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The Crystal Structure of Copper(II) Complexes with N-substituted *o*-Hydroxyacetophenone Imines: R=Methyl, n-Octyl, Benzyl, and 2-Phenylethyl

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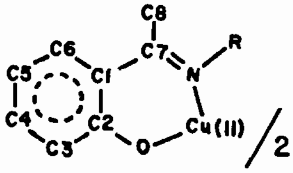
Crystal structures have been determined from three-dimensional X-ray diffraction data for a series of copper(II) complexes of N-substituted o-hydroxyacetophenone imines, $HO\text{-}C_6H_4\text{-}C(CH_3)=NR$, with R = methyl, n-octyl, benzyl, and 2-phenylethyl. The methyl complex was studied in two different crystalline forms. The structures of the complexes with R = isobutyl and H have been previously reported. In the yellow-brown, triclinic form of the methyl complex, the copper(II) has achieved 5-coordination by dimer formation through long (2.378Å) Cu-O bonds. In all other cases the copper is 4-coordinate, planar for R = H, CH_3, $i\text{-}C_4H_9$, C_8H_{17}, distorted tetrahedral for R = $CH_2\Phi$, $CH_2CH_2\Phi$. All of the complexes show deviations from planarity by exhibiting either a "twist" in the coordination polyhedron from planar toward tetrahedral geometry, a "step", or some combination of "twist" and "step". The largest "twist" is 29.°6 (for R = $CH_2CH_2\Phi$). The largest "step", defined as the distance by which the Cu atom is out of the plane defined by the benzene ring of the o-hydroxyacetophenone residue, is 1.33 Å (for R = $n\text{-}C_8H_{17}$). There are correlations between the "twist" and the chelate "bite" distance, and between the "step" and the values of the angles adjacent to the coordination polyhedron. The C-C bond adjacent to the benzene ring of the o-hydroxyacetophenone residue is significantly lengthened, up to 1.473(4)Å. The benzene ring itself is slightly distorted from planarity, exhibiting a tendency toward a "boat" conformation, and also contains three long and three short C-C bonds in the ring. These complexes are compared to a similar series of copper(II) complexes, the N-substituted salicyaldimines. The two series show similar structural properties, except that the valus for the "step" are larger for the N-substituted o-*hydroxyacetophenone imine complexes.*

Introduction

N-substituted ortho-hydroxyacetophenone imines form bis-chelates with copper(II), whose crystal and molecular structure in the solid state depend upon the



substituent, R. The colors of these solid Cu^{II} complexes are various shades of green or brown, a phenomenon extensively investigated by Professors D. Hall and T. N. Waters[1] for a similar series of complexes, the bis-chelates of N-substituted salicylaldimines. We have now completed the study of complexes where R = CH_3 (two crystalline forms, a yellow-brown five-coordinate form and a brown four-coordinate form), R = $n\text{-}C_8H_{17}$ (red-brown), R = $CH_2C_6H_5$ (green), and R = $CH_2CH_2C_6H_5$ (tan). These complexes are compared with the previously reported structures in this series where R = H (red-brown),[2] the unsubstituted compound, and R = $i\text{-}C_4H_9$ (brown).[3]

The stereochemistry of bis-chelates of metal(II) complexes has been summarized in an extensive review,[4] and the general features of the stereochemistry of the *o*-hydroxyacetophenone imine complexes reported here agree with those features found for similar previously reported complexes.

The complexes will be referred to by an abbreviation derived from their imine substituent, R. For example the two forms of the methyl substituted imine will be referred to as $CH_3(5)$ and $CH_3(4)$, to designate the five-coordinate and four- coordinate methyl complexes. A phenyl group will be abbreviated as φ. The numbering system for the independent atoms of each molecule will be as illustrated above, with the addition that the R group carbon atoms will be numbered sequentially beginning with C9 attached to the nitrogen atom, and that the second ligand moiety, when not related by symmetry to the

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(1) D. Hall, S.V. Sheat, and T.N. Waters, *J. Chem. Soc.*, A1968, 460 (1968).
(2) G. Marongiu and E.C. Lingafelter, *Acta Cryst.*, *B27*, 1195 (1971).
(3) Carlo A. Ghilardi and E.C. Lingafelter, *Acta Cryst.*, *B26*, 1807 (1969).
(4) R.M. Holm and M.J. O'Connor, « The Stereochemistry of Bis-Chelate Metal (II) Complexes », *Progress in Inorganic Chemistry, 14*, 241 (1971).

first, has its atom numbers larger by +20 except for the nitrogen and oxygen atoms which are simply N2 and O2, respectively.

Experimental Section

All the complexes were synthesized by Professor F. D. Thomas II. In general, equimolar amounts of *o*-hydroxyacetophenone and the appropriate primary amine were dissolved in 50 ml. absolute methanol to give a 1 M solution which was gently heated just to boiling, after which heating was discontinued. Fifty ml. of .25 *M* copper(II) acetate monohydrate in water was added dropwise with stirring. This was followed by dropwise addition of approximately 25 ml. of .5 *M* sodium acetate, and then 25 ml. of .5 *M* sodium hydroxide. Generally a dark oil would separate which solidified on cooling. The yield, based upon amount of copper acetate, was almost 100%. As the molecular weight of the primary amine increased, it became unnecessary to use the solutions of sodium acetate and/or sodium hydroxide to help the metal complex to precipitate. The solid complex was separated and recrystallized from either methanol, ethanol, or butanol.

A careful recrystallization of small green crystals of the methylsubstituted complex, obtained as described above, yielded two different crystalline forms. Slow evaporation of a green saturated solution of complex in ethanol gave yellow-brown crystals, CH_3(5), suitable for a single crystal X-ray study, as well as small brown crystals. Dissolving the methyl complex in tert-butanol gave a brown solution from which larger brown crystals, CH_3(4), were obtained. A powder pattern of the small green crystals showed that they were different in structure from either the yellow-brown or the brown crystals. No suitable green crystals of the methyl-complex were obtained.

The procedures used in general for solving the structures for all the complexes will be described. The collection of data was made with Mo Kα radiation, filtered through 0.001 inch of niobium foil, on a Picker automated diffractometer equipped with a scintillation counter and pulse-height discriminator. The take-off angle was set at 3.5°. The cell constants and their estimated standard deviation were obtained by a least squares fit of about 24 2Θ values (averages of $+2\Theta$ and -2Θ). For each crystal a density measured by flotation (using pentane and CCl_4) was compared to a calculated density, providing a check of the molecular weight and giving the number of molecules per unit cell, Z.

The intensity data were collected at room temperature ($\sim 24°C$) by the Θ–2Θscan method using the formula of Alexander and Smith:[5]

$$\text{scan range} = A + 1.0 \tan\theta.$$

The value of A was determined by measuring the width of some low order intense reflections. Stationary background measurements were made at the start and finish of each scan. Periodically the intensities of four or five standard reflections were remeasured after each group of about 150 reflections, and these values were used to calculate a scale factor for each group and also a stability constant, k, for all of the data collection. Intensities were measured in the range $0 < 2\Theta < 55°$. Measurements were recorded in truncated dekacounts and the intensities and their estimated standard deviations were calculated from:

$$I = S - \frac{ts}{2t_B}(B_1 + B_2) - 0.45(2\frac{ts}{2t_B} - 1)$$

$$\sigma_I^2 = \frac{1}{10}[S + (\frac{ts}{2t_B})^2(B_1 + B_2)] + k^2[S + \frac{ts}{2t_B}(B_1 + B_2)]^2 + 0.25.$$

S = dekacounts recorded during scan times t_S
B_i = dekacounts recorded during background time t_B
k = empirical stability constant

The terms 0.45 and 0.25 are corrections for the truncation of the counts to dekacounts. Lorentz and polorization factors were applied.

All calculations were carried out on either an IBM 7040-7094 direct coupled system (for the complexes abbreviated according to their imine substituent, as CH_3(5), n-C_8H_{17} and $CH_2CH_2\varphi$) or its successor, CDC 6400 system (for CH_3(4) and $CH_2\varphi$). The sets of programs used were written or adopted by J. M. Stewart; XRAY-63[6] for the direct coupled system and XRAY-70[7] for the CDC system. Scattering factors for copper, oxygen, nitrogen and carbon atoms were taken from Doyle and Turner[8] except for n-C_8H_{17} which used those from Cromer and Waber.[9] The hydrogen atom scattering factors were taken from Table 2 of Stewart, Davidson and Simpson.[10]

The copper positions for the various complexes were determined either from symmetry considerations or from three-dimensional Patterson syntheses. All other non-hydrogen atoms were located from three-dimensional Fourier syntheses. Refinement was by full-matrix least squares for CH_3(4), but the matrix for each of the other structures had to be divided into two blocks. The specific function minimized in the least squares program is given in Table I for each complex. Hydrogen atom positions were revealed by three-dimensional difference Fourier syntheses when possible; otherwise they were put in calculated positions. Least squares refinement, using anisotropic thermal parameters for the non-hydrogen atoms and isotropic for the hydrogen atoms, was considered complete when the shift/error < 1.0 for all parameters. There was no evidence of secondary extinction except in the data for $CH_2CH_2\varphi$. The thirty-eight reflections which suffered from secondary extinction were coded as such and had weights equal to zero in the least squares refinement. Final three-dimensional difference Fourier syntheses revealed no unusual peaks.

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(5) L.E. Alexander, and G.S. Smith, *Acta Cryst.*, *17*, 1195 (1964).

(6) J.M. Stewart, « Crystal Structure Calculation System X-Ray-63 for the IBM 709, 7090, 7094 ». Technical Report TR-64-6, Computer Science Center, University of Maryland and Research Computer Laboratory, University of Washington (1964).

(7) J.M. Stewart, « The X-Ray System of Crystallographic Programs for an Computer having a Pidgen FORTRAN Compiler », Version of July 70, Computer Science Center, University of Maryland (1970).

(8) P.A. Doyle, and P.S. Turner, *Acta Cryst.*, *A24*, 390 (1968).

(9) D. Cromer, and J. Waber, *Acta Cryst.*, *18*, 104 (1965).

(10) R.F. Stewart, E.R. Davidson, and W.T. Simpson, *J. Chem. Phys.*, *42*, 3175 (1965).

Table I. Summary of experimental data.

		$CH_3(5)$	CH_3 (4)	n—C_8H_{17}	$CH_2\varphi$	$CH_2CH_2\varphi$
shape		wedge	rectangular prism		hexagonal plate	flat plate
crystal dimensions in mm. along	*a*	0.36	0.28		0.4	
	b	0.20	0.10		0.4	
	c	0.32	0.16		0.1	
systematic absence		none	0k0 absent for k = odd; h0l absent for h = odd	none	0k0 absent for k odd; h0l absent for h+l=odd	hkl absent for h+k+l =odd; h0l absent for h = odd
space group		$P\bar{1}$ (1)	$P2_1/a$	$P\bar{1}$ (1)	$P2_1/n$	I2/a
reflections used for cell constant determination		28	28	23	20	23
cell dimensions with standard deviations	Å					
	a_o	9.194(2)	14.6999(9)	8.078(2)	17.645(6)	25.455(4)
	b_o	9.951(3)	7.8478 (4)	15.787(4)	8.465(3)	8.420(3)
	α	9.040(3)	6.899(1)	6.778(1)	16.509(3)	12.469(6)
	β					
	γ	90.89(2)	—	100.76(3)	—	—
	c_o	100.35(2)	93.282(6)	114.38(3)	97.17(1)	94.02(3)
	degrees	100.12(2)	—	78.40(5)	—	—
volume, $Å^3$		800.04	794.73	765.90	2446.31	2665.90
Z		2	2	1	4	4
calculated density g . cm^{-3}		1.452	1.461	—	1.41	1.32
experimental density g . cm^{-3}		1.452	1.499	—	1.39	1.34
Data Collection						
approximate reflections per data group		300	130	120	100	140
scan constant, A, degrees		2.3	2.0	—	.9	2.0
group scale factor variation, %		±2.0	±.3	±3.5	±6.9	±1.8
stability factor used		.003	.004	.009	.01	.004
unique reflections measured		3440	1811	2877	4426	3050
type of special reflections		—I (2)	—I	unobserved (6)	—I (8)	—I
special reflections		195	96	286	279	362
rejected reflections		0	5	—	6	38
type of R		R_wF^2 (3)	R_wI (5)	R_wR (7)	R_wF	R_wF^2
R value		.076	.061	.037	.037	.063
GOF		4.23 (4)	2.14	1.87	1.77	2.63
MoKα absorption coefficient, cm^{-1}		14.4	14.4	7.6	9.7	8.7
max-min transmission factors		.75—.59	.87—.80	—	.90—.68	—
absorption correction		no	yes (9)	no	no	no
anomalous dispersion correction		no	yes	no	yes	no

[1] No evidence for higher symmetry found. This is the reduced primitive cell. [2] All data were considered observed. Those with net negative intensity were coded as such to be included as negative F_o^2's in the least squares refinement. [3] The function minimized was $\Sigma w(F_o^2-F_c^2)^2$ where F_c is the calculated structure value and w is the statistical weight defined to be $(1/\sigma_{F_o2})^2$. The weighted residual index, R_wF^2, is defined as = $[\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$. [4] GOF is the «goodness of fit», the standard deviation of an observation of unit weight: $GOF=[\Sigma w(F_o^2-F_c^2)^2/n_o-n_v)]^{1/2}$ where n_o = number of observations and n_v = number of variables. [5] Refinement based upon minimizing $[\Sigma w(I_o-I_c)^2]$ with all reflections (±I) considered observed. Replace the F^2 by I in footnotes (2) and (3) to get the comparable I functions. [6] Reflections having intensity less than twice their estimated standard deviations were coded as « unobserved » and assigned intensity values of $I+2\sigma_I$ for special treatment in the least squares refinement. [7] The function minimized in the least squares refinement was $[\Sigma w(|F_o|-|F_c|)^2]$ with $w = (1/\sigma_F)^2$ except that any unobserved reflection with $F_c<F_o$ was given w = 0. The function used to calculated the residual was $R_wF=[\Sigma w(F_o-F_c)^2/\Sigma wF_o^2]^{1/2}$ and the standard deviation of an observation of unit weight is calculated by $GOF=[\Sigma w(F_o-F_c)^2/n_o-n_v)]^{1/2}$. [8] The refinement was carried out as a conventional F refinement as in (6) except that there were no « unobserved » reflections and the 279 reflections that had net negative intensity had their F_o set equal to 0.00. [9] Using the Tompa absorption program,[11] as modified by D. Cullen and E. Adman at the University of Washington.

Information specific to each complex is given in Table I. Final atomic parameters are listed in Tables II, III, IV, V and VI; observed and calculated structure factors are listed in Tables VII, VIII, IX, X and XI, for the complexes with R = $CH_3(5)$, $CH_3(4)$, n-C_8H_{17}, $CH_2\varphi$ and $CH_2CH_2\varphi$, respectively.

Discussion

All of the *o*-hydroxyacetophenone imine Cu^{II} complexes studied could be crystallized as discrete four-coordinate monomers, consisting of two bidentate ligands arranged trans to each other. In addition, the methyl complex is unique in that it could be crystallized in a second form in which the Cu^{II} is five-coordinate through long Cu-O bonds from one molecule to another, forming dimers, and could also be obtained in a third form for which no suitable crystals could be grown. Table XII gives general information about all of the complexes, and in particular gives the abbreviations used for the various unique parts of the unit cell of each complex.

The coordination of the ligand donor atoms about

(11) H. Tompa, « The Absorption Correction in Crystal Structure Analysis », IBM 1620 General Program Library, 8.4.014 (1966).

Table II. Final parameters of the five-coordinate form of bis-(*o*-hydroxyacetophenone methyliminato)copper(II), $CH_3(5)$.

