′	41°40′	11°0′	43°38′
β	—	39 40	3 06	37 25	23 40
γ		—	40 41	11 30	42 37
δ			—	38 34	22 44
ε				—	35 53

This agrees with the observation that our Cu–N values are close to the values found in the salicylaldoximates (columns 2 and 3).

The value of the angle between the two chelate ring planes is very much dependent on the different substituents on nitrogen. The value of 35°53′ in the ethyl derivative (present work) is about the same as that in the α-phenylethyl derivative (Starikova, 1966). The angle becomes zero when a phenyl group is introduced directly bonded to nitrogen atom. Further, the minor steric hindrance of the methyl derivative leads to the separation between copper atoms of 3·33 Å in a chain of octahedral molecules.

Table 4. *Distances* (Å × 10^3) *from least-squares planes*

	γ plane	α plane	δ plane	β plane
Cu	−281	−245	−99	−92
O	−52	−9		
O′			44	19
N	−10	−11		
N′			−57	−24
C(1)	10	26		
C(2)	−13	15		
C(3)	13	−616		
C(4)	−9	−50		
C(5)	7	−46		
C(6)	−8	−33		
C(7)	67	25		
C(8)	203	161		
C(9)	1579	1485		
C(1′)			−12	−39
C(2′)			6	−49
C(3′)			2	−26
C(4′)			−7	−41
C(5′)			4	−4
C(6′)			6	2
C(7′)			9	34
C(8′)			−55	9
C(9′)			1337	1411

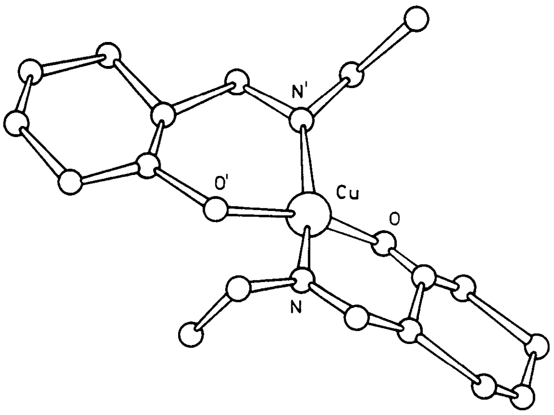

Fig. 1. A perspective view of the molecule.

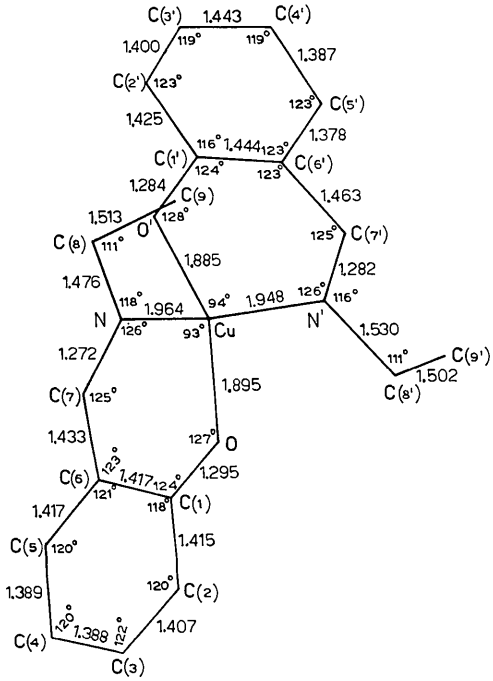

Fig. 2. Projection on (010).

Table 5. *Intramolecular bond lengths* (Å) *and intermolecular distances less than* 3·6 Å

Salicylaldimine group I

		e.s.d.
Cu—O	1·895	0·006
Cu—N	1·964	0·010
O—C(1)	1·295	0·014
C(1)-C(2)	1·415	0·015
C(2)-C(3)	1·407	0·020
C(3)-C(4)	1·388	0·022
C(4)-C(5)	1·389	0·018
C(5)-C(6)	1·417	0·017
C(6)-C(7)	1·433	0·017
C(1)-C(6)	1·417	0·017
N—C(7)	1·272	0·015
N—C(8)	1·476	0·018
C(8)-C(9)	1·513	0·024
O′—C(8)	2·951	0·021
O′—C(9)	3·584	0·020
O—C(8′)	2·959	0·015
Cu—C(9)	3·443	0·017
Cu—C(8)	2·968	0·018
Cu—C(8′)	3·000	0·012
Cu—C(9′)	3·649	0·012

Salicylaldimine group II

		e.s.d.
Cu—O′	1·885	0·007
Cu—N′	1·948	0·010
O′—C(1′)	1·284	0·015
C(1′)-C(2′)	1·425	0·020
C(2′)-C(3′)	1·400	0·027
C(3′)-C(4′)	1·443	0·028
C(4′)-C(5′)	1·387	0·024
C(5′)-C(6′)	1·378	0·019
C(6′)-C(7′)	1·463	0·017
C(1′)-C(6′)	1·444	0·017
N′—C(7′)	1·282	0·016
N′—C(8′)	1·530	0·014
C(8′)-C(9′)	1·502	0·020

In the present complex the ε and η coordination planes and the planes α and β of the salicyl chelates are also not coplanar. The respective angles are 11° and 23°40′, with distances of the copper atom from the planes of the chelates of 0·092 and 0·245 Å. This distance reaches its largest value, 0·45 Å, in the phenyl derivative (Wei, Stogsdill & Lingafelter, 1964), and is 0·38 Å in bis-(5-chlorosalicylaldoximato)copper(II) (Orioli, Lingafelter & Brown, 1964), and 0·065 Å in bis(salicylaldoximato)copper(II) (Jarski & Lingafelter, 1964).

Among the most important features of the present determination are the values of the bond angles in the coordination polyhedron. The tetrahedral angles between the oxygen and nitrogen atoms are very flattened and different (O–Cu–O′ 151·6°, N–Cu–N′ 156·6°). Their mean value and the mean value of the four other angles agree well with the values (92° and 153°) found in 2,2′-biphenylbis-(2-iminomethylenephenolato)copper(II) (Cheeseman, Hall & Waters, 1963) in which the two salicyl groups are bridged by a biphenyl group. The environment around the copper atom is best visualized as a tetrahedron in which both angles between the nitrogen atoms and between the oxygen atoms are flattened. The explanation of the tetrahedral arrangement is not clear. Whether it is mainly due to the Jahn–

Table 6. *Intramolecular bond angles* (°)

Tetrahedron angles

		e.s.d.
O -Cu-O′	151·7	0·6
N -Cu-N′	156·6	0·7
O -Cu-N	92·8	0·4
O′-Cu-N	91·1	0·4
O -Cu-N′	93·0	0·4
O′-Cu-N′	94·4	0·4