Atom		X/A	Y/B	Z/C	B11	B22	B33	B12	B13	B23
Positional parameters ($\times 10^5$) and Thermal parameters ($\times 10^2$).										
CU		41517(5)	61609(5)	55903(6)	202(2)	269(2)	299(2)	—55(1)	39(1)	—26(2)
N	1	49767(34)	75964(30)	43303(34)	369(16)	286(15)	256(16)	10(12)	0(12)	28(12)
N	2	30060(32)	48567(30)	67886(34)	274(14)	322(16)	253(16)	—34(12)	43(12)	12(12)
O	1	44598(27)	75085(26)	71670(31)	336(13)	381(14)	448(15)	—110(11)	178(11)	—140(12)
O	2	36310(23)	48072(22)	39551(25)	189(10)	324(12)	297(12)	—54(9)	49(9)	—45(11)
C	1	66174(39)	88591(35)	64365(42)	287(17)	225(17)	333(20)	—19(13)	71(14)	23(14)
C	2	57374(41)	83831(37)	75050(44)	329(18)	236(18)	347(21)	—24(14)	76(15)	—17(15)
C	3	62039(50)	88790(42)	90221(50)	486(24)	377(23)	365(24)	—65(18)	127(18)	—45(17)
C	4	75501(54)	97421(46)	94792(59)	562(27)	447(26)	348(25)	—76(20)	—30(21)	—68(20)
C	5	84602(56)	101348(51)	84593(57)	424(25)	468(27)	494(28)	—168(20)	—30(21)	—23(20)
C	6	80109(46)	97346(43)	69912(57)	361(21)	367(22)	450(26)	—81(16)	94(19)	42(19)
C	7	60930(41)	85775(37)	48297(41)	343(19)	257(18)	341(21)	54(14)	132(15)	49(15)
C	8	68555(77)	95003(66)	37852(76)	462(30)	543(33)	446(33)	0(25)	183(24)	116(24)
C	9	43296(65)	74954(57)	27118(60)	657(32)	435(28)	426(28)	—37(23)	12(24)	92(22)
C	21	12682(36)	37879(37)	46157(43)	198(16)	243(17)	325(20)	—33(13)	49(14)	—20(14)
C	22	22069(36)	41623(34)	35622(40)	201(15)	257(17)	326(19)	0(12)	38(13)	—22(14)
C	23	16536(43)	38433(43)	20423(48)	265(18)	466(23)	295(21)	—39(16)	53(16)	—50(17)
C	24	1927(45)	31851(44)	15275(48)	328(20)	517(25)	385(23)	—21(17)	—37(17)	—128(18)
C	25	—7390(48)	28484(47)	25414(55)	207(18)	491(25)	583(28)	—80(17)	—17(18)	—150(20)
C	26	—2254(42)	31179(41)	40300(55)	216(17)	357(21)	523(27)	—55(14)	115(17)	—71(18)
C	27	17851(40)	40082(37)	62357(44)	280(17)	267(18)	371(21)	—5(14)	129(15)	20(15)
C	28	8491(55)	32561(53)	72812(58)	546(26)	459(28)	524(28)	—149(22)	250(21)	34(22)
C	29	35288(57)	49990(60)	84207(54)	512(27)	554(30)	315(24)	—32(22)	26(19)	72(22)
Positional parameters ($\times^3$) and Thermal parameters ($\times 10$).										
H	3	553(4)	861(4)	975(4)	43(9)					
H	3	776(4)	1000(4)	1055(5)	57(11)					
H	5	922(5)	1067(4)	876(5)	62(13)					
H	6	853(3)	1000(3)	621(3)	31(7)					
H	81	648(5)	933(4)	283(5)	67(11)					
H	82	763(5)	932(4)	381(5)	75(12)					
H	83	644(6)	1040(6)	397(6)	131(18)					
H	91	502(6)	721(6)	208(7)	112(21)					
H	92	405(5)	845(5)	232(5)	71(13)					
H	93	338( )	680( )	260( )	95( )					
H	23	226(3)	404(3)	133(3)	23(7)					
H	24	—14(4)	304(4)	40(4)	42(9)					
H	25	—167(5)	252(4)	222(5)	57(11)					
H	26	—85(4)	294(4)	481(4)	42(9)					
H	281	35(6)	382(5)	764(6)	84(19)					
H	282	145(5)	290(5)	823(6)	85(16)					
H	283	48(4)	250(4)	690(4)	43(11)					
H	291	355(4)	413(4)	896(5)	58(12)					
H	292	457( )	555( )	864( )	70( )					
H	293	289(5)	551(5)	888(6)	77(15)					

Parameters come from a F^2 refinement. Estimated standard deviations are given in parentheses. Parameters without a standard deviation were not refined and are calculated or estimated parameters.

Anisotropic thermal parameters are of the form: $\exp(-1/4 \Sigma \Sigma B_{ij}h_ih_ja_i{*}a_j{*})$

Isotropic thermal parameters are of the form: $\exp(-B(\sin^2\theta)/\lambda^2)$

the copper atom is exactly planar for H1, $CH_3(4)$, i-C_4H_9 and n-C_8H_{17}, where the copper atom of each of these molecules is at a crystallographic center of symmetry. The other molecules are distorted from planarity by having some amount of "twist" in the coordination polyhedra from planar toward tetrahedral coordination. The other molecule of the asymmetric unit of the unsubstituted imine (designated as H2 and H3) is in a general position, but is nevertheless close to the planarity of H1 with a "twist" of only 7.8 degrees. The two complexes with the largest imine substituent groups, $CH_2\varphi$ and $CH_2CH_2\varphi$, show a considerable "twist" toward tetrahedral coordination. The five-coordinate $CH_3(5)$ has the basal plane of the square pyramidal coordination polyhedron also twisted toward tetrahedral coordination.

The N-substituted bis(*o*-hydroxyacetophenone iminato)Cu^{II} complexes reported here are quite similar to N-substituted bis(salicylaldiminato)Cu^{II} complexes. The difference in the ligand itself is small, the C7 atom in the former complexes has a methyl group (C8) attached to it, while for the latter complexes there is a hydrogen atom at this position. The salicylaldimine complexes are also discrete four-coordinate monomers, except for bis(N-methyl salicylaldiminato)Cu^{II} for which three different crystalline forms, α, β and γ, have been reported. These three forms are possibly directly comparable to the three forms found for bis-(*o*-hydroxyacetophenone methyliminato)Cu^{II}. The green α-form[12] consists of exactly planar four-coordinate

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(12) E.C. Lingafelter, G.L. Simmons, B. Morosin, C. Scheringer, and C. Freiburg, *Acta Cryst.*, *14*, 1222 (1961).

Table III. Final atomic parameters for the four-coordinate form of bis-(*o*-hydroxyacetophenone methyliminato)copper(II), $CH_3(4)$

Atom		X/A	Y/B	Z/C	B11	B33	B22	B12	B13	B33
Positional parameters ($\times 10^4$) and Thermal parameters ($\times 10^2$).										
CU		0( )	0( )	0( )	275(2)	245(2)	228(2)	—39(3)	49(1)	—39(3)
O	1	417(1)	1125(3)	—2173(3)	524(12)	314(10)	233(9)	—148(10)	90(9)	—57(8)
N	1	129(1)	2176(3)	1470(3)	297(11)	245(12)	218(10)	12(10)	79(9)	—33(9)
C	1	1342(2)	3184(4)	—407(4)	247(13)	223(14)	316(14)	9(11)	10(11)	47(12)
C	2	1133(2)	2127(4)	—2021(4)	304(15)	220(14)	289(14)	50(12)	62(12)	56(12)
C	3	1715(3)	2203(5)	—3585(5)	540(20)	300(17)	311(17)	88(16)	146(15)	27(15)
C	4	2473(3)	3199(6)	—3514(7)	392(20)	504(23)	556(23)	110(18)	267(18)	244(21)
C	5	2689(3)	4182(6)	—1926(7)	308(18)	586(24)	612(23)	—80(17)	51(17)	191(20)
C	6	2135(2)	4191(5)	—403(6)	360(17)	398(18)	445(18)	—98(14)	—34(14)	62(16)
C	7	729(2)	3325(4)	1200(4)	304(14)	201(13)	241(13)	22(12)	—29(11)	—7(11)
C	8	813(3)	4879(7)	2460(6)	559(21)	236(18)	426(17)	—41(22)	—24(16)	—72(19)
C	9	—525(3)	2439(6)	2976(7)	490(23)	400(22)	382(21)	43(19)	163(18)	—74(18)
Positional parameters ($\times^3$) and Thermal parameters ($\times 10$).										
H	3	158(2)	157(3)	—453(4)	18(2)					
H	4	275(2)	315(4)	—453(5)	42(4)					
H	5	324(2)	467(4)	—185(4)	38(4)					
H	6	228(2)	479(4)	69(4)	42(4)					
H	81	34(3)	500(8)	309(6)	127(17)					
H	82	88(2)	581(5)	189(5)	51(11)					
H	83	131(3)	476(7)	325(6)	96(14)					
H	91	—29(2)	223(4)	401(4)	33(9)					
H	92	—77(2)	355(4)	283(4)	40(9)					
H	93	—104(3)	181(5)	261(5)	77(13)					

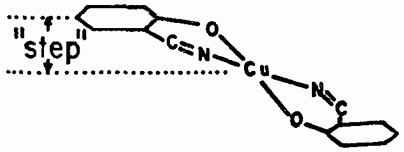
Parameters come from ± I refinement. Estimated standard deviations are given in parentheses. Parameters fixed by symmetry considerations have no standard deviations. Thermal parameters are as given in Table II.

monomers stacked such that the copper atoms are only 3.3 Å apart, and possibly the small green crystals, from which $CH_3(4)$ and $CH_3(5)$ were obtained by recrystallization, are of this form. The β-form,[1] whose color was not reported, consists of discrete four-coodinate monomers, as does $CH_3(4)$. The brown γ-form[14] has square pyramidal five-coordination through the formation of dimers by long Cu-O bonds (2.4 Å), just as in the yellow-brown $CH_3(5)$.

Table XII shows that the planar, or nearly planar, complexes of *o*-hydroxyacetophenone imine studied in this series are brown or red-brown. As the coordination undergoes a "twist" from square planar to tetrahedral, there tends to be a color change away from brown.

The O-N chelate "bite" distances, given in Table XVI for all the complexes, show a large range of values [from 2.691(4) to 2.771(3) Å]. However, there is a linear correlation between the oxygen-nitrogen atom chelate "bite" distance and the "twist" in the coordination polyhedron . The "bite" increases as the coordination becomes more tetrahedral. This trend can be understood in that the copper atom utilizes orbitals for square planar bonding that are directed 90 degrees apart, whereas for tetrahedral bonding the orbitals are directed 109 degrees apart. Hence, assuming a constant Cu-(donor atom) bond distance, as the coordination becomes more tetrahedral the "bite" increases.

All of the complexes show marked distortion of each molecule from planarity. In addition to the "twist" in the coordination polyhedron that some molecules show, all molecules exhibit a "step" effect where atoms are progressively found out of the plane



defined by the atoms in the benzene ring of the *o*-hydroxyacetophenone residue. The *o*-hydroxyacetophenone imine residue is hereafter referred to as the molecular skeleton since for every complex it consists of the same atoms. Table XIII gives the distances of various atoms from each unique benzene ring least squares plane. With respect to the coordination polyhedron, the two benzene rings of the molecular skeleton of each molecule are tipped in opposite directions except for $CH_2\varphi$ and $CH_2CH_2\varphi$ which are tipped in the same direction, giving an umbrella effect to the molecular skeleton.

The atoms defining the least squares plane of the benzene ring for the moieties R = H1, H2, H3, CH_3-(5)2 and $CH_2\varphi 2$ all lie within $-.011$ to $+.012$ Å (approximately $\pm 3\sigma$) from the least square plane. The remaining moieties, $CH_3(5)1$, $CH_3(4)$, i-C_4H_9, n-C_8H_{17}, $CH_2\varphi 1$ and $CH_2CH_2\varphi$, have their benzene ring atoms lying within a somewhat greater range of distances from $-.024$ to $+.036$ Å, which constitutes a significant deviation from the least square plane. The data to be noted are that similar atoms in the benzene

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(13) E.N. Baker, D. Hall, and T.N. Waters, *J. Chem. Soc., A*, 680 (1966).

(14) E. Frasson, C. Panattoni, and L. Sacconi, *J. Phys. Chem.*, *63*, 1908 (1959).

Table IV. Final atomic parameters for bis-(*o*-hydroxyacetophenone octyliminato)copper(II), n—C_8H_{17}

Atom		X/A	Y/B	Z/C	B11	B22	B33	B12	B13	B23
Positional parameters ($\times 10^4$) and Thermal parameters ($\times 10^2$).										
Cu		5000( )	5000( )	5000( )	515(2)	367(2)	327(2)	—74(2)	184(2)	51(1)
N	1	3612(3)	4481(1)	1999(3)	568(12)	390(10)	404(10)	—97(8)	216(9)	36(8)
O	1	2967(2)	5902(1)	4600(3)	618(10)	496(9)	368(8)	—18(7)	260(7)	84(6)
C	1	2512(3)	5903(1)	851(4)	373(12)	448(12)	353(11)	—60(9)	166(9)	71(9)
C	2	2519(3)	6327(2)	2907(4)	379(12)	447(12)	414(12)	—42(9)	189(10)	68(10)
C	3	2027(4)	7230(2)	3106(5)	557(14)	463(12)	487(13)	14(10)	243(11)	53(11)
C	4	1707(4)	7715(2)	1476(5)	603(15)	437(14)	674(17)	7(11)	252(13)	148(12)
C	5	1820(4)	7311(2)	—457(5)	595(15)	564(15)	570(15)	—11(11)	238(12)	246(13)
C	6	2172(3)	6426(2)	—776(4)	485(13)	559(14)	410(12)	—58(10)	207(10)	119(10)
C	7	2729(3)	4949(2)	408(4)	431(13)	469(13)	363(11)	—84(10)	202(10)	35(10)
C	8	1823(4)	4557(2)	—1919(4)	715(17)	575(15)	377(12)	—136(13)	158(12)	—25(11)
C	9	3656(5)	3529(2)	1722(5)	761(18)	395(12)	442(13)	—154(12)	248(13)	—3(10)
C	10	3079(4)	3280(2)	3379(5)	485(14)	410(12)	600(15)	—89(11)	263(12)	49(10)
C	11	3256(5)	2306(2)	3378(5)	581(16)	402(12)	584(15)	—97(11)	268(13)	45(11)
C	12	2881(5)	2076(2)	5216(5)	615(16)	428(13)	651(16)	—82(12)	324(14)	77(11)
C	13	3039(5)	1109(2)	5263(6)	819(20)	451(14)	764(19)	—110(14)	462(17)	71(13)
C	14	2530(6)	884(2)	6997(6)	808(21)	522(15)	757(20)	—110(15)	424(17)	124(14)
C	15	2680(5)	—74(2)	7068(6)	1037(24)	560(17)	952(23)	—149(16)	526(20)	159(15)
C	16	2079(6)	—281(3)	8740(7)	1223(30)	840(23)	1132(29)	—256(21)	552(24)	348(20)
Positional parameters ($\times^3$) and Thermal parameters ($\times 10$).										
H	3	206(3)	748(2)	446(4)	53(7)					
H	4	153(3)	837(2)	176(4)	63(7)					
H	5	160(3)	767(2)	—163(4)	62(6)					
H	6	223(3)	615(1)	—211(4)	46(6)					
H	81	195( )	386( )	—227( )	79( )					
H	82	36( )	479( )	—247( )	79( )					
H	83	235( )	479( )	—290( )	79( )					
H	91	505(3)	323(2)	197(4)	64(7)					
H	92	288(3)	333(2)	37(4)	51(7)					
H	101	192(4)	352(2)	318(4)	50(7)					
H	102	386(3)	356(1)	488(4)	50(6)					
H	111	457(3)	203(1)	354(4)	50(6)					
H	112	238(4)	205(2)	196(4)	59(6)					
H	121	160(4)	234(2)	511(4)	63(7)					
H	122	376(4)	234(2)	664(4)	65(7)					
H	131	435(4)	82(2)	546(5)	92(9)					
H	132	220(4)	83(2)	376(5)	85(8)					
H	141	112(4)	115(2)	666(5)	97(9)					
H	142	333(4)	116(2)	833(5)	68(8)					
H	151	410( )	—35( )	739( )	79( )					
H	152	183( )	—34( )	548( )	79( )					
H	161	223( )	—95( )	883( )	79( )					
H	162	299( )	0( )	1039( )	79( )					
H	163	72( )	1( )	848( )	79( )					

Parameters come from a F refinement. Estimated standard deviations are given in parentheses. Parameters fixed by symmetry considerations or not refined upon have no standard deviations. Thermal parameters are as given in Table II.

rings of the various moieties tend to be out of the least squares plane in the same direction. For the second group, where the deviations are more significant, only one atom does not follow the overall pattern. Atom C4 of the $CH_2\varphi 1$ benzene ring is a very small positive .001 Å out of the plane rather than being negative. Even for the first group, where the deviations are small, the trend is generally followed. CH_3-(5)2 follows the pattern completely. H3 follows the pattern except for atom C6. $CH_2\varphi 2$ follows the pattern except for atoms C1 and C4. Only H1 and H2 do not follow the pattern very well. Thus, the benzene ring tends to be bent, with atoms C2 and C5 "up" a mean of .015 and .011 Å, respectively, giving a "boat" conformation to the ring. The distortion of the benzene ring is a result of the various amounts of "step" and "twist" strain being transferred to the benzene ring through the O and C7 atoms. As will be discussed later under bond lengths, the benzene ring also has three long and three short bonds.

A comparison of the way other atoms in the ligand deviate from the plane defined by the benzene ring reveals some general trends for all the complexes. The distance by which the copper atom lies out of the plane defined by the benzene ring, hereafter simply called the "step", ranges from 0.109 Å (H3) to an extreme of 1.33 Å (n-C_8H_{17}), the largest value yet reparted in the chemical literature. The "step" in the independent molecule H1 is just the average of the values for H2 and H3, which comprise the two halves of the other independent molecule in the asymmetric unit. The O1 atom is always out of the benzene ring least square plane in a direction opposite to that of the C7 atom. The same relationship holds for the 02 and C27 atoms. The copper atom is always out of the plane in a direction arbitrarily defined as positive, but the other atoms are out of the plane in both positive and negative directions, for example atom C9(C29) shows a range of deviations from +.38 to −.39 Å. A larger range of deviations

Table V. Final atomic parameters for bis (*o*-hydroxyacetophenone benzyliminato)copper(II), $CH_2\varphi$.