Salicylaldimine angles

Group I		e.s.d.	Group II		e.s.d.
Cu—O—C(1)	127·4	0·7	Cu—O′—C(1′)	127·9	0·7
O—C(1)-C(2)	117·4	0·9	O′—C(1′)-C(2′)	119·7	0·9
O—C(1)-C(6)	124·5	0·9	O′—C(1′)-C(6′)	124·1	0·9
C(1)-C(2)-C(3)	119·8	1·1	C(1′)-C(2′)-C(3′)	122·7	1·3
C(1)-C(6)-C(5)	120·6	1·0	C(1′)-C(6′)-C(5′)	122·6	1·0
C(2)-C(3)-C(4)	121·7	1·2	C(2′)-C(3′)-C(4′)	118·6	1·5
C(3)-C(4)-C(5)	120·1	1·1	C(3′)-C(4′)-C(5′)	119·1	1·5
C(4)-C(5)-C(6)	120·0	1·1	C(4′)-C(5′)-C(6′)	123·0	1·2
C(5)-C(6)-C(7)	116·2	1·0	C(5′)-C(6′)-C(7′)	115·7	1·0
C(6)-C(1)-C(2)	118·1	1·0	C(6′)-C(1′)-C(2′)	116·0	0·9
C(6)-C(7)-N	124·9	0·9	C(6′)-C(7′)-N′	124·7	1·0
C(7)-C(6)-C(1)	123·3	0·9	C(7′)-C(6′)-C(1′)	122·7	1·0
C(7)-N—C(8)	116·3	1·1	C(7′)-N′—C(8′)	115·9	0·9
N—C(8)-C(9)	111·1	1·0	N′—C(8′)-C(9′)	110·6	0·9
Cu—N—C(7)	125·8	0·8	Cu—N′—C(7′)	125·6	0·8
Cu—N—C(8)	118·1	0·9	Cu—N′—C(8′)	118·5	0·7
N—C(7)-C(6)	124·9	0·9	N′—C(7′)-C(6′)	124·8	1·0

Table 7. *Bond lengths* (Å) *in salicyl complexes with copper*

Cu coordination	Octahedral			Planar		Tetrahedral		
	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)
Cu—O	1·90	1·92	1·91	1·88	1·90	1·89	1·93	1·89
Cu—N	1·99	1·94	1·96	1·99	1·96	1·95	1·97	2·01
O—C(1)	1·32	1·36	1·33	1·31	1·29	1·28	1·36	1·31
C(1)-C(2)	1·40	1·39	1·40	1·42	1·41	1·42	1·44	1·41
C(2)-C(3)	1·39	1·38	1·38	1·40	1·40	1·40	1·45	1·40
C(3)-C(4)	1·40	1·36	1·40	1·37	1·39	1·44	1·41	1·40
C(4)-C(5)	1·37	1·36	1·36	1·37	1·39	1·39	1·42	1·41
C(5)-C(6)	1·39	1·44	1·40	1·42	1·42	1·38	1·42	1·42
C(1)-C(6)	1·42	1·40	1·44	1·40	1·42	1·44	—	—
C(6)-C(7)	1·44	1·45	1·44	1·44	1·43	1·46	1·43	1·45
C(7)-N	1·31	1·25	1·26	1·30	1·27	1·28	1·30	1·30
N—C(8)	1·52	—	—	1·44	1·48	1·53	1·56	1·51

(1) Bis-(*N*-methyl salicylaldiminato)-Cu(II). Lingafelter et *al.* (1961).
(2) Bis(salicylaldoximato)-Cu(II). Jarski & Lingafelter (1964).
(3) Bis-(5-chlorosalicylaldoximato)-Cu(II). Orioli, Lingafelter & Brown (1964).
(4) Bis-(*N*-phenylsalicylaldiminato)-Cu(II). Wei et *al.* (1964).
(5) Bis-(*N*-ethylsalicylaldiminato)-Cu(II), salicyl group I. Present work.
(6) Bis-(*N*-ethylsalicylaldiminato)-Cu(II), salicyl group (II). Present work.
(7) Bis-(*N*-α-phenylethylsalicylaldiminato)-Cu(II), salicyl group I. Starikova (1966).
(8) Bis-(*N*-α-phenylethylsalicylaldiminato)-Cu(II), salicyl group II. Starikova (1966).

Table 8. *Observed and calculated structure factors for observed reflexions* (× 10)

H	F01	FC
K=0		
L=0		
01+	0216-	0206-
02+	1333-	1307-
03+	0209-	0178-
04+	1025+	0962+
05+	0510-	0523-
06+	0441-	0410-
07+	0521+	0505+
09+	0281-	0232-
10+	0252+	0220+
11+	0159+	0163+
12+	0134-	0149-
L=2		
00+	0736-	0760-
01+	1451-	1415-
01-	0897+	0839+
02+	0171+	0276+
02-	0250-	0242-
03+	0213-	0086-
03-	1243-	1149-
04+	0450-	0358-
04-	0256+	0219+
05+	0228+	0186+
05-	0984+	0912+
06+	0725+	0712+
06-	0778-	0728-
07+	0215-	0186-
07-	0399-	0394-
08+	0199-	0175-
08-	0387+	0363+
09+	0134+	0139+
10+	0210+	0202+
10-	0401-	0392-
11+	0212-	0212-
12-	0113+	0102+
L=4		
00+	0320-	0340-
01+	0357-	0155-
01-	0705-	0051-
02+	0155+	0062+
02-	0426+	0409+
03-	0436+	0504+
04+	0143+	0168+
04-	0936-	0971-
05+	0381+	0399+
05-	0237+	0236+
06+	0742-	0696-
06-	0580+	0546+
07+	0237-	0202-
07-	0209-	0191-
08+	0183+	0167+
08-	0518-	0515-
09+	0200+	0176+
09-	0220+	0233+
10+	0305-	0312-
10-	0402+	0416+
L=6		
00+	0190+	0350+
01+	0169+	0112+
01-	0492-	0514-
02+	0354-	0352-
02-	0157+	0073+
03+	0145+	0110+
03-	0266+	0369+
04+	0516+	0508+
04-	0767+	0720+
05+	0576-	0558-
05-	0233-	0266-
06+	0154+	0143+
07+	0366+	0353+
07-	0409+	0432+
08-	0120-	0141-
09-	0338-	0375-
10+	0282+	0078+
11-	0183+	0164+
12-	0160-	0151-
L=8		
00+	0338-	0324-
01+	0779-	0769-
01-	0814+	0860+
02+	0803+	0825+
02-	0114-	0052-
03+	0089+	0056+
03-	0478-	0505-
04+	0595-	0636-
05+	0288-	0268-
05-	0079+	0088+
06+	0932+	0924+
06-	0515-	0494-
07+	0226-	0190-
08+	0384-	0380-
08-	0419+	0428+
09-	0135+	0134+
10+	0169+	0195+
10-	0279-	0238-
12-	0137+	0104+