Atom	X/A	Y/B	Z/C	B11	B22	B33	B12	B13	B23
Positional parameters $(\times 10^4)$ and Thermal parameters $(\times 10^2)$.									
Cu 1	1709(2)	3742(4)	23723(2)	302(1)	355(2)	319(1)	—6(1)	9(1)	77(1)
N 1	—6695(11)	—10008(26)	18825(13)	267(10)	370(12)	367(11)	—12(8)	45(8)	107(9)
N 2	7913(12)	18421(27)	31284(12)	394(11)	320(12)	288(10)	34(9)	42(9)	17(9)
O 1	—1396(11)	20211(23)	16358(11)	573(11)	372(10)	395(10)	—56(9)	—133(9)	114(8)
O 2	7201(10)	—13652(22)	28547(11)	323(9)	363(10)	437(10)	—4(7)	—73(7)	61(8)
C 1	—8416(13)	3962(37)	5973(15)	237(11)	433(14)	307(12)	44(12)	29(9)	70(12)
C 2	—4229(14)	17627(36)	8715(16)	287(12)	421(16)	357(14)	48(11)	—8(11)	102(12)
C 3	—3461(18)	29624(43)	3047(21)	457(17)	444(19)	500(19)	—40(15)	—54(14)	177(15)
C 4	—6094(19)	28010(50)	—5073(21)	452(17)	592(22)	468(19)	74(16)	28(14)	262(17)
C 5	—9885(19)	14660(48)	—7821(21)	459(17)	624(23)	329(16)	126(16)	6(13)	88(16)
C 6	—11025(15)	3123(37)	—2423(16)	385(13)	488(16)	388(13)	26(13)	17(11)	2(13)
C 7	—10076(14)	—8879(34)	11354(17)	266(12)	411(15)	388(14)	0(11)	50(11)	7(12)
C 8	—15888(29)	—21138(65)	8040(29)	518(21)	729(28)	488(21)	—258(20)	—24(18)	38(21)
C 9	—8651(17)	—23280(40)	24135(21)	306(15)	392(17)	475(17)	—44(13)	18(13)	116(14)
C 10	—15080(15)	—19371(35)	28986(16)	304(13)	379(15)	352(13)	—47(11)	—6(10)	142(12)
C 11	—21959(18)	—27227(41)	27748(19)	411(16)	506(18)	391(16)	—122(14)	49(13)	3(14)
C 12	—27767(23)	—24126(47)	32362(23)	360(17)	647(23)	537(19)	—134(16)	68(15)	90(17)
C 13	—26782(23)	—12877(48)	38350(24)	526(20)	582(22)	556(20)	87(18)	168(17)	145(17)
C 14	—19985(23)	—4833(47)	39685(23)	706(23)	471(19)	474(18)	—63(18)	74(16)	—18(16)
C 15	—14193(19)	—7961(40)	35081(20)	397(16)	467(19)	477(17)	—120(14)	—1(14)	47(14)
C 21	18500(14)	512(32)	34171(15)	316(12)	375(16)	272(11)	5(10)	18(9)	53(10)
C 22	14590(15)	—13077(34)	30878(14)	342(13)	384(15)	230(11)	17(12)	32(10)	76(10)
C 23	18824(18)	—26917(40)	30168(17)	448(17)	377(17)	316(14)	38(14)	—1(12)	21(12)
C 24	26540(19)	—27491(48)	32388(19)	453(18)	552(20)	359(15)	187(16)	57(13)	70(14)
C 25	30376(19)	—14409(49)	35583(20)	318(16)	667(24)	533(18)	65(17)	—0(13)	109(16)
C 26	26428(18)	—865(45)	36473(20)	379(15)	513(21)	475(16)	—51(14)	—42(13)	18(14)
C 27	14675(16)	15648(34)	35083(16)	384(14)	368(15)	293(13)	—64(12)	45(11)	16(11)
C 28	18885(29)	28020(56)	40499(31)	601(24)	505(22)	538(23)	—59(19)	—79(20)	—41(19)
C 29	4025(19)	33511(38)	32300(19)	509(17)	309(15)	365(15)	15(14)	50(13)	50(12)
C 30	—1578(15)	32710(32)	38437(16)	382(13)	287(13)	314(13)	—4(11)	—6(11)	—23(11)
C 31	—8279(22)	40876(43)	37078(25)	581(20)	479(19)	534(20)	84(15)	107(17)	202(16)
C 32	—13380(24)	41292(48)	42697(29)	556(21)	617(24)	888(27)	174(18)	268(20)	203(20)
C 33	—11952(25)	33084(48)	49883(25)	653(23)	572(22)	562(21)	—38(18)	273(18)	—36(17)
C 34	—5375(23)	24699(51)	31254(23)	554(21)	821(26)	333(17)	9(18)	45(15)	75(17)
C 35	—265(20)	24393(45)	45675(20)	418(17)	719(23)	382(16)	109(16)	30(14)	101(15)
Positional parameters $(\times^3)$ and Thermal parameters $(\times 10)$.									
H 3	—7(2)	383(3)	47(2)	43(7)					
H 3	—52(2)	361(4)	—82(2)	53(8)					
H 5	—114(2)	134(3)	—130(2)	52(8)					
H 6	—130(1)	—64(3)	—41(1)	29(7)					
H 81	—190(2)	—231(4)	119(2)	74(11)					
H 82	—138(3)	—286(6)	55(3)	132(20)					
H 83	—195(2)	—173(5)	42(2)	87(13)					
H 91	—40(1)	—250(3)	277(2)	35(6)					
H 92	—96(1)	—328(3)	211(2)	36(7)					
H 11	—223(1)	—354(3)	238(1)	34(6)					
H 12	—321(1)	—290(3)	318(2)	38(7)					
H 13	—307(2)	—107(4)	417(2)	61(9)					
H 14	—191(2)	23(4)	438(2)	57(8)					
H 15	—95(1)	—26(3)	356(2)	39(7)					
H 23	162(1)	—354(3)	282(1)	25(6)					
H 24	289(2)	—375(4)	315(2)	51(8)					
H 25	358(2)	—149(3)	368(2)	60(8)					
H 26	288(2)	77(4)	385(2)	50(8)					
H 201	155(2)	343(5)	433(2)	86(14)					
H 282	215(2)	236(4)	445(2)	77(12)					
H 283	217(2)	341(5)	373(2)	80(13)					
H 291	15(1)	381(3)	270(2)	50(7)					
H 292	77(1)	415(3)	336(1)	31(6)					
H 31	—90(2)	450(4)	329(2)	48(9)					
H 32	—177(2)	473(4)	418(2)	65(9)					
H 33	—156(2)	331(4)	533(2)	65(9)					
H 34	—47(2)	193(4)	559(2)	60(9)					
H 35	42(2)	184(3)	466(2)	50(7)					

Parameters come from a F refinement. Estimated standard deviations are given in parentheses. Parameters with no standard deviations were not refined upon. Thermal parameters are as given in Table II.

Table VI. Final atomic parameters for bis(*o*-hydroxyacetophenone phenylethyliminato)copper(II), $CH_2CH_2\varphi$

Atom		X/A	Y/B	Z/C	B11	B22	B33	B12	B13	B23
Positional parameters $(\times 10^5)$ and Thermal parameters $(\times 10^2)$.										
CU		25000( )	—4277(6)	0( )	370(3)	467(3)	255(2)	0( )	—2(2)	0( )
N	1	29134(8)	—9133(26)	13617(17)	354(12)	520(16)	308(11)	49(10)	14(9)	48(10)
O	1	18930(6)	—823(22)	7218(12)	392(9)	754(14)	272(8)	103(9)	—3(7)	—53(9)
C	1	23055(10)	3149(32)	25017(19)	410(14)	343(14)	268(12)	—51(13)	29(10)	31(12)
C	2	18825(10)	4380(34)	17143(20)	405(14)	351(14)	298(12)	—12(13)	61(11)	28(13)
C	3	14050(11)	10879(33)	20047(23)	430(17)	499(18)	416(16)	70(13)	20(13)	—17(13)
C	3	13579(13)	16888(37)	29994(30)	546(20)	531(20)	576(21)	74(15)	160(17)	—33(16)
C	5	17689(16)	16569(39)	37478(26)	813(25)	535(20)	394(18)	—1(18)	114(18)	—134(14)
C	6	22310(12)	9639(33)	35068(22)	559(18)	431(19)	330(15)	—29(13)	21(13)	—39(12)
C	7	27919(10)	—5115(33)	23162(20)	370(14)	416(15)	295(12)	—54(13)	—34(11)	91(13)
C	8	31424(11)	—9503(34)	33111(22)	550(17)	703(22)	360(14)	92(14)	—60(12)	75(13)
C	9	34005(13)	—19030(34)	12140(24)	561(19)	476(18)	429(17)	—52(15)	—53(14)	6(13)
C	10	38830(13)	—8888(33)	12988(23)	653(20)	461(20)	505(17)	—109(16)	—66(14)	—7(13)
C	11	43673(13)	—19035(40)	11462(30)	412(18)	567(21)	605(21)	137(15)	—7(17)	15(16)
C	12	45589(14)	—29128(48)	19539(32)	527(22)	759(25)	919(28)	131(19)	—177(19)	194(20)
C	13	50064(21)	—37720(56)	18275(48)	634(31)	740(29)	1515(46)	234(24)	—394(27)	—21(29)
C	14	52752(19)	—36355(68)	9275(63)	473(28)	710(33)	2017(71)	96(23)	—194(32)	—469(39)
C	15	50820(21)	—26343(69)	1397(48)	715(34)	945(39)	1338(44)	—93(25)	376(29)	—369(29)
C	16	46246(17)	—17871(46)	2286(35)	687(26)	720(26)	811(26)	160(20)	172(21)	—2(20)
Positional parameters $(\times^3)$ and Thermal parameters $(\times 10)$.										
H	3	112(1)	113(3)	152(2)	35(8)					
H	4	106(1)	198(4)	317(3)	44(9)					
H	5	176(2)	205(4)	431(3)	54(12)					
H	6	252(1)	101(3)	401(2)	43(8)					
H	81	339(1)	—160(4)	315(3)	60(13)					
H	82	330(1)	3(4)	362(3)	69(13)					
H	83	289(1)	—126(4)	386(3)	72(12)					
H	91	349(1)	—283(4)	170(2)	35(8)					
H	92	338(1)	—245(4)	54(3)	44(9)					
H	101	385(1)	—18(4)	78(2)	47(9)					
H	102	392(1)	—37(4)	204(3)	58(9)					
H	12	425(3)	—331(8)	217(5)	174(29)					
H	13	519(2)	—455(7)	238(4)	150(18)					
H	14	559(2)	—427(7)	85(4)	158(22)					
H	15	520(2)	—250(7)	—36(4)	92(22)					
H	16	445(2)	—113(5)	—35(3)	93(16)					

Parameters come from an F^2 refinement. Estimated standard deviations are given in parentheses. Parameters without a standard deviation are fixed by symmetry considerations. Thermal parameters are as given in Table II.

from the plane (+.03 to −.89Å) occurs for C8(C28). The distance of atom C8(C28) out of the plane is that same plane. As the "step" increases the C8 atom is found increasingly out of the plane in the opposite direction.

Plots of the "step" vs. the deviations of atoms other than C8(C28) from the benzene ring least squares plane give scattered data points. For example, there is no good correlation between the "step" and the nitrogen atom deviation from the plane, perhaps because of the different substituent groups which are attached to the nitrogen atom. However, there are good correlations to be found if the deviations of atoms from the benzene ring plane are plotted vs. the deviation of the C7(C27) atom. The C7 atom is of interest because it is located in the middle of the "most crowded" part of the ligand. Figure 1 shows plots of the deviations of Cu, N, O, C8 and C9 atoms vs. deviation of the C7 atom from the benzene ring plane. With the exception of H(1,2,3), only the non-planar complexes are included in this plot. The data points for the planar complexes show considerable scatter and no conclusions can be drawn from them. Considering all non-planar complexes and H(1,2,3),

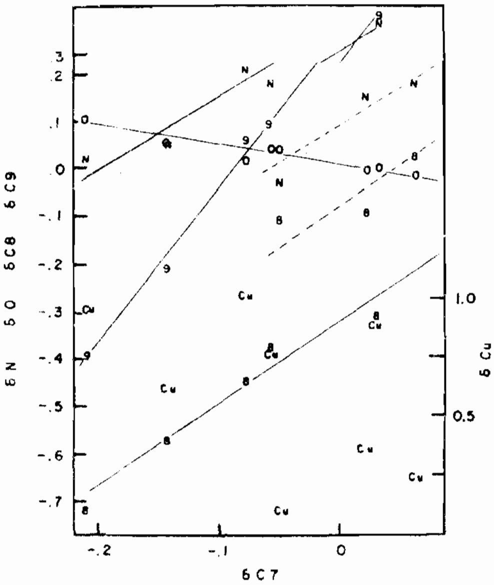

Figure 1. Correlations between the deviations of atoms Cu O, N, C8 and C9 (designated as Cu, O, N, 8 and 9 in the figure) *vs.* the deviation of atom C7 from the benzene ring least squares plane. [The dotted lines represent the correlation for H(1,2,3) atoms.]

Table VII. $CH_3(5)$ Observed and calculated structure factors.Columns are k, $10|F_o|$ and 10 F_c. F^2 values used are obtained by squaring values in the table. Reflections marked L hadnegative F^2_o.

Table VII. (Continued)

Table VII. (Continued)

7,K,0 [illegible]

7,K,1 [illegible]

7,K,-1 [illegible]

7,K,2 [illegible]

7,K,-2 [illegible]

7,K,3 [illegible]

7,K,-3 [illegible]

7,K,4 [illegible]

7,K,-4 [illegible]

7,K,5 [illegible]

7,K,-5 [illegible]

7,K,6 [illegible]

7,K,-6 [illegible]

7,K,7 [illegible]

7,K,-7 [illegible]

7,K,8 [illegible]

7,K,-8 [illegible]

7,K,-9 [illegible]

7,K,-10 [illegible]

8,K,0 [illegible]

8,K,1 [illegible]

8,K,-1 [illegible]

8,K,2 [illegible]

8,K,-2 [illegible]

8,K,3 [illegible]

8,K,-3 [illegible]

8,K,4 [illegible]

8,K,-4 [illegible]

8,K,5 [illegible]

8,K,-5 [illegible]

8,K,6 [illegible]

8,K,-6 [illegible]

8,K,7 [illegible]

8,K,-7 [illegible]

8,K,-8 [illegible]

8,K,-9 [illegible]

9,K,0 [illegible]

9,K,1 [illegible]

9,K,-1 [illegible]

9,K,2 [illegible]

9,K,-2 [illegible]

9,K,3 [illegible]

9,K,-3 [illegible]

9,K,4 [illegible]

9,K,-4 [illegible]

9,K,5 [illegible]

9,K,-5 [illegible]

9,K,-6 [illegible]

9,K,-7 [illegible]

9,K,-8 [illegible]

9,K,-9 [illegible]

10,K,0 [illegible]

10,K,1 [illegible]

10,K,-1 [illegible]

10,K,2 [illegible]

10,K,-2 [illegible]

10,K,3 [illegible]

10,K,-3 [illegible]

10,K,4 [illegible]

10,K,-4 [illegible]

10,K,-5 [illegible]

10,K,-6 [illegible]

10,K,-7 [illegible]

11,K,0 [illegible]

11,K,1 [illegible]

11,K,-1 [illegible]

11,K,2 [illegible]

11,K,-2 [illegible]

11,K,-3 [illegible]

11,K,-4 [illegible]

11,K,-5 [illegible]

11,K,-6 [illegible]

Table VIII. $CH_3(4)$ Observed and calculated structure factors. Columns are h, $10|F_o|$ and $10F_c$. I values used can be obtained from the F values by $I = Lp\ F^2$. Reflections marked N had negative net intensity. Dispersion included in F_c values. The sign given F_c is the sign of the real part of the structure factor.

[illegible]

Table IX. n—C_8H_{17}. Observed and calculated structure factors. Columns are k, 10|F_o| and 10F_c. Reflections marked * are « unobserveds ».

Table X. $CH_2\varphi$. Observed and calculated structure factors. Columns are h, $10|F_o|$ and $10F_c$. Reflections marked N had negative net intensity. Dispersion included in F_c values. The sign given F_c is the sign of the real part of the structure factor.

[illegible]

Table X. (Continued)

[illegible]

Table X. (Continued)

[illegible]

there are some remarkable trends revealed. The deviations of atoms N, C8 and C9 all show a similar correlation with respect to the deviation of atom C7. The slopes of the lines for H(1,2,3) for atoms N and C8 are parallel to, but closer together than, the corresponding lines for the non-planar substituted complexes, suggesting a smaller interaction when there is only a hydrogen atom on the imine nitrogen atom. The oxygen atom, which is on the other side of the ligand chelate, shows a correlation with an inverse slope. The copper atom deviation vs. the C7 deviation does not show a good correlation but the "up and down" scatter of the individual copper atom data points about their line has a pattern that is duplicated generally in the way other individual data points go "up and down" in this plot (except for the oxygen atom). Hence as the C7 atom deviation becomes more positive (in the direction of the copper atom), the other atoms also move in this direction, except the oxygen atom which does the opposite, with a smooth correlation except for some "up-down" scatter which is correlated with the "step".

Another way of looking at the "step" is to consider the dihedral angle between the benzene ring and the plane defined by the nitrogen, oxygen and copper atoms on the same side of the coordination polyhedra as the benzene ring. These "step" angles are given in Table XIII.

In a review[4] on bis-chelate metal(II) complexes, Holm and O'Connor conclude that for four-coordinate complexes with donor atoms O1, N1, O2 and N2 arranged *trans* about the copper atom, the stereochemistry (geometry of the coordination) of the complexes is planar when there are no substituent groups on the donor atoms larger than a hydrogen atom; and that when there are substituent groups on the ligand donor atoms larger than hydrogen, the stereochemistry of the complex is either stepped planar or pseudo-tetrahedral (twisted toward tetrahedral). Hence the expectation for imine-substituted bis(*o*-hydroxyacetophenone iminato)Cu^{II} complexes is that they would show various amounts of "step" and "twist". Presumably these complexes undergo "step" and "twist" effects to reduce strains in the molecule. The largest strains are postulated[13] as being primarily due to intramolecular forces, close contacts between atoms in the ligands about the same metal ion. Specific intermolecular forces may or may not be important.

The magnitude of the values of the "step" for the bis(*o*-hydroxyacetophenone iminato)Cu^{II} complexes are, in general, much larger than for similar types of complexes. The complexes which are most similar are the N-substituted bis(salicylaldiminato)Cu^{II} complexes, and a comparison listing of the "twist" and

Table XI. $CH_2CH_2\varphi$. Observed and calculated structure factors. Columns are l, $10|F_o|$ and $10F_c$. F^2 values used are obtained by squaring the F values in table. Reflections marked N had negative F_o^2.

0,0,L		
2	259E	-332
4	281	-285
6	1482	1471
8	790	793
10	294	279
12	312	313
14	212	253
16	293	257
2,0,L		
0	2260E	-2061
2	1430	1413
-2	701	-695
4	282	-323
-4	116	5
6	1103	-1108
-6	189	145
8	768	-793
-8	786	-733
10	469	461
-10	572	-574
12	458	-486
-12	453	-442
14	395	-363
-14	180	-144
16	158	-186
-16	263	-216
4,0,L		
0	2282E	2148
2	1618	1618
-2	1419	1413
4	1388	1371
-4	1768	1758
6	1222	1229
-6	23	-52
8	708	801
-8	964	865
10	355	-331
-10	618	604
12	628	633
-12	381	371
14	211	258
-14	156	118
-16	136	158
6,0,L		
0	729	757
2	694	-762
-2	458	-466
4	1748E	-187
-4	788	-777
6	334	-395
-6	129	-133
8	639	-878
-8	1066	-976
10	59N	187
-10	663	-673
12	378	-374
-12	276	-244
14	252	-191
-14	226	-173
-16	210	-143
8,0,L		
0	319E	441
2	117	-73
-2	832	841
4	1051	1048
-4	1339	1349
6	764	797
-6	535	542
8	579	591
-8	689	655
10	354	354
-10	567	544
12	336	346
-12	180	2
14	285	121
-14	382	244
10,0,L		
0	391E	-442
2	180	-286
-2	1027	-1027
4	1547	-1589
-4	683	-689
6	158	-143
-6	764	-761
8	399	-339
-8	683	-677
10	682	-673
-10	399	-429
12	368	-285
-12	54N	27
14	49N	17
-14	232	-237
12,0,L		
0	149	175
2	93	84
-2	1792	1813
4	615	618
-4	511	527
6	475	437
-6	491	509
8	398	391
-8	561	523
10	509	517
-10	195	164
12	368	347
-12	157	174
14	137	-29
-14	264	288
14,0,L		
0	978	-883
2	868	-867
-2	1241	-1222
4	318	-332
-4	392	-378
6	384	-376
-6	498	-494
8	159	-174
-8	274	-272
10	355	-378
-10	94	-136
12	371	-363
-12	262	-234
14	69N	-49
-14	182	-163
16,0,L		
0	684	683
2	329	336
-2	913	914
4	332	339
-4	348	349
6	390	403
-6	951	946
8	99	76
-8	48N	11
10	309	291
-10	485	407
12	288	292
-12	278	285
-14	88	139
18,0,L		
0	356	-338
2	913	-912
-2	277	-274
4	323	-334
-4	477	-513
6	389	-397
-6	366	-330
8	89	-38
-8	251	254
10	176	-247
-10	419	-434
12	245	-177
-12	264	-231
-14	157	-95
20,0,L		
0	380	316
2	886	934
-2	63N	-26
4	234	268
-4	320	341
6	258	269
-6	593	575
8	126	99
-8	167	137
10	234	268
-10	294	330
12	48N	28
-12	138	18
22,0,L		
0	83	-57
2	723	-762
-2	347	-334
4	38N	69
-4	92	-63
6	388	-263
-6	111	-131
8	448	-393
-8	317	-285
10	137	-133
-10	174	-178
-12	58N	-81
24,0,L		
0	47N	48
2	331	343
-2	334	296
4	266	211
-4	306	28
6	317	341
-6	247	257
8	149	156
-8	344	293
10	94	162
-10	189	168
26,0,L		
0	92	-91
2	103	-126
-2	267	-261
4	166	-156
-4	55N	-89
6	147	-131
-6	233	-239
8	143	-165
-8	174	-173
-10	58N	-97
28,0,L		
0	248	248
2	36	51
-2	234	234
4	56N	93
-4	185	135
6	213	238
-6	285	182
-8	218	131
30,0,L		
0	167	-126
2	79	-48
-2	243	-194
4	97	-83
-4	49N	-135
-6	137	-115
32,0,L		
0	223	173
2	142	127
-2	46	130
-4	118N	72
0,1,L		
1	1971E	1771
3	1461	1454
5	581	577
7	356	386
9	570	575
11	294	281
13	321	316
15	214	226
1,1,L		
0	539	530
2	744	-741
-2	1830	1814
4	74	-29
-4	45	-25
6	181	161
-6	140	162
8	301	321
-8	329	321
10	65	-46
-10	236	207
12	72	14
-12	126	115
14	108	79
-14	133	23
-16	138	42
2,1,L		
1	1821E	-1643
-1	1425E	-1293
3	271	-275
-3	936	-952
5	1155	-1149
-5	479	-489
7	522	-499
-7	44N	19
9	183	-179
-9	770	-767
11	243	-233
-11	378	-395
13	372	-338
-13	335	-308
15	222	-198
-15	218	-182
3,1,L		
0	304	303
2	774	-770
-2	662E	684
4	365	-313
-4	637	-606
6	422	-420
-6	74	84
8	40	-37
-8	74	69
10	36N	-44
-10	159	-184
12	135	-122
-12	78	-33
14	128	-112
-14	66	-42
-16	38N	-30
4,1,L		
1	915	917
-1	30	-11
3	2672	2678
-3	816	801
5	1228E	1176
-5	564	573
7	527	521
-7	468	488
9	338	330
-9	702	689
11	220	193
-11	429	421
13	316	304
-13	256	245
15	137	118
-15	167	141
5,1,L		
0	965	949
2	133	-147
-2	223	-229
4	679E	681
-4	475	489
6	97	2
-6	669E	612
8	19N	67
-8	113	40
10	254	245
-10	322	303
12	66	-15
-12	81	-13
14	89	63
-14	114	72
-16	103	48
6,1,L		
1	754	-762
-1	1077E	-1116
3	869	-871
-3	242	-237
5	891	-901
-5	716	-715
7	690	-688
-7	744	-759
9	517	-523
-9	644	-633
11	71N	-68
-11	448	-460
13	230	-236
-13	176	-123
15	111	-98
-15	158	-148
7,1,L		
0	285	277
2	679E	-612
-2	446	-441
4	28	-45
-4	47N	3
6	57N	-1
-6	116	33
8	340	-334
-8	133	-107
10	18N	0
-10	119	-129
12	40	-58
-12	29	-40
14	115	-71
-14	119	-53
8,1,L		
1	183	177
-1	954	960
3	923	928
-3	588	574
5	861	866
-5	678	680
7	694	708
-7	697	676
9	586	581
-9	520	534
11	179	131
-11	463	364
13	234	234
-13	43N	26
15	74	100
-15	119	148
9,1,L		
0	293	-298
2	512	519
-2	333	315
4	286	290
-4	242	238
6	213	192
-6	194	163
8	153	138
-8	232	238
10	134	59
-10	84	65
12	124	131
-12	85	30
14	36N	21
-14	110	15
10,1,L		
1	333	-350
-1	476	-462
3	334	-350
-3	1462	-1396
5	682	-686
-5	952	-992
7	614	-614
-7	459	-479
9	476	-464
-9	463	-443
11	334	-318
-11	342	-326
13	241	-185
-13	127	-62
-15	152	-134
11,1,L		
0	496	-493
2	42	-76
-2	614	-609
4	54	-19
-4	64	-114
6	38	-47
-6	84	-38
8	164	-184
-8	19N	-64
10	121	-86
-10	282	-207
12	91N	-36
-12	93	-34
14	92N	-23
-14	114	12
12,1,L		
1	598	561
-1	119	134
3	560E	596
-3	1172	1193
5	340	324
-5	682	692
7	428	421
-7	356	343
9	444	431
-9	169	142
11	463	366
-11	285	238
13	217	176
-13	188	155
-15	175	129
13,1,L		
0	147	-147
2	84	-97
-2	17	-19
4	351	341
-4	347	340
6	260	293
-6	79	132
8	26N	21
-8	191	-217
10	59N	83
-10	94	190
12	96	92
-12	61N	95
14	110	50
-14	85N	23
14,1,L		
1	626	-618
-1	727	-726
3	941	-949
-3	828	-827
5	312	-291
-5	613	-622
7	282	-277
-7	931	-917
9	386	-376
-9	99	88
11	316	-277
-11	332	-334
13	183	-231
-13	153	-186
15,1,L		
0	377	-383
2	159	-189
-2	97	-116
4	138	-157
-4	342	-344
6	125	-111
-6	373	-367
8	67	3
-8	116	35
10	77	-97
-10	214	-132
12	89	-66
-12	127	-112
-14	57	-48
16,1,L		
1	484	494
-1	602E	655
3	513	527
-3	499	480
5	183	175
-5	284	273
7	150	181
-7	427	422
9	276	270
-9	129	-88
11	197	212
-11	361	386
13	208	189
-13	179	170
17,1,L		
0	279	-235
2	295	266
-2	45	44
4	63	72
-4	56	-4
6	91N	51
-6	54N	47
8	128	110
-8	65N	42
10	83	-1
-10	83N	-58
12	81	95
-12	146	140
-14	64	50
18,1,L		
1	746	-728
-1	282	-284
3	441	-421
-3	333	-321
5	470	-469
-5	378	-363
7	168	-141
-7	365	-345
9	174	-155
-9	60	3
11	212	-199
-11	285	-311
-13	212	-160
19,1,L		
0	161	-145
2	421	-415
-2	60	34
4	64N	-18
-4	261	-271
6	67	-138
-6	282	-267
8	91	-58
-8	118	-121
10	98	-62
-10	116	89
12	58N	-61
-12	28	-82
20,1,L		
1	855	852
-1	80	95
3	339	334
-3	183	174
5	200	201
-5	202	221
7	285	242
-7	403	394
9	169	159
-9	189	175
11	92	125
-11	195	184
-13	137	126
21,1,L		
0	263	258
2	152	135
-2	128	-48
4	118	-19
-4	232	-215
6	145	-95
-6	89	130
8	190	147
-8	151	166
10	148	85
-10	80N	5
-12	96	-6
22,1,L		
1	499	-513
-1	212	-166
3	122	-116
-3	115	-140
5	344	-324
-5	99	-68
7	494	-361
-7	366	-369
9	118	-138
-9	228	-234
11	121N	-65
-11	147	-137
23,1,L		
0	402	-252
2	88	54
-2	18	-153
4	81	34
-4	83	-69
6	254	-233
-6	44N	-41
8	96	-48
-8	95	-69
10	109N	-6
-10	77	-60
-12	104N	1
24,1,L		
1	134	155
-1	239	222
3	190	183
-3	330	237
5	312	240
-5	118	91
7	204	206
-7	291	337
9	162	158
-9	172	190
-11	183	107
25,1,L		
0	46	67
2	90	-40
-2	63	41
4	129	94
-4	52	4
6	106	37
-6	63	33
8	88N	-6
-8	66N	33
-10	142N	3
26,1,L		
1	142	-138
-1	157	-195
3	135	-76
-3	184	-203
5	264	-250
-5	158	-117
7	131	-145
-7	207	-241
-9	109	-135
27,1,L		
0	82	-7
2	44	-73
-2	39	-106
4	57	2
-4	113	-61
6	44N	-31
-6	23	34
8	51N	-53
-8	108	-103
-10	112	22
28,1,L		
1	147	103
-1	205	201
3	65	20
-3	247	240
5	194	180
-5	165	146
7	40	108
-7	166	128
-9	94	125
29,1,L		
0	48	53
2	32	-36
-2	30N	46
4	80	71
-4	132	60
6	134	43
-6	62	-2
-8	16	30
30,1,L		
1	105	-123
-1	181	-158
3	133	-43
-3	204	-158
5	129	-134
-5	113	-90
-7	58	-72
31,1,L		
0	102N	-52
2	57	-21
-2	53	6
4	118	-73
-4	39N	-15
-6	110N	-36
32,1,L		
1	39N	50
-1	180	106
-3	160	118
0,2,L		
0	1156	1139
2	94N	-50
4	677	671
6	170	132
8	359	363
10	93N	25
12	487	407
14	206	197
1,2,L		
1	866E	799
-1	2149E	2183
3	130	-162
-3	179	183
5	143	137
-5	591	-571
7	668	671
-7	566	563
9	384	392
-9	640	633
11	236	-225
-11	30N	-16
13	281	197
-13	148	112
15	170	181
-15	174	136
2,2,L		
0	3183E	-3015
2	1672	-1696
-2	397	391
4	1039	-1028
-4	1110E	-1152
6	584	-598
-6	345	-376
8	439	-444
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14	136	-134
-14	168	-185
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-9	318	-287
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13	234	-263
-13	171	-145
15	124	-137
-15	36	-67
4,2,L		
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5,2,L		
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-3	400	435
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7	313	327
-7	296	312
9	180	-85
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11	289	285
-11	39	47
13	187	197
-13	248	205
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-15	32	38
6,2,L		
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2	1131	-1137
-2	255	-253
4	1179	-1169
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6	521	-534
-6	429	-443
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-8	743	-742
10	73	-71
-10	452	-443
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-12	135	-187
14	132	-116
-14	185	-129
7,2,L		
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-7	64	-92
9	228	243
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11	373	-376
-11	73N	-55
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-13	190	-194
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8,2,L		
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-12	130	38
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9,2,L		
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7	357	344
-7	149	184
9	73	-83
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13	239	185
-13	58	71
-15	17	59
10,2,L		
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6	604	-637
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12	294	-296
-12	127	-91
14	29	-69
-14	58	-139
11,2,L		
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-1	538	-527
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7	187	-211
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-9	176	-197
11	231	-197
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13	138	-114
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-15	93	-83
12,2,L		
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2	268	291
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-4	677E	721
6	316	321
-6	565	553
8	188	118
-8	235	231
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12	330	315
-12	155	139
14	46	27
-14	287	176
13,2,L		
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-1	346	329
3	514	-511
-3	368	383
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7	289	272
-7	139	-83
9	198	231
-9	183	187
11	188	161
-11	138	162
13	94N	47
-13	93	-6
14,2,L		
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12	236	-238
-12	281	-271
-14	150	-156
15,2,L		
1	199	-223
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3	544	-534
-3	518	-531
5	99	-65
-5	239	-191
7	188	-129
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-11	66	-87
13	48N	9
-13	69N	-42
16,2,L		
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2	611	614
-2	588	584
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6	333	340
-6	396	399
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-12	197	204
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17,2,L		
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3	259	269
-3	519	518
5	152	157
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-7	64N	-88
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11	183	189
-11	125	141
-13	64	78
18,2,L		
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-2	368	-392
4	157	-181
-4	152	-147
6	243	-231
-6	412	-398
8	137	-182
-8	162	-120
10	170	-174
-10	260	-271
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-12	172	-187
19,2,L		
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5	117	-188
-5	236	-288
7	117	94
-7	298	-296
9	171	-185
-9	77	19
11	132	-142
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20,2,L		
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6	391	304
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8	198	140
-8	98	86
10	79	94
-10	248	254
-12	141	101
21,2,L		
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-1	161	151
3	98	116
-3	60	-12
5	58	7
-5	97	108
7	158	108
-7	267	203
9	169	172
-9	81N	-22
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-11	119N	81
22,2,L		
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4	247	-231
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6	290	-288
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8	123	-93
-8	231	-177
10	168	-136
-10	246	-243
-12	56	-64
23,2,L		
1	238	-233
-1	247	-216
3	94	-4
-3	76	-46
5	192	-182
-5	66	-187
7	136	-98
-7	117	-145
9	119	-91
-9	50	-44
-11	63	-84
24,2,L		
0	91N	-5
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-2	234	218
4	166	123
-4	129	57
6	217	185
-6	173	181
8	94	159
-8	110	167
-10	164	133
25,2,L		
1	262	261
-1	56	-47
3	117	-90
-3	164	113
5	137	93
-5	181	169
7	176	160
-7	139N	81
9	86	3
-9	105N	72
26,2,L		
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2	151	-129
-2	229	-249
4	163	-123
-4	166	-160
6	143	-206
-6	194	-183
8	82N	-82
-8	182	-162
-10	79	-79
27,2,L		
1	178	-193
-1	103	-137
3	29	4
-3	65N	-58
5	95N	-39
-5	22N	-44
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-7	74	-56
-9	121	-41
28,2,L		
0	146	92
2	114	87
-2	143	156
4	102	67
-4	95	92
6	92	117
-6	135	133
-8	115	115
29,2,L		
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-1	126	49
3	60	73
-3	151	118
5	112	53
-5	125	44
-7	137	68
30,2,L		
0	193	-161
2	81	-59
-2	203	-169
4	56	-18
-4	165	-92
-6	84	-69
31,2,L		
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-1	101	-61
3	79	-33
-3	118	-70
-5	45N	-3
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0,3,L		
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3	115	-110
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7	58N	-21
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11	276	269
13	233	264
15	137	99
1,3,L		
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2	416	437
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4	614	604
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6	426	435
-6	314	322
8	457	462
-8	424	416
10	184	180
-10	265	240
12	134	166
-12	124	125
14	226	219
-14	158	167
2,3,L		
1	855	-857
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5	427	-429