H	F01	FC
L=10		
00+	0890-	0852-
01+	1848+	1726+
01-	0822-	0858-
02+	0525+	0493+
02-	0835+	0812+
03+	0513-	0568-
03-	0185-	0144-
04+	0278-	0270-
04-	0338-	0432-
05+	0581+	0587+
05-	0155+	0102+
06-	0409+	0430+
07+	0445-	0416-
07-	0365-	0386-
08+	0111+	0100+
08-	0254-	0229-
09+	0114+	0124+
09-	0438+	0446+
11-	0219-	0236-
L=12		
00+	0642+	0642+
01+	0116-	0070-
01-	0199-	0163-
02+	0598-	0600-
02-	0904-	0897-
03-	0215+	0259+
04+	0195+	0164+
04-	0354+	0372+
05+	0531-	0525-
05-	0262-	0297-
06+	0130-	0141-
06-	0152-	0130-
07+	0368+	0373+
07-	0404+	0368+
08+	0139+	0121+
08-	0343-	0351-
09-	0109-	0147-
10-	0114+	0097+
11-	0137+	0103+
12-	0124-	0145-
L=14		
00+	0122-	0064-
01+	0356-	0291-
01-	0711+	0661+
03+	0277+	0278+
03-	0525-	0605-
04+	0225-	0194-
04-	0210+	0231+
05+	0168+	0112+
05-	0636+	0658+
06+	0311+	0290+
06-	0325-	0297-
07+	0248-	0260-
07-	0181-	0199-
08+	0223-	0212-
08-	0239+	0267+
09-	0322+	0324+
10-	0173-	0154-
L=16		
00+	0384-	0366-
01+	0201+	0190+
01-	0099-	0032-
02+	0233+	0226+
02-	0495+	0526+
03+	0350-	0316-
03-	0359+	0400+
04-	0209-	0185-
05+	0287+	0292+
05-	0125-	0112-
06-	0144+	0105+
07-	0293-	0337-
08+	0133+	0153+
08-	0201-	0229-
10-	0130+	0167+
11-	0156-	0119-
L=18		
00+	0255+	0227+
01-	0423-	0413-
02+	0229-	0238-
02-	0339-	0343-
03+	0115+	0116+
03-	0163-	0161+
04+	0312+	0257+
04-	0121-	0122-
05+	0243-	0221-
05-	0207-	0217-
06+	0235-	0262-
06-	0153+	0180+
07+	0157+	0203+
07-	0281+	0324+
08-	0124-	0106-
09-	0168-	0205-

H	F01	FC
L=20		
01-	0428+	0422+
02+	0187+	0171+
02-	0391-	0357-
03+	0128+	0077+
04+	0253-	0217-
04-	0157+	0118+
05+	0177-	0163-
05-	0131+	0071+
06+	0192+	0181+
06-	0217-	0254-
08-	0278+	0301+
10-	0093-	0154-
L=22		
00+	0219-	0230-
01+	0324+	0259+
01-	0214-	0256-
02+	0115+	0154+
02-	0195+	0201+
03+	0165-	0182-
03-	0168+	0232+
04-	0166-	0191-
05+	0131+	0230+
06-	0136+	0135+
07-	0142-	0121-
L=24		
00+	0136+	0161+
01+	0133+	0084+
01-	0186-	0168-
02-	0184-	0192-
03-	0212+	0250+
04-	0185+	0219+
05-	0217-	0220-
L=26		
01-	0170+	0223+
03-	0121-	0148-
K=1		
L=0		
01+	1115-	1235-
02+	1422-	1240-
03+	0353+	0390+
04+	0726-	0682-
05+	0161-	0146-
06+	0492+	0458+
08+	0242-	0232-
11+	0119-	0163-
L=1		
00+	1100+	1136+
01+	1213-	1508-
01-	0270+	0372+
02+	0225+	0174+
02-	0597-	0692-
03+	1023+	1010+
03-	0960-	0919-
04+	0419+	0348+
04-	0782+	0813+
05+	0494-	0441-
05-	0310+	0279+
06+	0336+	0333+
06-	0528-	0465-
07-	0204+	0135+
08+	0237-	0239-
09+	0157-	0123-
09-	0166-	0197-
10+	0276+	0311+
11-	0198+	0245+
L=2		
00+	0516-	0488-
01+	1369+	1313+
01-	0789-	1012-
02+	1055+	0932+
02-	0750+	0796+
03+	0389-	0345-
04+	0155+	0111+
05+	0849+	0806+
06-	0414+	0429+
07+	0343-	0325-
07-	0243-	0227-
09-	0267+	0276+
10+	0133-	0122-
11-	0215-	0241-
L=3		
00+	0569-	0577-
01+	0532+	0429+
01-	0591+	0683+
02+	0118+	0091+
02-	0450-	0326-
03+	0809-	0695-
03-	0158-	0191-
04+	0229-	0245-
04-	0808-	0781-
05+	0453+	0387+
05-	0626+	0620+

H	F01	FC
L=3		
06-	0136+	0133+
07+	0362-	0349-
07-	0410-	0417-
09+	0279+	0267+
09-	0160+	0161+
11-	0136-	0152-
L=4		
00+	0288+	0313+
01+	0546+	0445+
01-	0962-	1261-
02+	0238-	0212-
03+	0153+	0132+
03-	0146+	0175+
04+	0182-	0138-
05+	0477-	0454-
05-	0636-	0604-
06+	0190-	0167-
07+	0371+	0337+
07-	0347+	0276+
08-	0310-	0314-
09-	0364-	0383-
L=5		
00+	0734+	0572+
01+	0501+	0438+
01-	0460-	0544-
02+	0464-	0359-
03+	0045-	0105-
03-	0406+	0402+
04+	0245+	0233+
05-	0500-	0448-
06+	0406-	0357-
06-	0321+	0309+
07+	0283+	0270+
07-	0353+	0360+
10+	0154-	0147-
11+	0111+	0134+
L=6		
00+	0376-	0258-
01+	0511-	0462-
01-	0377+	0473+
02+	0430+	0371+
02-	0378-	0419-
03+	0277+	0286+
04+	0169-	0181-
04-	0357+	0407+
05+	0278-	0230-
05-	0209+	0140+
06+	0257+	0228+
07+	0216+	0162+
07-	0172+	0161+
08+	0328-	0325-
08-	0338+	0339+
L=7		
00+	0371+	0296+
01+	0558-	0488-
01-	0377+	0455+
02+	0377+	0223+
02-	0515-	0506-
03+	0176+	0181+
04+	0160+	0118+
04-	0378+	0403+
05+	0778-	0732-
05-	0163-	0159-
06+	0436+	0401+
06-	0380-	0387-
07+	0175+	0162+
08-	0234+	0201+
09+	0187-	0194-
10+	0127+	0186+
11-	0151+	0161+
L=8		
00+	0705-	0649-
01+	0273-	0170-
01-	0091-	0039-
02+	0568+	0510+
02-	0497+	0655+
03+	0232-	0183-
04+	0101-	0119-
05+	0277+	0218+
05-	0121+	0138+
07+	0206-	0222-
07-	0467-	0504-
09+	0147+	0134+
09-	0253+	0286+
L=9		
00+	0791-	0751-
01-	0303+	0343+
02+	0741+	0644+
02-	0454+	0557+
03+	0104-	0091-
03-	0376-	0438-
04+	0828-	0685-
05+	0288+	0251+

H	F01	FC
L=9		
05-	0499+	0532+
06+	0398+	0392+
07+	0206-	0219-
07-	0438-	0467-
08+	0136-	0112-
09-	0246+	0262+
10-	0113-	0147-
11-	0140-	0149-
L=10		
00+	0678+	0700+
01+	0478+	0363+
02+	0363-	0345-
02-	0212-	0246-
03+	0365-	0347-
03-	0216+	0264+
04+	0527+	0532+
04-	0244+	0209+
05+	0378-	0330-
05-	0452-	0431-
06+	0299-	0294-
06-	0211+	0205+
07+	0226+	0207+
08+	0136+	0150+
08-	0148-	0104-
10-	0111+	0128+
L=11		
01+	0693+	0663+
01-	0558-	0653-
02+	0507-	0436-
03+	0413-	0339-
03-	0286+	0393+
04+	0400+	0368+
05+	0332+	0295+
06+	0160-	0160-
06-	0309+	0306+
08-	0279-	0265-
10-	0165+	0186+
L=12		
00+	0119+	0152+
01+	0726-	0645-
01-	0402+	0500+
02+	0220+	0175+
02-	0253-	0344-
03+	0304+	0278+
03-	0299-	0318-
04+	0210-	0177-
04-	0307+	0293+
05+	0182-	0152-
06+	0450+	0465+
06-	0275-	0272-
07+	0215+	0229+
08+	0121-	0111-
08-	0320+	0328+
10-	0261-	0287-
L=13		
00+	0242+	0282+
01+	0348-	0331-
01-	0117+	0147+
02-	0358-	0400-
03+	0265+	0236+
03-	0117-	0121-
04+	0238-	0240-
04-	0268+	0296+
05+	0242-	0211-
05-	0157+	0137+
06+	0193+	0161+
06-	0403-	0437-
07-	0161+	0167+
08+	0196-	0240-
09+	0009-	0070-
L=14		
00+	0519-	0480-
02+	0190+	0143+
02-	0288+	0300+
03+	0142-	0156-
03-	0145-	0162-
04-	0293-	0340-
05+	0242-	0230-
06-	0159+	0105+
07+	0211-	0219-
07-	0214-	0240-
09-	0209+	0210+
L=15		
00+	0395-	0334-
01+	0185+	0177+
01-	0138+	0160+
02+	0254+	0232+
02-	0257+	0312+
03-	0216-	0237-
04+	0186-	0179-
04-	0203-	0228-
05+	0162+	0155+

H	F01	FC
L=15		
05-	0315+	0326+
06-	0252+	0267+
07+	0152-	0140-
07-	0199-	0181-
L=16		
00+	0136+	0189+
01+	0329+	0083+
02-	0133-	0165-
03-	0386+	0488+
04+	0235+	0209+
04-	0275+	0294+
06-	0171+	0162+
07-	0161+	0144+
L=17		
00+	0302+	0247+
01+	0181+	0153+
01-	0301-	0381-
03+	0277-	0250-
03-	0143+	0143+
04+	0178+	0178+
04-	0167-	0177-
06+	0207-	0247-
08-	0157-	0120-
10-	0249+	0150+
L=18		
00+	0202+	0138+
02+	0133+	0124+
03+	0166+	0176+
05+	0170-	0168-
05-	0181-	0183-
06+	0117+	0151+
06-	0239-	0216-
08-	0140+	0172+
10-	0111-	0065-
L=19		
02+	0198-	0166-
02-	0162-	0192-
03+	0173+	0154+
03-	0250+	0272+
04-	0191+	0209+
05+	0211-	0238-
06-	0199-	0224-
07-	0328+	0178+
09-	0280-	0131-
L=20		
00+	0151-	0178-
02-	0230+	0255+
03+	0261-	0229-
04-	0191-	0258-
09-	0116+	0105+
L=21		
00+	0278-	0258-
02+	0232+	0222+
05-	0200+	0176+
07-	0126-	0095-
08-	0106+	0106+
L=22		
01-	0200-	0244-
03-	0195+	0208+
07-	0123+	0125+
L=23		
01-	0184-	0241-
05-	0176-	0174-
L=24		
01-	0114+	0140+
02-	0151-	0141-
05-	0134+	0130+
L=25		
02-	0133-	0180-
04-	0142+	0158+
L=26		
00+	0094-	0111-
02-	0200+	0168+
K=2		
L=0		
01+	0696-	0746-
02+	0432-	0388-
03+	0135-	0128-
04+	0768+	0663+
L=1		
01-	0343+	0353+
03-	0831-	0776-
04+	1009-	1021-
04-	0221-	0143-
05+	0241+	0214+
05-	0565+	0505+
06+	0327+	0324+
07+	0381-	0415-
07-	0317-	0291-
08-	0303+	0295+

H	F01	FC
L=2		
00+	0097+	0122+
02+	0398-	0304-
02-	0618-	0470-
03+	0307+	0235+
03-	0308-	0259-
04-	0237-	0171-
05+	0338-	0259-
05-	0446+	0375+
10-	0243+	0072+
L=3		
00+	0438+	0500+
01+	0141+	0218+
02+	0503-	0489-
02-	0633+	0622+
03+	0457-	0527-
03-	0922+	0813+
04+	0476+	0446+
04-	0637-	0581-
05+	0347+	0309+
05-	0660-	0613-
06+	0440-	0462-
06-	0520+	0491+
08+	0365+	0437+
08-	0460-	0459-
L=4		
00+	0321-	0295-
01+	0115-	0056-
02+	0201-	0224-
03+	0307+	0269+
03-	0186-	0101-
04-	0352-	0260-
06-	0196+	0171+
07+	0337+	0376+
L=5		
00+	0441+	0545+
01+	0367-	0386-
01-	0127-	0107-
02+	0401-	0403-
02-	0600-	0642-
03+	0384+	0380+
03-	0303+	0229+
04-	0639+	0592+
05+	0392-	0428-
05-	0431-	0394-
06-	07[illegible]1-	0698-
07+	0405+	0445+
07-	0313+	0280+
08-	0333+	0331+
L=6		
00+	0175-	0150-
01+	0380-	0404-
01-	0329+	0284+
02+	0285+	0243+
03+	0275+	0274+
03-	0182-	0130-
04-	0143-	0092-
05+	0231-	0197-
05-	0355-	0306-
L=7		
00+	0306-	0304-
01+	0517-	0516-
01-	0627+	0670+
02+	0721+	0822+
04+	0679-	0719-
04-	0179+	0111+
05-	0610+	0599+
06+	0378+	0418+
06-	0258-	0269-
07-	0312-	0311-
08+	0254-	0249-
08-	0240+	0214+
L=8		
00+	0253-	0249-
01-	0346-	0332-
02+	0470+	0423+
02-	0555-	0412-
03-	0213+	0164+
04-	0214+	0186+
05+	0216-	0207-
05-	0293+	0287+
L=9		
00+	0441-	0383-
01+	0526+	0622+
01-	0873-	0887-
02-	0394+	0430+
03+	0619-	0667-
03-	0246+	0232+
04+	0301+	0287+
04-	0435-	0381-
05+	0281+	0228+
06+	0229-	0243-
06-	0573+	0527+