Table XI. (Continued)

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-13	190	-165
15	92	-60
-15	103	-90
3,3,L		
0	812	-812
2	372	-365
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4	734	-728
-4	337	-341
6	248	-248
-6	491	-458
8	315	-328
-8	261	-243
10	246	-223
-10	468	-467
12	111	-131
-12	161	-183
14	178	-194
-14	116	-118
4,3,L		
1	849	846
-1	560	561
3	216	227
-3	395	392
5	420	413
-5	204	201
7	480	482
-7	218	235
9	157	121
-9	465	461
11	92	-6
-11	376	363
13	183	205
-13	142	130
15	174	74
-15	65N	64
5,3,L		
0	340	359
2	566	597
-2	913E	474
4	674	693
-4	667	607
6	373	382
-6	430	451
8	318	331
-8	281	187
10	261	256
-10	386	385
12	284	132
-12	99	69
14	139	126
-14	83	134
6,3,L		
1	579	-583
-1	516	494
3	993	-988
-3	386	-383
5	680	-680
-5	292	-324
7	474	-477
-7	269	-267
9	249	-245
-9	462	-472
11	185	-96
-11	182	-178
13	161	-153
-13	125	-98
15	124	-62
-15	42N	-84
7,3,L		
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2	566E	-607
-2	274	-276
4	163	-162
-4	518	-514
6	428	-438
-6	384	-286
8	339	-335
-8	385	-325
10	218	-205
-10	418	-465
12	137	-141
-12	78N	-45
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-14	133	-187
8,3,L		
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-1	269	276
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7	412	414
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9	330	330
-9	488	479
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4	606	695
-4	436	436
6	390	376
-6	267	293
8	349	395
-8	148	164
10	133	82
-10	336	359
12	220	233
-12	184	179
14	138	103
-14	82	44
10,3,L		
1	273	267
-1	162	-194
3	505	-498
-3	417	-390
5	532	-540
-5	365	-391
7	224	-213
-7	423	-422
9	394	-397
-9	111N	-41
11	161	-157
-11	182	-129
13	120	-117
-13	38N	-82
-15	156	-123
11,3,L		
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2	542	-516
-2	365	-379
4	487	-492
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6	233	-243
-6	423	-434
8	156	-186
-8	77	87
10	219	-179
-10	230	-265
12	214	-229
-12	248	-224
14	110	-67
-14	96	-69
12,3,L		
1	186	174
-1	612	595
3	446	448
-3	586	588
5	245	240
-5	437	446
7	198	76
-7	668	694
9	329	369
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11	268	229
-11	94	71
13	159	119
-13	136	87
13,3,L		
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2	567	566
-2	204	173
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6	66	74
-6	627	843
8	258	213
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-10	186	205
12	119	125
-12	132	170
-14	139	138
14,3,L		
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9	258	-218
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-13	117	-77
15,3,L		
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2	487	-493
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4	85N	77
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-6	211	-230
8	242	-237
-8	181	-112
10	128	-125
-10	153	-148
12	135	-125
-12	119	-141
-14	198	-121
16,3,L		
1	586	536
-1	484	469
5	371	359
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7	147	141
-7	169	174
9	126	103
-9	99	96
11	197	165
-11	149	156
-13	34N	56
17,3,L		
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4	239	269
-4	331	297
6	231	247
-6	298	292
8	157	143
-8	179	193
10	149	117
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12	141	118
-12	119	150
18,3,L		
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3	111	-125
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5	26	-92
-5	49N	-7
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9	29N	-50
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-13	89	-21
19,3,L		
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20,3,L		
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9	149	51
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21,3,L		
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-4	29	184
6	186	176
-6	283	281
8	181	157
-8	238	178
10	152	113
-10	96	13
-12	78	129
22,3,L		
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-3	341	-288
5	179	-149
-5	179	-140
7	81	-99
-7	213	-179
9	64	-82
-9	64N	-84
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23,3,L		
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4	81	-98
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6	221	-179
-6	122	-184
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-8	184	-187
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24,3,L		
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26,3,L		
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7	72	-92
-7	167	-119
-9	148	-88
27,3,L		
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-4	118	-110
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-6	89	-37
-8	98	-137
28,3,L		
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31,3,L		
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14	56N	37
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13	271	273
-13	323	319
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8	158	-147
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-14	113	-63
3,4,L		
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10	158	148
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13	119	-145
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6	147	175
-6	286	310
8	396	411
-8	362	356
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12	121	60
-12	164	136
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9,4,L		
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7	735	729
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9	122	-126
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11	239	222
-11	267	268
13	263	203
-13	94	94
10,4,L		
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6	208	-196
-6	328	-330
8	446	-437
-8	192	-178
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12	42	-62
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-14	47	-29
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-9	191	-195
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-11	268	-244
13	222	-191
-13	152	-87
12,4,L		
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4	25	8
-4	267	247
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10	55N	65
-10	75	80
12	49N	36
-12	88N	50
-14	88N	60
13,4,L		
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-1	173	147
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5	67N	-6
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9	181	162
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-11	234	217
13	64N	57
-13	84	79
14,4,L		
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-4	229	-239
6	213	-211
-6	191	-198
8	43	-33
-8	80	63
10	184	-130
-10	139	-53
12	72N	-78
-12	116	-36
15,4,L		
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-1	371	-306
3	543	-545
-3	337	-319
5	170	-119
-5	317	-321
7	236	-216
-7	48N	-29
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-9	200	-191
11	203	-212
-11	145	-151
-13	76	-81
16,4,L		
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-2	318	326
4	25	10
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6	90	34
-6	164	174
8	101	34
-8	84	134
10	27N	68
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12	34	86
-12	42	66
17,4,L		
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-1	170	211
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-5	181	138
7	167	149
-7	326	341
9	195	165
-9	201	199
11	163	175
-11	87	100
-13	122	133
18,4,L		
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-2	181	-181
4	55	10
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6	223	-237
-6	59N	-41
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-8	135	-114
10	75	-6
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-12	51N	-59
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-1	265	-240
3	232	-226
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9	169	-146
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11	207	-162
-11	57N	-79
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2	184	178
-2	234	251
4	144	168
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8	132	28
-8	26	76
10	47	17
-10	150	146
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21,4,L		
1	178	173
-1	295	262
3	178	207
-3	169	171
5	277	257
-5	184	184
7	153	135
-7	223	221
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-11	94	97
22,4,L		
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2	69	-73
-2	43	-51
4	162	-162
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6	211	-191
-6	84	-125
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-8	112	-27
-10	160	-149
23,4,L		
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-1	161	-144
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-5	181	-192
7	189	-123
-7	187	-211
9	116	-64
-9	78	-57
24,4,L		
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-6	160	92
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-8	95	52
-10	119	104
25,4,L		
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3	64	37
-3	156	142
5	163	142
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7	160	126
-7	151	127
-9	73	28
26,4,L		
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2	96	-96
-2	92	-85
4	68	-45
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6	87	-118
-6	19	-76
-8	121	-66
27,4,L		
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-1	88N	-13
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-3	84	-172
5	111	-71
-5	168	-111
-7	77	-114
28,4,L		
0	36	-36
2	77N	65
-2	159	116
4	44N	4
-4	84	84
-6	64	63
29,4,L		
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-1	152	62
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-5	94N	41
30,4,L		
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9	48	-47
11	12	126
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1,5,L		
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2	483	483
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-4	257	245
6	277	287
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8	313	322
-8	325	315
10	300	275
-10	304	356
12	128	86
-12	106	72
14	205	234
-14	207	194
2,5,L		
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-1	98	9
3	135	-128
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5	25N	-68
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7	96	-59
-7	88	29
9	86	69
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11	22	3
-11	179	-191
13	117	-81
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3,5,L		
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2	262	-250
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-4	269	-284
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-6	378	-375
8	308	-339
-8	370	-378
10	231	-214
-10	284	-271
12	123	-133
-12	178	-145
14	183	-154
-14	128	-163
4,5,L		
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-5	146	158
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9	91	61
-9	120	24
11	51	-35
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13	59N	52
-13	38	42
5,5,L		
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2	443	423
-2	499	503
4	543	525
-4	252	250
6	388	367
-6	331	344
8	215	213
-8	251	274
10	186	194
-10	238	243
12	288	192
-12	177	167
-14	187	158
6,5,L		
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-1	224	213
3	92	-127
-3	194	-161
5	195	-159
-5	132	-133
7	23N	-95
-7	189	-88
9	58	-13
-9	166	-167
11	51N	19
-11	108	-60
13	18N	-7
-13	95N	-39
7,5,L		
0	468	-477
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4	518	-519
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6	437	-458
-6	561	-552
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-8	203	-190
10	238	-211
-10	251	-262
12	178	-280
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8,5,L		
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-1	203	-256
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-5	39N	29
7	55N	47
-7	263	252
9	164	151
-9	78N	12
11	91N	95
-11	161	-87
13	53N	-4
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9,5,L		
0	520	521
2	196	220
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4	236	265
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6	392	374
-6	447	460
8	238	170
-8	69	26
10	269	189
-10	292	312
12	121	181
-12	147	115
10,5,L		
1	166	-188
-1	156	-127
3	137	-144
-3	161	-172
5	219	198
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-7	490	-501
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11	63N	-14
-11	149	144
13	38N	19
-13	137N	1
11,5,L		
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2	493	-496
-2	402	-399
4	473	-483
-4	368	-361
6	286	-261
-6	511	-501
8	266	-262
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10	141	-168
-10	239	-226
12	239	-283
-12	125	-96
12,5,L		
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-1	436	434
3	449	-467
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5	282	283
-5	138	-123
7	37	72
-7	48N	66
9	164	111
-9	133	98
11	106N	19
-11	57N	-17
-13	91N	-46
13,5,L		
0	288	279
2	538	546
-2	398	393
4	149	7
-4	303	385
6	177	173
-6	260	256
8	259	266
-8	190	194
10	180	141
-10	197	199
12	176	154
-12	148	91
14,5,L		
1	73	39
-1	281	-273
3	71N	2
-3	252	-236
5	243	-253
-5	39N	-72
7	119	97
-7	123	-9
9	58	-16
-9	122	-19
11	105	-79
-11	106	-33
-13	111	15
15,5,L		
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2	433	-469
-2	374	-343
4	273	-247
-4	295	-238
6	187	-178
-6	192	-160
8	293	-272
-8	216	-283
10	157	-126
-10	196	-186
-12	163	-78
1	199	203
-1	86	72
3	115	-116
-3	124	111
5	109	97
-5	59N	-18
7	43N	-13
-7	136	-18
9	97	-54
-9	66N	18
11	91	91
-11	168	52
17,5,L		
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2	290	279
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4	187	129
-4	228	224
6	191	182
-6	148	161
8	163	178
-8	199	186
10	140	124
-10	164	177
-12	143	94
18,5,L		
1	92	-69
-1	67	-87
3	83	-116
-3	113	-144
5	103	-53
-5	63	96
7	11	-29
-7	83	-23
9	94	10
-9	162N	-1
-11	186	-78
19,5,L		
0	244	-231
2	218	-191
-2	246	-257
4	382	-302
-4	169	-113
6	168	-156
-6	161	-154
8	117	-121
-8	187	-168
10	139	-140
-10	115	-104
20,5,L		
1	69	102
-1	119	-62
3	116	161
-3	79	78
5	93	49
-5	60	-7
7	87	-5
-7	80	17
9	64	-7
-9	61	65
-11	79	84
21,5,L		
0	165	129
2	189	166
-2	188	159
4	212	171
-4	195	167
6	266E	181
-6	183	175
8	72	108
-8	172	176
-10	33	8
22,5,L		
1	90	-23
-1	39N	-6
3	91N	-57
-3	60N	-18
5	86	-71
-5	23N	-13
7	28N	23
-7	128	99
-9	111	-89
23,5,L		
0	181	-203
2	260	-158
-2	65	-117
4	164	-118
-4	181	-128
6	191	-149
-6	169	-121
8	131	-72
-8	266	-187
24,5,L		
1	93N	-18
-1	60	-68
3	138	86
-3	34N	99
5	38	79
-5	97	80
7	70	14
-7	75	-18
-9	91N	39
25,5,L		
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4	144	102
-4	168	167
6	139	156
-6	127	98
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3	135	-46
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Table XI. (Continued)