Table 8 (*cont.*)

H	F01	FC
K=2 L=9		
07-	0206-	0162-
10+	0159-	0213-
L=10		
01+	0254+	0223+
02-	0173+	0125+
03+	0240-	0227-
04+	0341-	0362-
05+	0284+	0330+
05-	0192-	0196-
L=11		
00+	0705+	0721+
01+	0476-	0534-
01-	0256+	0222+
02-	0747-	0746-
03+	0676+	0736+
04+	0443+	0492+
04-	0703+	0646+
05+	0546-	0632-
05-	0405-	0354-
06-	0224-	0228-
07-	0299+	0277+
L=12		
00+	0417+	0415+
04+	0215+	0237+
05+	0204+	0206+
L=13		
00+	0511-	0506-
01-	0413+	0387+
02+	0261+	0266+
02-	0227+	0228+
03-	0594-	0590-
04+	0419-	0438-
05-	0486+	0443+
06-	0237-	0232-
07-	0361-	0376-
09+	0170+	0264+
10-	0269-	0298-
L=15		
00+	0371-	0214-
01+	0372+	0392+
01-	0359-	0310-
02-	0342+	0326+
03+	0209-	0279-
03-	0347+	0311+
04-	0386-	0401-
05-	0355-	0332-
06-	0319+	0310+
L=16		
01-	0209-	0199-
03-	0250-	0211-
06-	0326+	0318+
L=17		
00+	0406+	0396+
02+	0222-	0242-
05-	0226-	0235-
L=18		
02-	0363+	0343+
L=19		
00+	0281-	0287-
01+	0206-	0216-
02+	0243+	0288+
03-	0252-	0242-
04+	0186-	0231-
05-	0243+	0234+
06+	0160+	0193+
L=21		
01+	0239+	0264+
01-	0285-	0281-
02-	0267+	0254+
03+	0206-	0184-
03-	0211+	0193+
04-	0311-	0326-
05+	0123+	0197+
06-	0189+	0228+
L=23		
07-	0152+	0175+
L=25		
01-	0156+	0201+
K=3 L=0		
01+	0766-	0904-
02+	0662+	0576+
03+	0924+	0871+
04+	0461-	0450-
05+	0439-	0442-
06+	0321+	0330+
08+	0169-	0159-
10+	0200+	0215+
L=1		
01+	0455+	0523+
01-	0156-	0180-
02+	0320-	0324-
02-	0462+	0469+
03+	1018-	1025-
03-	0195+	0207+
04+	0334-	0263-
04-	0317-	0304-
05+	0158+	0164+
06-	0260+	0225+
07+	0188-	0176-
08+	0221+	0208+
08-	0166-	0191-
09-	0232+	0252+
10+	0166-	0058-
L=2		
00+	0500-	0550-
01+	0200+	0195+
01-	0597-	0600-
02+	0197+	0281+
02-	0807+	0828+
03+	0790-	0779-
03-	0276+	0287+
04-	0669-	0663-
05+	0444+	0438+
05-	0221+	0208+
06-	0350+	0353+
07+	0222-	0200-
07-	0296-	0309-
08+	0265+	0295+
08-	0162-	0163-
09-	0138+	0153+
10-	0098+	0092+
L=3		
01-	0260+	0270+
02+	0317-	0359-
02-	0301-	0292-
03+	1022+	1025+
03-	0599+	0546+
04+	0379+	0338+
04-	0143+	0156+
05+	0298-	0283-
07+	0260+	0275+
07-	0370+	0325+
09-	0200-	0205-
10+	0139+	0046+
10-	0131+	0156+
L=4		
00+	0432+	0489+
01-	0779-	0818-
02+	0196-	0207-
02-	0449-	0371-
03+	0166+	0102+
03-	0839+	0851+
04+	0321+	0278+
04-	0259+	0223+
05+	0111-	0118-
05-	0551-	0558-
06+	0342-	0380-
06-	0203-	0190-
07+	0231+	0221+
07-	0462+	0490+
09+	0284-	0354-
09-	0163-	0170-
10-	0115+	0135+
L=5		
00+	0188-	0207-
01+	0530-	0537-
01-	0327+	0334+
02+	0133+	0115+
02-	0160+	0134+
03+	0539+	0473+
03-	0649-	0655-
04+	0391-	0373-
04-	0409+	0364+
05-	0190+	0176+
06-	0297-	0318-
07-	0335-	0320-
08+	0140-	0161-
10-	0197-	0164-
L=6		
01+	0178-	0220-
01-	0238+	0284+
02+	0238+	0239+
02-	0543-	0521-
03+	0472+	0465+
03-	0428+	0357+
04+	0322-	0333-
04-	0238+	0239+
05+	0298-	0280-
05-	0369+	0341+
06+	0238+	0249+
L=6		
06-	0531-	0520-
07+	0259+	0212+
08+	0177-	0166-
08-	0264+	0258+
11-	0112+	0119+
L=7		
00+	0301-	0252-
01-	0167-	0174-
02-	0343+	0341+
03+	0245-	0235-
03-	0184+	0121+
04-	0320-	0342-
05-	0164+	0138+
06-	0166+	0171+
07+	0119-	0098-
08+	0186+	0193+
09-	0122+	0128+
10-	0143-	0080-
11-	0170-	0179-
L=8		
00+	0161-	0152-
01+	0510+	0484+
02-	0110+	0020+
03+	0385-	0411-
03-	0272-	0325-
04+	0376-	0362-
04-	0500-	0473-
05+	0341+	0358+
05-	0253+	0243+
07+	0180-	0181-
07-	0159-	0129-
08-	0108+	0132+
09+	0201+	0211+
09-	0268+	0210+
10+	0086-	0069-
10-	0173-	0077-
L=9		
00+	0282+	0325+
01+	0098+	0077+
01-	0158-	0146-
02+	0419-	0421-
02-	0404-	0350-
03+	0215+	0202+
03-	0176+	0112+
04+	0200+	0178+
05-	0299-	0315-
06+	0197-	0212-
07+	0190+	0225+
07-	0183+	0188+
09+	0092-	0154-
L=10		
00+	0467+	0425+
01+	0191+	0181+
01-	0557-	0561-
02+	0749-	0654-
02-	0206-	0195-
03+	0221-	0215-
03-	0694+	0675+
04+	0493+	0486+
04-	0210+	0174+
05-	0475-	0483-
06+	0128-	0162-
07-	0140+	0118+
08+	0180+	0195+
09+	0158-	0195-
09-	0146-	0151-
L=11		
01-	0266+	0251+
02+	0414+	0398+
03+	0146+	0131+
03-	0294-	0257-
04+	0437-	0483-
04-	0240+	0252+
05+	0137-	0152-
05-	0149+	0113+
07-	0152-	0137-
08-	0234+	0218+
11-	0108+	0068+
L=12		
00+	0202-	0152-
01+	0568-	0538-
01-	0592+	0562+
02+	0140+	0168+
03+	0533+	0579+
03-	0348-	0379-
04+	0223-	0220-
04-	0413+	0398+
05+	0289-	0310-
05-	0297+	0269+
06+	0204+	0228+
06-	0388-	0380-
08+	0155-	0222-
08-	0221+	0193+
L=13		
00+	0130-	0109-
01+	0214+	0196+
01-	0147-	0122-
02-	0286+	0303+
03+	0316-	0304-
04+	0287+	0288+
04-	0353-	0311-
05+	0270+	0275+
05-	0194+	0169+
06-	0274+	0288+
07+	0000-	0037-
08-	0232-	0216-
L=14		
00+	0674-	0607-
01+	0230+	0214+
01-	0119+	0107+
02+	0136+	0121+
02-	0497+	0458+
03-	0131-	0104-
04+	0204-	0216-
04-	0367-	0373-
05+	0182+	0203+
05-	0258+	0233+
06-	0262+	0307+
07-	0234-	0211-
08-	0179-	0218-
09-	0177+	0154+
L=16		
01+	0187+	0170+
01-	0204-	0155-
02+	0139-	0153-
02-	0197+	0105+
03-	0121+	0076+
05-	0289-	0321-
07-	0220+	0244+
10-	0113+	0090+
L=15		
02+	0365-	0327-
02-	0221-	0196-
03-	0218+	0239+
05-	0400-	0442-
L=17		
00+	0139-	0136-
01+	0282-	0283-
01-	0131+	0088+
02-	0270+	0264+
04-	0197+	0180+
10-	0089-	0056-
L=18		
01+	0202-	0189-
03+	0238+	0228+
03-	0129-	0109-
04-	0224+	0233+
05+	0164-	0166-
06-	0112-	0077-
L=19		
01+	0209+	0180+
02+	0139+	0143+
03-	0163-	0165-
04-	0186-	0198-
06-	0232+	0179+
L=20		
00+	0201-	0207-
02+	0211+	0232+
02-	0245+	0243+
04+	0153-	0170-
04-	0132-	0148-
05-	0150+	0153+
07-	0123-	0132-
L=21		
02-	0132-	0098-
03-	0125+	0111+
05-	0137-	0116-
L=22		
00+	0200+	0147+
01-	0146-	0138-
02+	0250-	0256-
02-	0142-	0076-
03-	0250+	0242+
04+	0250+	0238+
05-	0264-	0193-
06-	0157+	0077+
L=23		
01+	0160-	0166-
03-	0111-	0130-
04-	0139+	0179+
L=24		
01-	0157+	0147+
02-	0124-	0127-
04-	0099+	0112+
06-	0160-	0176-
K=4 L=0		
01+	0135-	0114-
02+	0727+	0797+
03+	0536-	0549-
04+	0410-	0430-
05+	0384+	0406+
06+	0131+	0094+
07+	0318-	0335-
09+	0218+	0260+
L=1		
00+	0500-	0455-
01+	0365-	0425-
02+	0270-	0215-
02-	0112+	0091+
03-	0176-	0169-
04-	0227-	0185-
05+	0146+	0098+
05-	0132+	0097+
06+	0259+	0250+
07+	0148-	0185-
07-	0182-	0184-
10+	0161+	0019+
10-	0187-	0043-
L=2		
00+	0316+	0431+
01+	0327+	0407+
01-	0390-	0490-
02+	0687-	0717-
02-	0219-	0205-
03+	0276+	0248+
03-	0531+	0538+
04+	0832+	0896+
04-	0165-	0134-
05+	0120-	0089-
05-	0355-	0334-
06+	0451-	0429-
06-	0338+	0331+
07-	0322+	0317+
08+	0278+	0312+
08-	0312-	0317-
09+	0210-	0257-
L=3		
00+	0196+	0257+
01+	0343+	0372+
01-	0448-	0480-
02+	0205+	0161+
03+	0202-	0151-
03-	0206+	0201+
05+	0236-	0273-
05-	0209-	0216-
06+	0232-	0239-
07-	0277+	0270+
08+	0147+	0122+
10-	0162+	0128+
L=4		
00+	0281+	0298+
01+	0504-	0557-
01-	0195+	0260+
02-	0182-	0224-
03+	0641+	0660+
03-	0438-	0428-
04+	0317-	0313-
04-	0481+	0486+
05+	0361-	0373-
06-	0461-	0463-
07+	0162+	0191+
07-	0160+	0140+
08-	0244+	0248+
09-	0198-	0219-
10-	0166-	0155-
L=5		
00+	0262+	0205+
01-	0112+	0139+
02+	0190-	0171-
02-	0406-	0370-
03+	0229+	0206+
03-	0254+	0206+
04-	0247+	0272+
05+	0116-	0124-
06-	0126-	0099-
07+	0124+	0142+
07-	0226+	0188+
08+	0127+	0139+
10+	0163-	0044-
10-	0109-	0247-
L=6		
00+	0483-	0537-
01+	0107-	0098-
01-	0161-	0118-
02+	0547+	0594+
02-	0736+	0752+
03-	0463-	0458-
04+	0459-	0471-
04-	0361-	0321-
05-	0267+	0239+
06+	0210+	0229+
L=6		
06-	0127+	0133+
07+	0261-	0283-
09-	0184+	0198+
10-	0152-	0160-
L=7		
00+	0218-	0240-
02-	0271-	0300-
03-	0300+	0259+
06-	0435-	0446-
08+	0188-	0229-
08-	0127+	0132+
09-	0124+	0127+
L=8		
00+	0185+	0154+
01+	0466+	0479+
01-	0284-	0280-
02+	0276-	0239-
02-	0482+	0488+
03+	0385-	0364-
03-	0693+	0715+
04+	0290+	0295+
04-	0467-	0477-
05-	0313-	0336-
06+	0221-	0245-
07-	0210+	0182+
08+	0254+	0312+
08-	0295-	0299-
L=9		
00+	0197-	0166-
01+	0132+	0133+
01-	0169-	0103-
03-	0116+	0112+