27,5,L		
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28,5,L		
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-1	90N	4
3	83	49
-3	111	77
-5	118	39
29,5,L		
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-2	14	34
0,6,L		
0	36	-4
2	117	124
4	25	66
6	222	-244
8	43N	-58
10	30N	63
12	111	1
1,6,L		
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-1	580	512
3	317	330
-3	494	405
5	374	353
-5	311	345
7	217	214
-7	95	71
9	205	288
-9	410	371
11	175	129
-11	158	166
13	127N	188
-13	133	193
2,6,L		
0	96	120
2	58	12
-2	47	-79
4	221	-237
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6	206	215
-6	94	95
8	57	-13
-8	83	53
10	19N	-19
-10	35	-45
12	86	77
-12	158	-93
3,6,L		
1	287	-276
-1	336	-323
3	513	-519
-3	384	-389
5	296	-306
-5	383	-393
7	223	-191
-7	126	-163
9	196	-172
-9	329	-316
11	150	-173
-11	129	-89
13	172	-118
-13	190	-186
4,6,L		
0	147	-125
2	114	91
-2	93N	-27
4	187	156
-4	61	-62
6	73	-65
-6	139	-121
8	33N	-11
-8	73N	-37
10	99	-16
-10	99	-7
12	64	-52
-12	52	95
5,6,L		
1	81	93
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3	625	644
-3	349	313
5	248	263
-5	347	335
7	295	283
-7	288	261
9	201	172
-9	213	247
11	186	198
-11	145	94
13	180	185
-13	177	183
6,6,L		
0	194	196
2	63	-72
-2	163	192
4	188	-88
-4	268	-259
6	153	-125
-6	67	64
8	54	114
-8	49	-9
10	41N	3
-10	44N	-14
12	93	24
-12	171	-133
7,6,L		
1	867	-836
-1	379E	-437
3	412	-387
-3	61	-42
5	225	-206
-5	987	-962
7	246	-246
-7	177	-169
9	159	-145
-9	179	-189
11	289	-198
-11	151	-153
-13	146	-166
8,6,L		
0	241	-194
2	102	121
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4	80N	3
-4	289	218
6	41	-63
-6	117	141
8	126	-11
-8	95	-115
10	33N	73
-10	113	-137
12	72N	-11
-12	67	77
9,6,L		
1	251	217
-1	446	436
3	523	531
-3	71	-23
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-5	586	587
7	287	286
-7	286	184
9	245	196
-9	92	144
11	163	187
-11	112	90
-13	134	122
10,6,L		
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2	159	-157
-2	287	276
4	164	198
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6	168	96
-6	311	-315
8	68	-176
-8	114	-59
10	75N	-47
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12	114	77
-12	117	-17
11,6,L		
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3	158	-162
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5	81N	54
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-7	72	-82
9	132	-94
-9	278	-278
11	158	-161
-11	118	-134
12,6,L		
0	124	86
2	168	-190
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4	268	-236
-4	132	-119
6	125	-31
-6	58N	32
8	193	193
-8	69N	15
10	87N	-38
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-12	73N	-36
13,6,L		
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3	386	372
-3	204	217
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7	342	396
-7	79	66
9	135	61
-9	187	158
11	81	119
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14,6,L		
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-2	31	-51
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6	99	-42
-6	47	72
8	38N	-29
-8	34N	-52
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-10	13N	33
-12	115	42
15,6,L		
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-1	388	-287
3	323	-346
-3	243	-237
5	186	12
-5	193	-213
7	208	-292
-7	147	-186
9	87N	-82
-9	105	-158
-11	84	-98
16,6,L		
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2	63	-65
-2	46	-15
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-10	87N	-12
17,6,L		
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3	275	297
-3	193	187
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-5	128	144
7	129	147
-7	96	130
9	108	88
-9	189	148
-11	73	79
18,6,L		
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-2	94	-105
4	97	-84
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6	163	-24
-6	74	46
8	96	32
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19,6,L		
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3	227	-196
-3	161	-172
5	177	-169
-5	182	-147
7	188	-153
-7	136	-142
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20,6,L		
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21,6,L		
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-3	134	88
5	130	129
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22,6,L		
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2	95	33
-2	79N	-18
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23,6,L		
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3	88	-82
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5	140	-138
-5	146	-98
-7	127	-141
24,6,L		
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25,6,L		
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26,6,L		
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27,6,L		
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5	93	-18
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1,7,L		
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2	361	366
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-4	331	327
6	212	172
-6	144	136
8	35	116
-8	215	194
10	161	202
-10	163	170
12	83N	61
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2,7,L		
1	92N	-59
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3	36	-50
-3	142	145
5	158	177
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3,7,L		
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-4	145	-163
6	219	-236
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8	61	-83
-8	162	-195
10	264	-185
-10	86	-70
12	84	-98
-12	101	-81
4,7,L		
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3	68	-67
-3	165	-148
5	163	-57
-5	170	-128
7	52	-45
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9	31	-45
-9	42N	-34
11	38	-48
-11	142	-37
5,7,L		
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2	231	216
-2	312	361
4	262	283
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6	243	236
-6	366	373
8	121	148
-8	208	237
10	197	197
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-12	53	96
6,7,L		
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3	169	133
-3	158	146
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7	24	62
-7	64	-20
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-9	84	51
11	95	62
-11	36	7
7,7,L		
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2	79	-26
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6	172	-181
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8	124	-86
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-10	125	-82
-12	156	-138
8,7,L		
1	92	-1
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9	144	-14
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11	99	-48
-11	49N	-26
9,7,L		
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4	147	78
-4	149	114
6	263	237
-6	375	376
8	180	152
-8	136	115
10	175	128
-10	121	167
10,7,L		
1	64N	93
-1	129	78
3	296	277
-3	85N	39
5	34N	-30
-5	77N	31
7	119	24
-7	116	38
9	21N	4
-9	66	43
11	74	46
-11	34	49
11,7,L		
0	362	-321
2	159	-151
-2	216	-191
4	131	56
-4	162	-162
6	267	-264
-6	136	-117
8	191	-152
-8	167	-156
10	102	-66
-10	166	-195
12,7,L		
1	43N	-15
-1	149	-82
3	173	-122
-3	62N	-3
5	35N	-22
-5	93	-54
7	103	-43
-7	51N	-34
9	42N	-43
-9	79	-22
-11	58	-76
13,7,L		
0	149	189
2	237	220
-2	279	272
4	56	134
-4	229	242
6	278	231
-6	98	16
8	197	169
-8	134	75
10	49	19
-10	196	186
14,7,L		
1	36	57
-1	126	15
3	177	179
-3	43N	9
5	87N	-23
-5	99	43
7	120	83
-7	133	69
9	71	32
-9	72	28
15,7,L		
0	63N	-61
2	199	-201
-2	236	-264
4	229	-222
-4	139	-137
6	60	-18
-6	125	-124
8	113	-112
-8	97	-92
-10	160	-137
16,7,L		
1	119	-44
-1	62	-12
3	9	-6
-3	87	-6
5	118	-72
-5	124	-92
7	130	-95
-7	95N	-48
9	33N	-9
-9	87	-36
17,7,L		
0	85	56
2	165	144
-2	268	252
4	190	199
-4	156	82
6	121	68
-6	88N	42
8	122	123
-8	111	113
18,7,L		
1	82	6
-1	26	34
3	86	37
-3	97	40
5	49	47
-5	111	80
7	35	54
-7	68	61
-9	84N	-14
19,7,L		
0	95	-85
2	133	-119
-2	94	-138
4	232	-191
-4	126	-134
6	133	-95
-6	46	-58
-8	172	-156
20,7,L		
1	65	-61
-1	6N	15
3	116	-48
-3	86N	-32
5	45N	4
-5	46	-71
-7	121	-85
21,7,L		
0	136	119
2	139	81
-2	93	92
4	86	132
-4	19	95
6	68	97
-6	53	31
22,7,L		
1	74	91
-1	92	70
3	134	-47
-3	103	30
5	101N	-42
-5	112	5
23,7,L		
0	142	-98
2	78N	-36
-2	101	-92
4	151	-149
-4	31N	-85
24,7,L		
1	38	-36
-1	48N	-56
3	110N	6
-3	53N	-37
25,7,L		
0	111	96
-2	79	48
0,8,L		
0	262	-233
2	79	-39
4	82	-53
6	116	-110
8	175	-152
10	98N	-42
1,8,L		
1	116	119
-1	133	133
3	247	277
-3	137	159
5	135	152
-5	213	227
7	33	-32
-7	128N	22
9	135	151
-9	175	138
-11	114	134
2,8,L		
0	132	178
2	125	-121
-2	200	170
4	96	119
-4	113	87
6	118	111
-6	76	87
8	142	148
-8	54N	60
10	26	-9
-10	131	96
3,8,L		
1	89	-129
-1	148	-113
3	292	-281
-3	173	-168
5	121	-32
-5	143	-133
7	195	-133
-7	93	-72
9	179	-137
-9	97	-122
4,8,L		
0	16N	-56
2	112	-77
-2	96	-89
4	193	-161
-4	236	-178
6	33N	-49
-6	80	-78
8	46	-31
-8	84	-3
10	87	-13
-10	67	-85
5,8,L		
1	79	65
-1	185	188
3	271	269
-3	164	163
5	86	81
-5	176	178
7	82	136
-7	59N	58
9	98N	69
-9	91	122
6,8,L		
0	153	134
2	127	73
-2	145	133
4	132	77
-4	213	214
6	27N	39
-6	29	39
8	125	67
-8	43	23
10	112N	46
-10	176	108
7,8,L		
1	76	-59
-1	71	-85
3	246	-285
-3	48	-59
5	59N	-84
-5	259	-346
7	155	-128
-7	51	-28
9	92	-77
-9	38	-54
8,8,L		
0	69	13
2	231	-202
-2	90N	-49
4	105	-122
-4	179	-126
6	102	27
-6	142	-44
8	102	-64
-8	74N	-13
10	48	-38
-10	78N	-48
9,8,L		
1	228	217
-1	87	168
3	186	165
-3	87	-64
5	77N	18
-5	348	372
7	117	118
-7	33N	58
9	126	94
-9	101	98
10,8,L		
0	208	167
2	178	131
-2	112	145
4	118	98
-4	79	-17
6	90N	-1
-6	161	134
8	137	85
-8	111	58
-10	122	68
11,8,L		
1	161	-131
-1	188	-188
3	147	-146
-3	182	48
5	43	31
-5	154	-214
7	171	-214
-7	21N	-96
9	119	-68
-9	138	-76
12,8,L		
0	72	-38
2	77	-63
-2	154	-146
4	55N	-84
-4	95	86
6	85	-24
-6	142	-86
8	113	-91
-8	59	-21
13,8,L		
1	126	129
-1	206	186
3	58	138
-3	27N	65
5	66	-37
-5	94	114
7	187	211
-7	68N	77
-9	94	107
14,8,L		
0	88	77
2	118	83
-2	76N	83
4	89N	76
-4	64	33
6	208	146
-6	127	131
8	142	25
-8	96	25
15,8,L		
1	118	-86
-1	144	-182
3	163	-135
-3	98N	-33
5	131N	-6
-5	79	-94
7	46	-154
-7	129	-45
16,8,L		
0	47N	-44
2	92	-74
-2	78	-54
4	121N	13
-4	34	-14
6	139	-133
-6	12	-64
-8	41	-47
17,8,L		
1	89N	57
-1	187	175
3	99N	69
-3	142	22
5	97	49
-5	98	94
-7	118N	31
18,8,L		
0	68N	-14
2	118	68
-2	95	65
4	98	34
-4	186	91
6	115	118
-6	184	78
19,8,L		
1	148	-48
-1	184	-156
3	29N	-68
-3	93N	-49
5	71	-101
-5	89N	-49
20,8,L		
0	41	-16
2	119	-135
-2	116	-48
4	87N	-5
-4	94	-34
21,8,L		
1	99N	-22
-1	82	76
3	95	74
-3	38	92
22,8,L		
0	118	47
-2	51	66
0,9,L		
1	37	-138
3	60N	-74
5	143	-134
7	149	-137
9	72	-33
1,9,L		
0	113N	-39
2	177	181
-2	132	92
4	153	132
-4	118	144
6	83	31
-6	43N	117
8	103N	-4
-8	90N	16
2,9,L		
1	106	93
-1	26N	61
3	43N	77
-3	145	47
5	138	65
-5	208	177
7	127	79
-7	108N	69
9	85	49
-9	86N	24
3,9,L		
0	93	-119
2	159	-168
-2	96	-136
4	49N	-48
-4	64	39
6	22	-43
-6	157	-137
8	36	-25
-8	152	-134
4,9,L		
1	188	-182
-1	111	-127
3	35	-23
-3	41N	-2
5	145	-98
-5	231	-231
7	61	-76
-7	13	-24
-9	95	-74
5,9,L		
0	73N	53
2	69N	38
-2	162	151
4	83N	55
-4	144	-33
6	179	120
-6	138	104
8	59	38
-8	127	65
6,9,L		
1	51	77
-1	132	111
3	122	180
-3	68	80
5	44	21
-5	139	123
7	88	57
-7	72N	29
7,9,L		
0	180	-144
2	89	-88
-2	29N	-85
4	95N	-36
-4	60N	-7
6	88	-125
-6	54	-114
8	110	-13
-8	100	-49
8,9,L		
1	103	-79
-1	68	-99
3	188	-158
-3	146	-125
5	93N	-6
-5	87N	-4
7	101	-88
-7	132	-73
9,9,L		
0	98	82
2	80N	32
-2	99N	78
4	85N	20
-4	71	46
6	121	111
-6	137	102
-8	47	18
10,9,L		
1	38N	24
-1	169	150
3	138	146
-3	35N	104
5	72N	17
-5	98	-29
7	77	59
-7	181	185
11,9,L		
0	79	-89
2	113	-92
-2	86	-53
4	130	-3
-4	87	-83
6	155	-187
-6	118	-77
12,9,L		
1	116	1
-1	186	-153
3	52	-82
-3	38	-85
5	63	-116
-5	40N	-14
-7	68	-57
13,9,L		
0	78	55
2	103	73
-2	56N	76
4	187	56
-4	68	47
6	86N	42
-6	141	55
14,9,L		
1	119	38
-1	130	185
3	124	73
-3	26N	16
5	167	117
-5	93	76
15,9,L		
0	26N	-32
2	24N	-56
-2	41	-92
4	79	-55
-4	96	-65
16,9,L		
1	134	-51
-1	72N	-58
3	64	-38
-3	112	-49
-5	94N	-47
17,9,L		
0	107	52
2	33N	59
-2	113N	93
-4	115N	34
18,9,L		
1	92	69
-1	77	5
-3	88N	86
0,10,L		
0	14	-36
2	116N	-58
4	231	-173
6	14	-26
1,10,L		
1	63N	37
-1	111	-54
3	139	140
-3	117N	76
5	35	5
-5	89	42
2,10,L		
0	87	96
2	44	77
-2	45	-23
4	132	120
-4	159	127
6	111	-20
-6	79	89
3,10,L		
1	92	-51
-1	77N	-45
3	86	-69
-3	61N	-9
5	113	-1
-5	21N	-71
4,10,L		
0	47	-122
2	166	-57
-2	51	-42
4	144	-76
-4	99	-135
6	91N	4
-6	88	-95
5,10,L		
1	62	49
-1	77N	47
3	139	34
-3	50N	-39
5	107	12
-5	128	56
6,10,L		
0	64	59
2	154	130
-2	20N	7
4	78	69
-4	166	152
7,10,L		
1	55N	-13
-1	35N	-83
3	49N	-51
-3	19	-1
5	56	-18
-5	82	-59
8,10,L		
0	95	-66
2	51	-119
-2	52	-61
4	113	-65
-4	147	-49
9,10,L		
1	63	11
-1	70N	51
3	89	38
-3	92	19
-5	84N	33
10,10,L		
0	94	44
2	58	94
-2	78N	76
4	69N	47
-4	94N	15
11,10,L		
1	53	-13
-1	46	-49
3	103	-45
-3	114	-7
12,10,L		
0	103	-69
2	60N	-71
-2	87	-69
13,10,L		
1	120N	17
-1	76	74

Table XII. Description of n-substituted *o*-hydroxyacetophenone imine copper(II) complexes.

Imine Substituent Group R	Z	Space Group	Coordination Number	« Twist » [e] Degrees	Color Transmitted	Color Reflected	The C1-C7 bond « Rotation » in Degrees
H1 [a]	3	P1	4	0.	brown	red-brown	4.3
H2			4	7.8	yellow-brown	yellow-brown	6.3
H3							1.6
$CH_3(5)1$ [b]	2	P1	5	11.0			17.2
$CH_3(5)2$							16.5
$CH_3(4)$ [c]	2	$P2_1/a$	4	0.	brown	brown	18.7
i-C_4H_9	2	$P2_1/a$	4	0.	red-brown	redder-brown	24.1
n-C_8H_{17}	1	P1	4	0.	red-brown	redder-brown	17.3
$CH_2\varphi1$ [d]	4	$P2_1/n$	4	26.44	green	pale green	15.7
$CH_2\varphi2$							16.0
$CH_2CH_2\varphi$	4	12/a	4	29.6	tan	black	14.2

[a] This is one crystal (designated as H(1.2,3)). The unit cell has three independent parts designated H1, H2 and H3, which give two independent molecules, H1 associated with a copper atom located at a center of symmetry, and H2 and H3 associated with a copper atom in a general position. [b] This is the five-coordinate dimer form of $R=CH_3$. The two molecules of the dimer are related by a center of symmetry. ach molecule is composed of two independent parts (the ligands), hence $CH_3(5)1$ and $CH_3(5)2$ with $CH_3(5)2$ corresponding to the higher numbered atoms. [c] This is the four-coordinate form of $R=CH_3$. [d] One crystal of $R=CH_2\varphi$ with one independent molecule in the unit cell. Each molecule is composed of two independent parts (the two ligands), hence the 1 and 2, where the 2 corresponds to the higher numbered atoms. [e] The « twist » is defined as the dihedral angle between the plane defined by the atoms N1, O1 and Cu and the plane defined by the atoms N2, O2 and Cu.

Table XIII. Distances [a] of atoms out of the benzene ring least squares plane.

	H1	H2	H3	$CH_3(5)1$	$CH_3(5)2$	$CH_3(4)$	i-C_4H_9	n-C_8H_{17}	$CH_2\varphi1$	$CH_2\varphi2$	$CH_2CH_2\varphi$
C1 [b]	.011 Å	.001	—.005	—.024	—.006	—.011	—.010	—.020	—.009	.002	—.019
C2	.003	—.002	.006	.032	.010	.017	.020	.036	.019	.005	.028
C3	—.007	.001	—.002	—.012	—.003	—.010	—.014	—.022	—.015	—.008	—.015
C4	.008	.000	—.003	—.015	—.008	—.004	—.004	—.009	.001	.005	—.009
C5	.001	.001	.004	.023	.012	.010	.015	.026	.009	.002	.018
C6		—.001	.000	—.003	—.005	—.003	—.008	—.010	—.005	—.006	—.004
C7	.062	.023	—.050	—.208	—.076	—.123	—.141	—.177	—.057	.034	—.143
C8	.025	—.093	—.115	—.718	—.451	—.633	—.781	—.888	—.380	—.314	—.573
C9				—.393	.059	—.072	.000	—.050	.097	.378	—.213
O1	—.021	—.010	.034	.093	.022	.024	.042	.139	.037	—.003	.049
N1	.173	.153	—.033	.017	.026	.172	.251	.244	.173	.366	.048
Cu [c]	.239	.368	.109	.966	1.026	.955	1.119	1.332	.777	.899	.608
Step Angles, given in degrees											
	13.3	4.8		41.1	41.1	38.9	43.4	54.5	30.3	33.9	24.7

[a] All distances given in Å. The direction of the Cu atom out of the plane defined to be positive. [b] Atoms defining the benzene ring are in brackets. [c] This is the « step » distance, the distance the Cu atom is out of benzene ring plane.

Table XIV. « Step » and « Twist » values for the n-substituted salicylaldimine copper(II) complexes.

R	Ref.	$(N\text{-}R\ sim)_2Cu^{II}$ [a] « step » Å	« twist » (°)	$(hap\ R\text{-}imine)_2Cu^{II}$ [b] « step » Å	« twist » (°)
H	13	.15	0.	.239 [c]	5.2 [c]
$CH_3(4)$	14	— [d]	0.	.955	0.
$CH_3(5)$	1	.12	12.	.996 [c]	11.0
α-form C_2H_5	15	.12 [c]	9.4 [c]		
β-form C_2H_5	16, 17	.27	35.6		
n-C_3H_7	18	.13	0.	1.119	0.
i-C_3H_7	19	.17 [e]	59.7		
n-C_4H_9	20	.37	0.	1.332	0.
i-C_4H_9					
	21	.34 [c]	53.6	.838 [c]	26.4
n-C_8H_{17}				.608	29.6
φ	22	.45	0.		
$CH_2\varphi$					
$CH_2CH_2\varphi$					

[a] N-substituted bis(salicylaldiminato)Cu^{II}. [b] Imine-substituted bis(*o*-hydroxyacetophenone iminato)Cu^{II}. [c] Average value. [d] Only reported as being isomorphous with the Ni analog. [e] Atom C7 included as part of benezne ring least squares plane.

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(15) G.R. Clark, D. Hall, and T.N. Waters, *J. Chem. Soc., A*, 2808 (1969).

(16) C. Panattoni, G. Bombieri, and R. Graziani, *Acta Cryst.*, *23*, 537 (1967).

(17) E.N. Baker, G.R. Clark, D. Hall, and T.N. Waters, *J. Chem. Soc., A*, 251 (1967).

(18) G. Bombieri, C. Panattoni, E. Forsellini, and R. Graziani, *Acta Cryst.*, *B25*, 1208 (1969).

Table XV. Nonbonding Distances (Å) in the Region about C8(C28).