05-	0142-	0123-
07+	0146-	0132-
L=10		
00+	0191+	0185+
01+	0557-	0566-
01-	0159+	0134+
02+	0308-	0318-
02-	0568-	0565-
03+	0532+	0594+
03-	0130-	0115-
04-	0553+	0592+
05+	0219-	0258-
06-	0318-	0295-
07-	0143+	0147+
08+	0202-	0239-
08-	0146+	0143+
09-	0230-	0254-
L=11		
00+	0266+	0263+
01-	0120+	0128+
02+	0221-	0228-
02-	0253-	0228-
03+	0202-	0167-
03-	0107-	0088-
04-	0144+	0063+
05+	0222-	0226-
L=12		
00+	0420-	0366-
01-	0188+	0163+
02+	0545+	0561+
02-	0333+	0312+
03+	0342-	0355-
03-	0359-	0351-
04-	0199-	0187-
05+	0195+	0216+
05-	0462+	0440+
06-	0125+	0083+
07+	0304-	0293-
07-	0315-	0304-
09+	0180+	0237+
09-	0206+	0226+
L=13		
00+	0247-	0301-
01-	0331+	0315+
02+	0212+	0204+
02-	0175+	0196+
03+	0244+	0236+
03-	0131-	0101-
04+	0161-	0207-
04-	0195-	0214-
09-	0116+	0124+
L=14		
01+	0282+	0253+
01-	0197-	0167-
02+	0266-	0250-
03-	0335+	0302+
04+	0288+	0317+
04-	0276-	0260-
05-	0232-	0222-
06+	0169-	0195-
06-	0325+	0340+
07-	0212+	0186+
08-	0234-	0257-
L=15		
00+	0180-	0166-
02-	0130+	0082+
03-	0158+	0158+
07-	0124-	0138-
08-	0164-	0174-
L=16		
01+	0252-	0254-
01-	0404+	0395+
02+	0208-	0211-
02-	0248-	0244-
03+	0267+	0255+
03-	0139-	0103-
04-	0191+	0180+
05+	0214-	0233-
06-	0125-	0109-
08-	0125+	0102+
L=17		
00+	0161-	0147-
01-	0172-	0186-
L=18		
00+	0170-	0138-
01-	0169+	0163+
02-	0184+	0163+
03-	0229-	0210-
09-	0124+	0097+
L=19		
01-	0212+	0198+
02-	0159+	0145+
07-	0118-	0064-
L=20		
01-	0213-	0199-
03+	0290-	0228-
03-	0264+	0269+
04-	0185-	0196-
05-	0138-	0149-
06-	0146+	0144+
08-	0123-	0125-
L=22		
00+	0210+	0193+
02-	0219-	0211-
03+	0200+	0229+
04-	0210+	0223+
06-	0105-	0123-
L=23		
02-	0118-	0131-
K=5 L=0		
01+	0328+	0349+
02+	0158-	0165-
03+	0096-	0044-
04+	0224+	0221+
05+	0175+	0137+
06+	0169-	0126-
08+	0155+	0174+
L=1		
01+	0571+	0677+
01-	0508-	0645-
02+	0168+	0172+
02-	0465+	0492+
03+	0362-	0383-
03-	0313+	0297+
04+	0450+	0444+
04-	0428-	0428-
05+	0303+	0265+
05-	0184-	0159-
06+	0244-	0246-
06-	0357+	0315+
07+	0258-	0262-
08+	0269+	0304+
08-	0265-	0264-
09+	0100+	0117+
09-	0221+	0198+
L=2		
01+	0226-	0228-
03+	0286+	0271+
05+	0535-	0535-
05-	0372-	0341-
06+	0125-	0119-
07-	0204+	0197+
09-	0237-	0260-
L=3		
00+	0351+	0424+
01+	0163-	0147-
02+	0523-	0541-
02-	0398-	0394-
03-	0272+	0256+
04+	0138+	0136+
04-	0348+	0323+
05+	0292-	0272-
05-	0527-	0554-
06-	0258-	0224-
07+	0285+	0261+
L=3		
07-	0332+	0320+
09+	0207-	0217-
09-	0269-	0299-
L=4		
00+	0141-	0155-
02+	0202+	0174+
02-	0325+	0330+
03-	0273-	0206-
04+	0149-	0143-
04-	0201+	0182+
05+	0201+	0171+
06+	0172+	0200+
10-	0152-	0118-
L=5		
00+	0140-	0143-
01+	0460-	0510-
01-	0121+	0146+
02+	0274+	0275+
02-	0431+	0390+
03+	0246+	0217+
03-	0450-	0460-
04+	0249-	0252-
06+	0201+	0176+
08+	0159-	0160-
08-	0268+	0275+
09-	0140+	0124+
L=6		
00+	0140-	0143-
01+	0459+	0461+
01-	0238-	0194-
02+	0154-	0135-
03+	0274-	0264-
03-	0274+	0264+
04-	0228-	0221-
05-	0314-	0307-
L=7		
01+	0270+	0253+
01-	0324-	0276-
02+	0390+	0375+
02-	0345+	0306+
03+	0332-	0328-
03-	0228+	0230+
04+	0150+	0152+
04-	0269-	0247-
05+	0252+	0251+
05-	0265+	0264+
06+	0164-	0179-
06-	0152+	0147+
07+	0280-	0321-
08+	0175+	0205+
08-	0243-	0316-
09+	0090+	0135+
09-	0139+	0123+
L=8		
00+	0267+	0214+
01+	0172-	0147-
02+	0355-	0361-
02-	0256-	0226-
03+	0112+	0113+
03-	0211+	0207+
04+	0191+	0051+
04-	0507+	0498+
07+	0187+	0164+
07-	0152+	0096+
08+	0122-	0114-
L=9		
00+	0391+	0375+
01+	0183+	0166+
01-	0328-	0282-
02+	0253-	0227-
02-	0397-	0393-
03+	0228+	0237+
03-	0406+	0377+
04+	0190+	0185+
05+	0233-	0218-
05-	0280-	0247-
06+	0263-	0228-
07+	0240+	0243+
07-	0327+	0337+
L=10		
01+	0161-	0101-
01-	0152+	0145+
02+	0332+	0282+
02-	0120-	0123-
03-	0439-	0413-
04-	0163+	0117+
08-	0161+	0186+
09+	0085+	0078+
L=11		
00+	0180-	0175-
01+	0644-	0683-
01-	0609+	0591+
02+	0263+	0217+
02-	0159+	0156+