Sum of van der Waals Radii		H1	H2	H3	$CH_3(5)1$	$CH_3(5)2$	$CH_3(4)$	$i\text{-}C_4H_9$	$n\text{-}C_8H_{17}$	$CH_2\varphi1$	$CH_2\varphi2$	$CH_2CH_2\varphi$
4.0 [a]	C8-C9				2.796(8)	2.770(7)	2.784(7)	2.844	2.904(4)	2.807(6)	2.835(6)	2.856(4)
3.5	C8-N1	2.407	2.419	2.420	2.450(7)	2.429(6)	2.429(6)	2.467	2.457(3)	2.443(5)	2.447(5)	2.460(4)
3.2	C8-H6	2.417	2.493	2.524	2.43 (3)	2.47 (3)	2.55 (3)	2.574	2.64 (3)	2.47 (3)	2.50 (3)	2.49 (3)
3.4	C9-O2 [b]				2.929(6)	2.818(6)	2.858(5)	2.956	2.999(4)	2.917(4)	2.912(4)	2.912(4)
2.9	N1-O2 [b]	2.659	2.706	2.674	2.822(4)	2.727(4)	2.764(3)	2.795	2.812(3)	2.775(3)	2.790(3)	2.786(3)

[a] Values for the radii are taken from Pauling[23]. The radii are C8(methyl group) = 2.0 Å, C9(methylene) = 2.0 Å, N = 1.5 Å, O = 1.40 Å and H = 1.2 A. [b] Interligand distances.

Table XVI. Molecular skeleton bond distance in Å.

	H1	H2	H3	$CH_3(4)$	$i\text{-}C_4H_9$	$n\text{-}C_8H_{17}$
Cu-O	1.876(2)	1.894(2)	1.898(2)	1.873(2)	1.891(2)	1.906(2)
Cu-N	1.922(3)	1.926(3)	1.917(3)	1.990(2)	2.003(2)	1.982(2)
N-C7	1.281(4)	1.284(4)	1.289(4)	1.282(4	1.294(3)	1.291(3)
C7-C1	1.456(5)	1.449(5)	1.453(5)	1.473(4)	1.465(4)	1.470(3)
C7-C8	1.515(8)	1.512(7)	1.506(7)	1.498(6)	1.514(4)	1.508(3)
C1-C2	1.422(6)	1.418(6)	1.419(6)	1.408(4)	1.419(4)	1.427(4)
C2-C3	1.416(5)	1.409(5)	1.421(5)	1.416(5)	1.416(4)	1.398(3)
C3-C4	1.363(5)	1.365(5)	1.368(5)	1.360(6)	1.375(4)	1.369(5)
C4-C5	1.390(6)	1.386(7)	1.393(7)	1.362(5)	1.376(4)	1.377(5)
C5-C6	1.369(5)	1.360(6)	1.361(6)	1.366(6)	1.368(4)	1.363(4)
C6-C1	1.409(5)	1.406(4)	1.415(5)	1.408(5)	1.412(4)	1.404(4)
C2-O	1.310(4)	1.311(3)	1.314(4)	1.314(4)	1.313(3)	1.321(3)
N-C9				1.471(5)	1.482(3)	1.475(3)
O-N	2.715(4)	2.706(4)	2.728(4)	2.702(3)	2.714(3)	2.687(3)

	$CH_2\varphi1$	$CH_2\varphi2$	$CH_2CH_2\varphi$	$CH_3(5)1$	$CH_3(5)2$	Range	Weighted Mean
Cu-O	1.886(2)	1.884(2)	1.865(2)	1.890(3)	1.920(2)	.055 (.033)	1.889 1.886 [a]
Cu-N	1.977(2)	1.990(2)	1.977(2)	1.973(3)	1.985(3)	.086 (.030)	1.975 1.986 [b]
N-C7	1.305(3)	1.298(3)	1.295(3)	1.296(4)	1.294(4)	.024	1.293
C7-C1	1.457(4)	1.465(4)	1.453(4)	1.452(5)	1.457(5)	.024	1.461
C7-C8	1.513(6)	1.511(5)	1.522(4)	1.505(8)	1.511(7)	.024	1.511
C1-C2	1.408(4)	1.415(4)	1.409(3)	1.404(6)	1.409(5)	.023	1.414
C2-C3	1.402(5)	1.402(4)	1.403(4)	1.415(6)	1.388(5)	.033	1.406
C3-C4	1.370(5)	1.366(5)	1.353(5)	1.368(6)	1.381(5)	.028	1.368
C4-C5	1.362(5)	1.369(5)	1.352(5)	1.370(8)	1.370(7)	.041	1.371
C5-C6	1.354(5)	1.359(5)	1.365(5)	1.349(7)	1.350(7)	.020	1.362
C6-C1	1.407(4)	1.408(4)	1.392(4)	1.420(5)	1.420(5)	.028	1.408
C2-O	1.321(3)	1.313(3)	1.315(3)	1.317(4)	1.355(4)	.025	1.316
N-C9	1.492(4)	1.469(4)	1.516(4)	1.472(6)	1.464(6)	.052	1.482
O-N	2.771(3)	2.753(3)	2.754(3)	2.691(4)	2.726(4)	.084	2.725
Cu-O2′				2.378(2) [c]			

[a] with the $CH_3(5)2$ Cu-O2 distance deleted. [b] with the R=H1, H2 and H3 distances deleted. [c] the 5-coordinate link that forms the dimer.

"step" values for these two similar types of Cu^{II} complexes is given in Table XIV. The bis difference between the ligands comprising these two types of complexes is given in Table XIV. The big difference acetophenone imine ligand has an additional methyl group (C8, C28). Assuming that this extra methyl group adds appreciably to the intramolecular force or strain that gives rise to large values of the "step", the nonbonding distances between acurately located atoms in the region about the methyl groups (C8, C28) were examined. As shown in Table XV each nonbonding distance is significantly less than the sum of the van der Waals radii. It can be seen that in all cases the nonbonding distances increase when the value for the "step" is greater than 1.0 Å.

There seems to be no simple relationship between the imine substituent group, R, and either the "twist" or the "step". Likewise the "twist" has no simple relationship to the "step". Crystal packing forces and intramolecular forces which vary with the different substituted imine R groups are difficult to assess.

Bond distances within that part of the molecule that is similar for all complexes, the molecular skeleton, are tabulated in Table XVI. The range of values

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(19) P.L. Orioli and L. Sacconi, *J.A.C.S.*, *88*, 277 (1966).

(20) D. Hall, R.H. Summer, and T.N. Waters, *J. Chem. Soc.*, *A*, 420 (1969).

(21) T.P. Cheeseman, D. Hall, and T.N. Waters, *J. Chem. Soc.*, *A*, 685 (1966).

(22) L. Wei, R.M. Stogsdill, and E.C. Lingafelter, *Acta Cryst.*, *17*, 1058 (1964).

(23) L. Pauling, *The Nature of the Chemical Bond*, Cornell University Press; Ithaca, New York, 3rd Edition, p. 260.

Table XVII. Bond angles in main skeleton.

	H1	H2	H3	CH$_3$(4)	i-C$_4$H$_9$	n-C$_8$H$_{17}$
O-Cu-N	91.3(1)	90.2(1)	91.3(1)	88.70(9)	88.30(20)	87.40(7)
Cu-O-C2	128.5(2)	128.0(2)	127.9(2)	121.1(2)	118.4(2)	114.8(2)
Cu-N-C7	130.8(2)	131.4(3)	131.3(3)	125.2(3)	123.4(2)	122.0(2)
O-C2-C1	124.9(3)	124.6(3)	125.4(3)	123.6(3)	123.2(2)	122.8(2)
O-C2-C3	117.1(3)	118.0(3)	117.1(3)	118.7(3)	118.9(2)	119.5(2)
C3-C2-C1	118.0(3)	117.5(3)	117.6(3)	117.7(3)	117.8(2)	117.7(3)
C2-C3-C4	122.4(4)	122.1(4)	122.3(4)	121.7(3)	121.1(2)	122.1(3)
C3-C4-C5	119.5(4)	120.2(4)	120.0(4)	120.5(4)	120.9(2)	119.9(3)
C4-C5-C6	120.0(4)	119.5(4)	119.1(4)	120.0(4)	119.4(2)	119.8(3)
C5-C6-C1	122.2(4)	122.2(4)	123.0(4)	121.7(4)	121.9(2)	122.1(3)
C2-C1-C6	117.9(3)	118.6(3)	118.0(3)	118.4(3)	118.5(2)	118.0(2)
C2-C1-C7	121.8(3)	122.4(3)	122.5(3)	121.6(3)	121.0(2)	120.8(3)
C6-C1-C7	120.3(3)	119.0(3)	119.6(3)	119.9(3)	120.2(2)	121.1(2)
N-C7-C1	121.9(3)	121.3(3)	121.4(3)	120.8(3)	121.0(2)	119.9(2)
N-C7-C8	118.4(3)	118.9(3)	118.8(3)	121.5(3)	122.7(2)	122.6(2)
C1-C7-C8	119.7(3)	119.9(3)	119.8(3)	117.7(3)	116.2(2)	117.5(2)
C7-N-C9				119.1(3)	119.5(2)	122.7(2)
Cu-N-C9				115.7(2)	116.9(2)	115.3(2)
O1-Cu-N2				91.30(9)	91.60(20)	92.60(7)

	CH$_2\varphi$1	CH$_2\varphi$2	CH$_2$CH$_2\varphi$	CH$_3$(5)1	CH$_3$(5)2	Range	Ave.
O-Cu-N	91.65(9)	90.53(9)	91.54(8)	88.26(12)	88.51(1)	4.25	89.79
Cu-O-C2	122.8(2)	122.3(2)	125.4(2)	120.8(3)	119.2(2)	13.7	122.7
Cu-N-C7	125.1(2)	126.2(2)	126.0(2)	123.9(3)	124.4(3)	9.4	126.3
O-C2-C1	124.6(3)	124.2(3)	124.5(2)	123.3(3)	123.0(3)	2.1	124.0
O-C2-C3	117.1(3)	117.7(3)	116.6(2)	117.2(4)	117.5(3)	2.4	117.8
C3-C2-C1	118.4(3)	118.2(2)	118.8(2)	119.5(3)	119.5(3)	2.0	118.2
C2-C3-C4	121.9(3)	122.1(3)	121.1(3)	120.8(4)	121.7(4)	1.3	121.8
C3-C4-C5	120.1(4)	120.2(4)	120.7(3)	119.8(5)	119.2(4)	1.7	120.1
C4-C5-C6	119.1(3)	119.3(3)	119.6(3)	120.7(4)	120.5(4)	1.6	119.7
C5-C6-C1	123.7(3)	123.1(3)	122.7(3)	122.4(5)	122.4(4)	1.6	122.5
C2-C1-C6	116.7(3)	117.2(3)	116.9(2)	116.6(4)	116.7(4)	2.0	117.6
C2-C1-C7	123.4(2)	122.8(2)	122.8(2)	122.4(3)	123.0(3)	2.0	122.2
C6-C1-C7	119.8(3)	120.0(3)	120.2(2)	120.7(4)	120.3(4)	2.1	120.1
	121.9(2)	121.1(2)	122.2(2)	120.7(4)	121.3(4)	1.3	121.2
N-C7-C8	120.1(3)	121.0(3)	121.4(2)	121.9(4)	119.8(4)	4.3	120.6
C1-C7-C8	118.1(3)	117.9(3)	116.4(2)	117.4(3)	119.0(3)	3.7	118.1
C7-N-C9	119.9(2)	121.1(2)	120.4(2)	118.5(4)	119.6(4)	4.2	120.1
Cu-N-C9	114.8(2)	112.7(2)	113.6(2)	117.5(3)	115.6(3)	4.8	115.3
O1-Cu-N2	92.04(9)	91.88(9)	92.16(8)	89.41(12)	92.90(11)	7.5	91.74
			N-Cu-O2′	94.2(1)			
			N2-Cu-O2′	95.6(1)			
			O1-Cu-O2′	104.1(1)			
			O2-Cu-O2′	81.5(1)			

in bond distances for the coordination polyhedra is 1.865 to 1.920 Å for Cu-O bonds and 1.917 to 2.003 Å for Cu-N bonds. The Cu-O2 distance for CH$_3$(5) is long at 1.920 Å but this is the oxygen atom that gives dimer formation. By participating as the fifth coordinating ligand atom in another molecule, the Cu-O2 bond is weakened, as is the O2-C22 bond, which will be discussed later. The distance of this oxygen atom of one molecule to the copper atom of the other molecule is 2.378(2) Å. The shorter Cu-N distances for H(1,2,3) are similar to those found for the corresponding Ni^{II} and Cu^{II} unsubstituted salicylaldimines and have been previously discussed[2] as being "normal" for an unsubstituted imine. Omitting the Cu-O distance for CH$_3$(5) and the Cu-N distances for H(1,2,3) for the reasons discussed above, the range of the remaining values is .041 Å (approximately 20 sigma) for the Cu-O bond distances and .030 Å (approximately 10 sigma) for the Cu-N bond distances. Hence there are significant variations in the bond lengths in the coordination polyhedra. However, there is no simple correlation between Cu-O or Cu-N bond distances with either "step", "twist", or imine substituent (other than H(1,2,3)). Other series of complexes, for example the salicylaldimines,[24] show a similar range of values for the bond lengths in the coordination polyhedron, and we conclude that this is a normal range.

A comparison of the bond distance for each bond type other than Cu-O and Cu-N for each molecule in the series with respect to the weighted average for that bond type shows reasonable values and no unusual trends despite the variations in "step" and "twist" for each molecule. There are only two individual bond distances that differ from the weighted mean bond length by more than four standard deviations (delta/sigma>4). The first exception is the C22-O2 bond distance in CH$_3$(5) ,delta/sigma = 10), but this is the oxygen atom that participates in the five-coordination. The other exception is the N-C9 bond distance for CH$_2$CH$_2\Phi$ (delta/sigma = 8.5). There is no apparent explanation for this latter case.

(24) E.C. Lingafelter and R.L. Braun, *J.A.C.S.*, *88*, 2951 (1966).

The C1-C7 bond distances for these *o*-hydroxyacetophenone imine Cu^{II} complexes are generally longer than those found in salicylaldimine complexes.[24] An analysis of the angles in the system C2-C6-C1-C7-C9-N shows (Table XII) that the "p_z" orbitals on C1 and C7 are rotated out of alignment by up to 24.1 degrees. There is no correlation between the rotation and the bond length, contrary to the suggestion of Ghilardi and Lingafelter,[3] but the rotation increases linearly as the "step" increases.

The C-C bonds in the benzene ring of the molecular skeleton fall into two groups, as is found in salicylaldimine complexes.[24] The three C-C bonds nearest to the metal atom are longer than the three farthest C-C bonds. Figure 2 compares the experimental and theoretical bond length values and shows that they agree satisfactorily except for the previously noted C1-C7 distances.

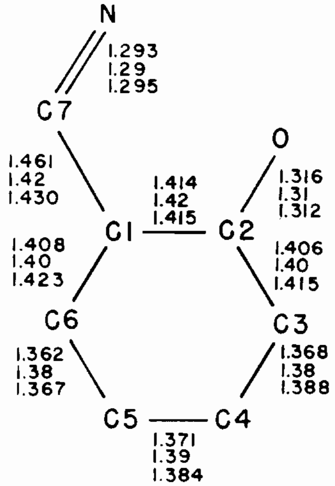

Figure 2. Bond distances in the molecular Skeleton. Upper values are weighted mean values found for the *o*-hydroxyacetophenone imine complexes. The middle values are theoretical values calculated by the simple Hückel M.O. method.[24] The lower values are the mean experimental values found for the comparable salicylaldimine complexes.

An analysis of the bond angles in the molecular skeleton shows a normal range of bond angle values for each type of bond angle except for those in the coordination polyhedra. Table XVII shows that the Cu-O-C2 bond angle has the largest range of values (114.8° to 128.4°, approximately 70 sigma) for a bond type in this series. Figure 3 shows however, that there is a correlation between the Cu-O-C2 bond angle and the "step". As the copper atom "steps" out of the plane, the Cu-O-C2 angle decreases. In Figure 3 the dotted line shows a theoretical curve calculated to show for a simple model the relationship between the "step" and the Cu-O-C2 angle. The model assumes the O, C7, and N atoms to be held fixed to a rigid benzene ring. All bond lengths are held constant and the variation in the bond angle Cu-O-C2 is calculated as a function of the distance the copper atom is out of the plane defined by the benzene ring. The calculated curve does not present the experimental points, but does show that the relationship between the Cu-O-C2 bond angle and "step" is curved and not linear. There is no simple relationship between the Cu-O-C2 bond angle and "twist".

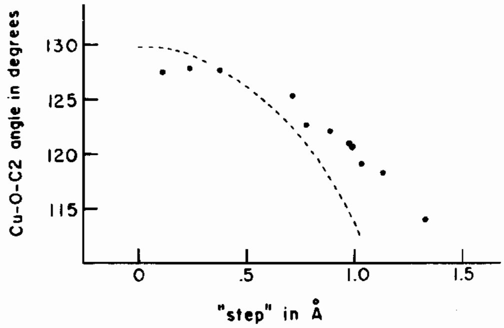

Figure 3. Plot of the Cu-O-C2 bond angle value *vs.* the « step », the distance the Cu Atom is out of the benzene ring plane. A simple rigid model calculation for this relationship is given by the dotted line.)