Table 8 (*cont.*)

H FOB	FC
K=5	
L=11	
03+0138+	0140+
03-0467-	0461-
04+0230-	0201-
05-0216+	0204+
06+0298+	0296+
06-0180-	0199-
07-0152-	0150-
08+0181-	0199-
08-0222+	0237+
L=12	
00+0120+	0090+
02+0143-	0093-
03+0177-	0114-
04+0150+	0143+
04-0224-	0205-
05-0150+	0149+
06+0207-	0239-
06-0158+	0123+
08-0151-	0143-
L=13	
00+0146-	0122-
01-0149-	0117-
02-0333+	0305+
03+0368-	0345-
03-0228+	0190+
04-0394-	0417-
06-0219+	0178+
07+0174-	0205-
07-0138-	0114-
08-0140-	0148-
09-0190+	0228+
L=14	
01-0185+	0167+
02-0125-	0142-
03+0230+	0188+
07-0140+	0117+
L=15	
02+0290-	0299-
02-0339-	0314-
03+0200+	0172+
03-0229+	0189+
04+0180+	0203+
04-0179+	0154+
05+0160-	0137-
07-0225+	0220+
09-0280-	0247-
L=16	
01+0250-	0235-
02+0270+	0252+
02-0168+	0143+
04+0200-	0149-
04-0147-	0178-
L=17	
01-0241+	0199+
03+0180+	0193+
03-0242-	0244-
06-0159-	0125-
08-0083+	0113+
L=18	
02-0140+	0148+
03+0180-	0211-
L=19	
00+0263-	0282-
02-0245+	0192+
04-0130-	0100-
05-0106+	0092+
08-0129-	0069-
L=20	
01-0128-	0138-
02-0135-	0111-
03-0139+	0147+
L=21	
00+0227+	0244+
02+0240-	0243-
02-0200-	0153-
07-0124+	0135+
L=23	
01-0143+	0164+
03-0103-	0155-
K=6	
L=0	
01+0178+	0165+
02+0228+	0285+
03+0127-	0073-
05+0156+	0157+
06+0129+	0126+
07+0158-	0146-
09+0156+	0178+
L=1	
00+0380+	0402+
01+0211+	0204+
01-0154-	0173-
02+0504-	0518-
02-0307-	0299-
03-0442+	0452+
04+0445+	0419+
05+0261-	0253-
05-0435-	0441-
06+0285-	0319-
06-0237+	0246+
07+0164+	0185+
07-0217+	0238+
08+0142+	0159+
08-0188-	0188-
09+0115-	0121-
09-0205-	0252-
L=2	
00+0123-	0115-
01+0176+	0160+
01-0178-	0170-
02+0159-	0163-
02-0116-	0124-
03+0154-	0132-
03-0288+	0275+
05-0259-	0246-
07-0144+	0145+
08+0161+	0231+
L=3	
00+0092-	0049-
01+0436-	0516-
01-0278+	0272+
02+0208+	0199+
03+0271+	0292+
03-0205-	0175-
04-0335+	0338+
05+0120+	0110+
06+0233+	0242+
06-0153-	0176-
08+0271-	0307-
08-0273+	0295+
09-0168-	0176-
L=4	
01+0191-	0177-
01-0101+	0076+
03+0218+	0199+
03-0199-	0178-
04-0160+	0131+
L=5	
00+0444-	0431-
01+0229+	0213+
01-0184-	0186-
02+0224+	0226+
02-0435+	0421+
03+0186-	0188-
03-0098-	0056-
04+0115-	0106-
04-0231-	0221-
05+0133+	0136+
05-0117-	0090-
06-0162+	0140+
07+0182-	0174-
07-0224-	0231-
09-0129+	0154+
L=6	
02+0191+	0184+
02-0279+	0281+
03+0149-	0140-
03-0105+	0112+
04+0095-	0074-
L=7	
00+0366+	0345+
01-0191+	0146+
01-0276-	0272-
02+0328-	0310-
02-0324-	0317-
03-0139+	0082+
04+0206+	0198+
05+0152-	0165-
06+0240-	0276-
06-0199+	0186+
07+0154+	0162+
07-0251+	0275+
08-0117-	0116-
L=8	
00+0118-	0148-
01-0138-	0118-
02+0149-	0082-
02-0110-	0113-
03-0205+	0174+
04+0135+	0140+
04-0246-	0244-
05+0140+	0125+
06+0109-	0142-
07-0152+	0189+
L=9	
00+0456+	0478+
01+0354-	0274-
01-0456+	0468+
03+0270+	0277+
03-0447-	0438-
04+0291-	0242-
04-0391+	0363+
05+0152-	0168-
06+0208+	0247+
06-0270-	0272-
08-0211+	0230+
L=10	
00+0308+	0287+
01-0166+	0172+
02-0149-	0177-
03+0151+	0155+
04-0166+	0144+
06-0119-	0149-
07+0137+	0149+
08-0139+	0155+
L=11	
00+0437-	0293-
01-0179-	0129-
02+0235+	0280+
02-0390+	0389+
03+0249-	0237-
03-0133-	0155-
04-0209-	0177-
05+0264+	0280+
05-0249+	0260+
07+0148-	0215-
07-0242-	0287-
09-0149+	0139+
L=12	
00+0158-	0124-
01+0170-	0213-
02+0235+	0223+
02-0205+	0174+
03-0135-	0140-
04+0158-	0056-
04-0137-	0128-
05-0082+	0133+
06-0123+	0113+
07-0127-	0089-
L=13	
00+0247+	0220+
01-0207-	0195-
02+0400-	0322-
03-0233+	0210+
05-0140-	0131-
07-0168+	0120+
08-0173-	0235-
L=14	
00+0144+	0100+
02+0130-	0134-
03-0128+	0097+
L=15	
00+0192+	0064+
01+0260-	0249-
01-0256+	0240+
02-0207-	0179-
03-0202-	0182-
04-0143+	0105+
05-0140+	0110+
06-0139-	0121-
08-0163+	0195+
L=16	
03+0150+	0148+
06-0096-	0098-
L=17	
00+0118-	0106-
02+0180+	0209+
02-0240+	0222+
03+0200-	0191-
04-0134-	0113-
L=18	
01+0120-	0138-
03-0096-	0113-
L=19	
01+0220+	0265+
01-0244-	0203-
03-0145+	0157+
04+0200+	0156+
05-0123-	0107-
06-0193+	0127+
L=20	
01+0180+	0166+
L=21	
01-0111+	0126+
03-0098-	0086-

Teller effect will perhaps become clearer after further investigation of the influence of the alkyl chains. In order to throw some light on this question we are studying the structure of bis(*N*-n-propylsalicylaldiminato)copper(II) and of bis(*N*-n-heptylsalicylaldiminato)nickel(II).

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A Method of Positioning a Known Molecule in an Unknown Crystal Structure

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A function is proposed for determining the position of a known molecule of known orientation relative to a crystallographic symmetry element in an unknown crystal structure. A Fourier-series summation with appropriate coefficients is used to express the correlation between the observed Patterson function of the crystal and the set of cross-Patterson vectors of a model structure. The point of maximum correlation gives the value of the intermolecular vector between molecules related by the chosen symmetry element. The function has been tested on sperm whale myoglobin.

Introduction

A number of methods exist for determining the orientation of a known molecule in an unknown crystal structure (Rossmann & Blow, 1962; Nordman & Nakatsu, 1963; Tollin & Cochran, 1964). Several methods have also been used to solve the subsequent translational problem of positioning the molecule rela-