The Cu-N-C7 bond angle shows the second largest range of values (122.0° to 131.4°, approximately 30 sigma) for a given type of bond in the molecular skeleton of this series. This bond angle also decreases as the "step" increases, but with a linear rather than the curved relationship that is shown in Figure 3. The more linear relationship may be deceiving however, since throughout this series of complexes there is a range of values for (1) the amounts by which C7 and N atoms (as well as the Cu atom) are out of the plane defined by the benzene ring, (2) the rotation about the C1-C7 bond, and (3) the "twist".

It was previously noted that the O-N "bite" increases as the "twist" increases. It would be expected that as the bite increases the O1-Cu-N1 angle would

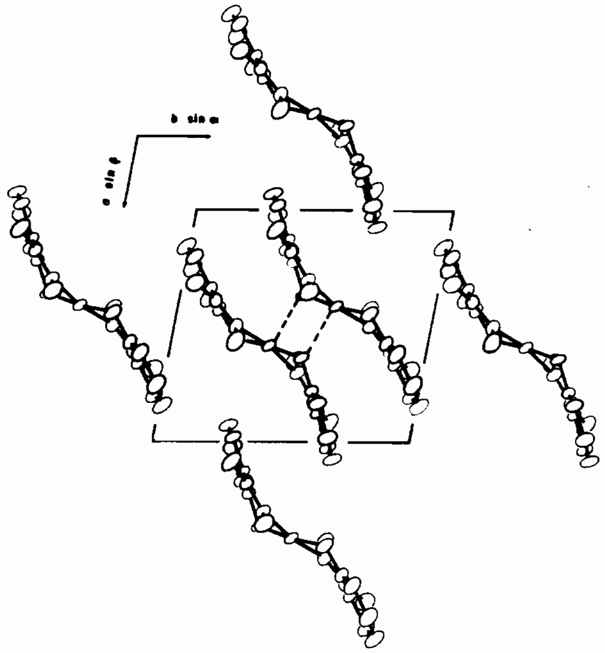

Figure 4. Packing diagram of the five-coordinate form of bis(o-hydroxiacetophenone methyliminato)Cu^{II}, CH_3(5). The dotted lines show the dimer linkage. View is down the *c* axis.

increase, and this relationship holds. The "bite" distances for H(1,2,3) are smaller since the Cu-N bond distances tend to be shorter for the unsubstituted complex.

Table XVIII. R Group bond distances (Å) and angles (de-grees).

$R = n\text{-}C_8H_{17}$

C9-C10	1.518(6)	C11-H112	.99(2)	N1-C9-C10	109.6(2)	C11-C12-H121	111(2)
C10-C11	1.514(4)	C12-H121	1.01(3)	C9-C10-C11	113.6(3)	-H122	109(2)
C11-C12	1.520(6)	C12-H122	1.01(2)	C10-C11-C12	112.4(3)	C12-C13-H131	110(2)
C12-C13	1.512(4)	C13-H131	1.03(3)	C11-C12-C13	114.0(3)	-H132	109(2)
C13-C14	1.513(7)	C13-H132	1.04(3)	C12-C13-C14	113.8(3)	C13-C14-H141	108(2)
C14-C15	1.503(5)	C14-H141	1.07(3)	C13-C14-C15	114.6(3)	-H142	105(2)
C15-C16	1.510(7)	C14-H142	.95(3)	C14-C15-C16	113.5(3)	C14-C15-H151	108[a]
C9-H91	1.09(3)	C15-H151	1.09[a]	N1-C9-H91	107(1)	-H152	108
C9-H92	.91(2)	C15-H152	1.08	-H92	112(2)	C15-C16-H161	114
C10-H101	.90(3)	C16-H161	1.07	C9-C10-H101	111(2)	-H162	108
C10-H102	1.02(2)	C16-H162	1.12	-H102	108(2)	-H163	111
C11-H111	1.03(3)	C16-H163	1.06	C10-C11-H111	109(1)		
				-H112	110(1)		

$R = CH_2\varphi$

		b			b
C9-C10	1.505(4)	1.503(4)	N1-C9-C10	113.1(3)	113.2(3)
C10-C11	1.377(4)	1.364(5)	C9-C10-C11	121.6(3)	119.7(3)
C10-C15	1.389(4)	1.381(4)	C9-C10-C15	120.9(3)	123.6(3)
C11-C12	1.376(5)	1.371(6)	C10-C11-C12	122.0(3)	122.0(4)
C12-C13	1.368(6)	1.367(6)	C11-C12-C13	119.8(3)	120.4(4)
C13-C14	1.373(6)	1.355(6)	C12-C13-C14	119.4(4)	118.4(4)
C14-C15	1.373(5)	1.367(6)	C13-C14-C15	120.7(4)	121.2(4)
			C14-C15-C10	120.7(4)	121.3(3)
C9-H91	.95(2)	1.01(3)	N1-C9-H91	104(2)	113(2)
C9-H92	.96(3)	.94(2)	N1-C9-H92	112(2)	109(2)
C11-H11	.95(3)	.77(3)	C10-C11-H11	117(1)	122(2)
C12-H12	.89(3)	.93(3)	C11-C12-H12	124(2)	121(2)
C13-H13	.97(3)	.92(3)	C12-C13-H13	120(2)	118(2)
C14-H14	.91(3)	.88(3)	C13-C14-H14	120(2)	115(2)
C14-H15	.92(3)	.93(3)	C14-C15-H15	124(2)	121(2)

[a] No standard deviation means the hydrogen atom position was not refined. [b] These are values for the second half of the asymmetric unit for this column.

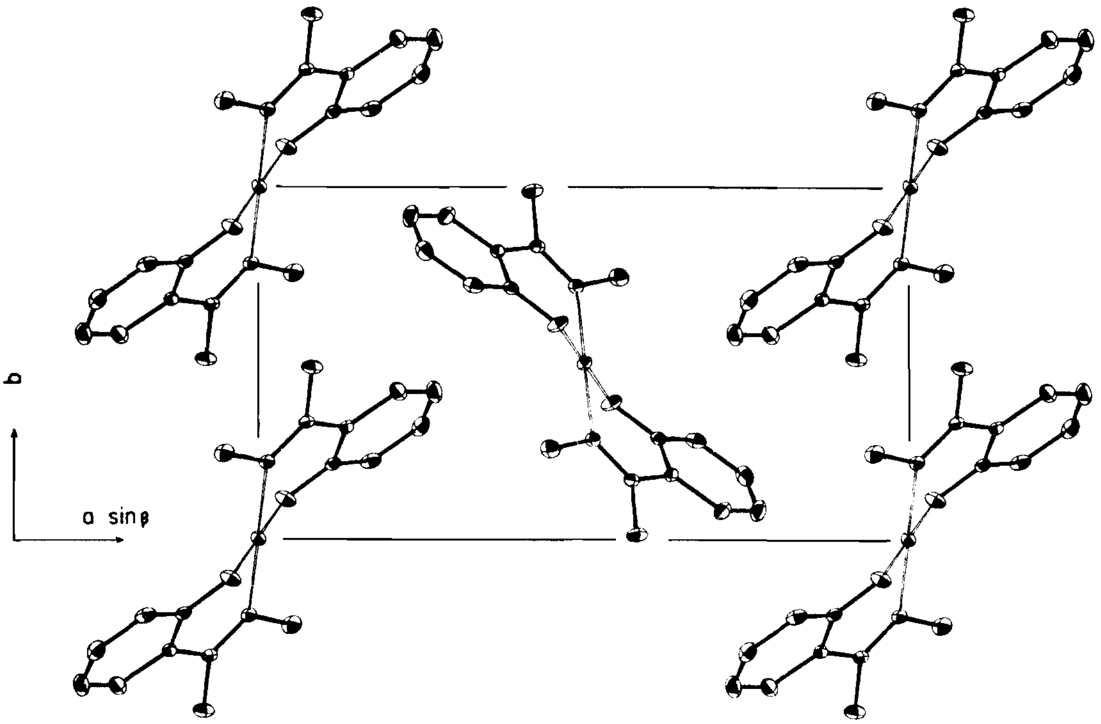

Figure 5. Packing diagram of the four-coordinate form of bis (o-hydroxyacetophenone methyliminato)Cu^{II}), $CH_3(4)$. View is down the c axis. The copper atom of the molecule in the center of the figure is at (1/2, 1/2, 1/2).

The other angles where there is a moderate range of bond angle values (four to five degrees, which is approximately 13 sigma) involve the C7-C8 bond and the N-C9 bond. This is the region where the different substituent groups, R, are attached to the imine and where various amounts of "step" and "rotation" are present. More importantly, this is also the region that suffers most from close intramolecular contacts. Considering this, the range of values is not surprising, but there are no simple correlations to be found among these factors. All other remaining bond angles of the molecular skeleton show a range of values (1.3 to 2.4 degrees, which is approximately three sigma) that may be considered to be a normal distribution about a given mean bond angle value.

Bond angles and distances for atoms not in the molecular skeleton and for the hydrogen atoms, are presented in Tables XVIII and XIX.

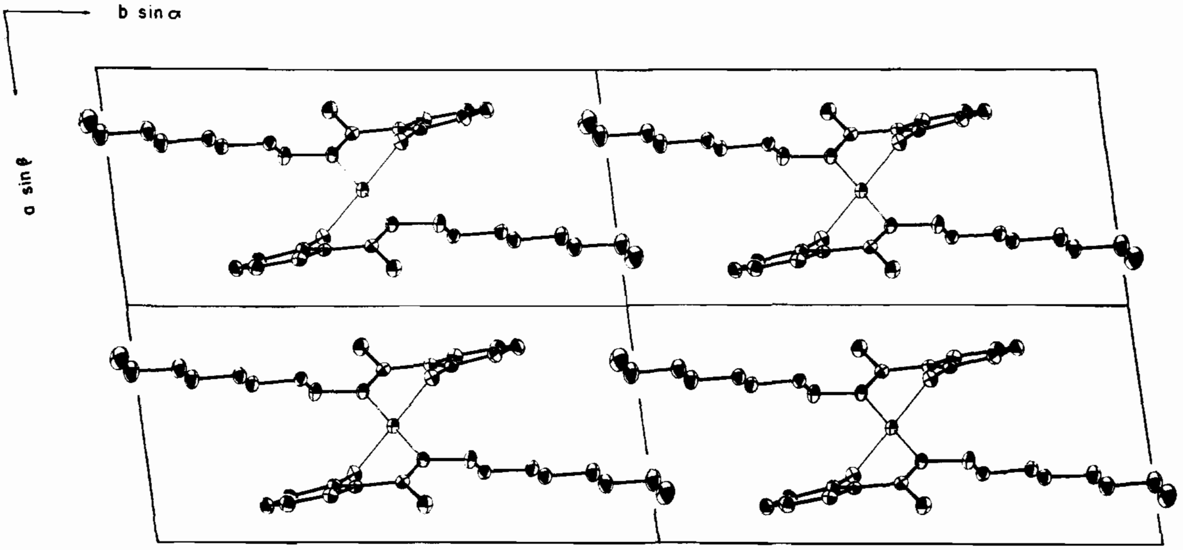

Figure 6. Packing diagram for bis(*o*-hydroxyacetophenone n-octyliminato)Cu^{II}, n-C_8H_{17}. View is down the *c* axis.

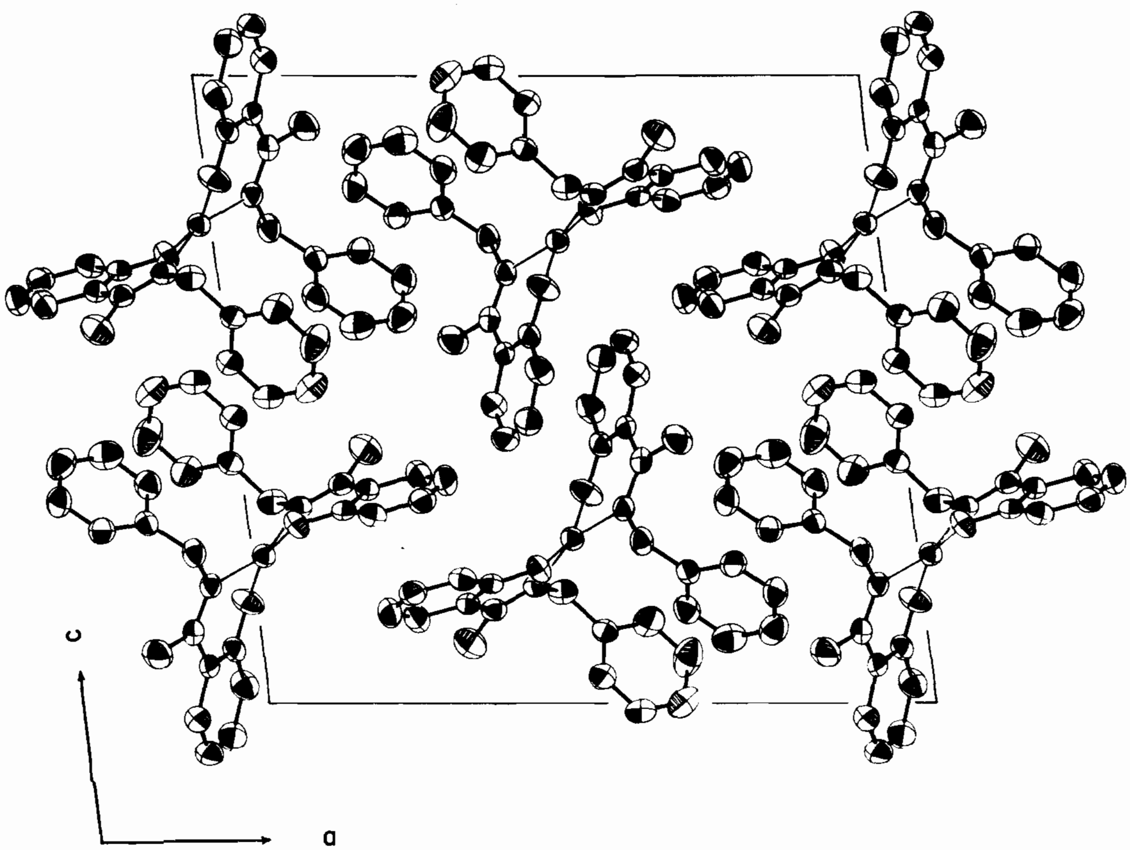

Figure 7. Packing diagram for bis(*o*-hydroxyacetophenone benzyliminato)Cu^{II}, $CH_2φ$. View is down the *b* axis.

Table XIX. Bond distances and angles involving hydrogen atoms in main skeleton.

	$CH_3(4)$	$CH_3(5)1$	$CH_3(5)2$	$n\text{-}C_8H_{17}$	$CH_2\varphi 1$	$CH_2\varphi 2$	$CH_2CH_2\varphi$
C3-H3	.84(3)	.99(4)	.93(3)	.92(3)	.90(3)	.90(2)	.92(3)
C4-H4	.84(3)	.97(4)	1.02(4)	1.00(3)	.89(3)	.97(3)	.83(3)
C5-H5	.94(3)	.80(4)	.86(4)	1.00(3)	.89(3)	.96(3)	.78(4)
C6-H6	.91(3)	.93(3)	.99(4)	.95(3)	.92(3)	.88(3)	.93(3)
C8-H81	.85(5)	.88(4)	.88(6)	1.08	.92(4)	.95(4)	.87(4)
C8-H82	.84(4)	.76(5)	1.03(5)	1.09	.86(5)	.85(3)	.99(4)
C8-H83	.94(4)	1.05(6)	.82(4)	1.08	.90(4)	.92(4)	1.00(4)
C9-H92	.79(3)	1.00(6)	1.00(4)				
C9-H93	.95(3)	1.09(5)	1.00				
C9-H91	.93(4)	1.00	.98(6)				
C2-C3-H3	116(2)	119(2)	122(2)	115(2)	118(2)	116(2)	120(2)
C3-C4-H4	112(2)	113(2)	117(2)	119(2)	116(2)	116(2)	119(2)
C4-C5-H5	117(2)	117(3)	120(3)	120(2)	120(2)	118(2)	122(3)
C5-C6-H6	121(2)	126(2)	124(2)	120(2)	121(2)	121(2)	119(2)
C7-C8-H81	110(4)	115(3)	109(3)	119	109(2)	112(2)	111(2)
C7-C8-H82	116(2)	107(3)	115(3)	118	113(3)	110(2)	109(2)
C7-C8-H83	108(3)	100(3)	108(3)	108	114(2)	107(2)	105(2)
N1-C9-H91	111(2)	113(3)	117(2)				
N1-C9-H92	109(2)	112(2)	108				
N1-C9-H93	107(2)	106	109(3)				

Values without a standard deviation indicate an atom in a calculated position which was not refined upon.

There are no unusual intramolecular contact distances except in the region around the C8(C28) methyl hydrogen atoms ,as previously discussed. There are also no unusual intermolecular contact distances.

Packing diagrams for $CH_3(5)$, $CH_3(4)$, n-C_8H_{17}, and $CH_2\Phi$ may be seen in Figures 4, 5, 6, and 7, respectively. There is no packing diagram for $CH_2CH_2\Phi$ since there are no clear views along an axis. It has already been noted that $CH_2\Phi$ and $CH_2CH_2\Phi$ are different in that their molecular skeletons have their benzene rings tipped in the same direction, giving an umbrella effect to the molecular skeleton. But, what is even more unusual for these complexes is that their imine substituent groups pack in the same direction with their benzyl and phenyl planes tilted toward one another. In $CH_2CH_2\Phi$, the phenyl rings are related to each other through a two-fold axis through the copper atom. In $CH_2\Phi$ the benzyl rings are almost perpendicular (81.2°) to each other.

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