

# The Crystal Structure of bis-(*N*-phenylsalicylaldiminato)copper(II)

By L. WEI, R. M. STOGSDILL AND E. C. LINGAFELTER

Department of Chemistry, University of Washington, Seattle 5, Washington, U.S.A.

(Received 30 August 1963)

The crystal structure of bis-(*N*-phenylsalicylaldiminato)copper(II),  $[\text{OC}_6\text{H}_4\text{CHNC}_6\text{H}_5]_2\text{Cu}$ , has been determined from three-dimensional X-ray diffraction data,  $h0l$  through  $h5l$ . The cell has dimensions  $a = 12.15$ ,  $b = 7.96$ ,  $c = 11.94$  Å,  $\beta = 111^\circ 44'$ , space group  $P2_1/n$ , and contains two molecules.

The coordination of the copper(II) ion is planar with  $\text{Cu}-\text{O} = 1.88$  Å and  $\text{Cu}-\text{N} = 1.99$  Å. The molecule, although centrosymmetric, is markedly non-planar, the two salicylaldimine groups being parallel but not coplanar, with a separation of 0.89 Å. The phenyl groups are roughly perpendicular to the remainder of the molecule.

## Introduction

The cell dimensions and space group of bis-(*N*-phenylsalicylaldiminato)copper(II),  $[\text{OC}_6\text{H}_4\text{CHNC}_6\text{H}_5]_2\text{Cu}$ , have been reported by von Stackelberg (1947) and a report on a preliminary study of the structure has been given by Block (1958). We have now completed a three-dimensional determination of the crystal structure from X-ray diffraction data.

## Experimental

The Schiff base, *N*-phenylsalicylaldimine, was prepared by the reaction between aniline and salicylaldehyde in ethanol-water solution. To this solution was added the stoichiometric amount of copper(II) acetate and the mixture was refluxed for one hour. The product, separated as a dark brown powder, was recrystallized from ethanol, yielding rhomb-shaped monoclinic plates on  $\{10\bar{1}\}$ , bounded by  $\{110\}$ .

Cell dimensions were determined from rotation, zero-level Weissenberg, and precession photographs, with  $\text{Cu } K\alpha$  radiation ( $\lambda = 1.5418$  Å). Calibration was made by superposition of diffraction patterns of  $\text{NaCl}$  ( $a = 5.6394$  Å) on the films used for measurement. The cell dimensions are:

$$a = 12.145, b = 7.956, c = 11.935 \text{ \AA} \text{ (all } \pm 0.01 \text{ \AA);}$$

$$\beta = 111^\circ 44'.$$

The cell contains two molecules. Density calculated is  $1.412 \text{ g.cm}^{-3}$ , observed  $1.396 \text{ g.cm}^{-3}$ . Systematic absence of  $h0l$  for  $h+l$  odd and of  $0k0$  for  $k$  odd indicate the space group to be  $P2_1/n$ . With appropriate changes of axes, these results agree satisfactorily with those reported by earlier investigators.

Intensities were obtained from a set of integrated equi-inclination Weissenberg photographs,  $h0l$  through  $h5l$ , with  $\text{Cu } K\alpha$  radiation. Camera integration was carried out in one direction only, normal to the rotation axis. Diffraction spots were then scanned

normal to the integration direction with a Moll type densitometer feeding into a Leeds & Northrup amplifier and recorder having a logarithmic slide wire. The areas under the densitometer tracings were measured with a planimeter and used as relative intensities. The range of intensities, 1 to 10,000 was obtained by the use of multiple films and a range of exposure times. The intensities from the several films for a given level were placed on the same scale by comparison of common spots. The several levels were then placed on a common scale by the use of intensities from an integrated  $hk0$  Weissenberg photograph.

Of the 2451 reflections within the limiting sphere, 1682 (68.4%) were examined and intensities measured for 1475. 207 reflections were found to be too weak for measurement.

Lorentz and polarization factors were applied and observed structure factors calculated by data reduction programs for the IBM 709 computer written in this Laboratory. No correction was made for absorption.

The atomic scattering factors used were those of Viervoll & Øgrim (1949) for copper, Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955) for nitrogen and carbon, and McWeeny (1951) for oxygen and hydrogen. No correction was made for anomalous dispersion.

## Structure determination

The presence of two copper atoms in a cell of space group  $P2_1/n$  requires that they be in a twofold set of special positions. They were therefore placed at  $0, 0, 0$  and  $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$  and an electron-density projection on  $(010)$  was calculated with all  $h0l$  phases equal to zero. All of the atoms appeared clearly, although not completely resolved, on this projection and their  $x$  and  $z$  parameters were refined by a series of two-dimensional difference syntheses to  $R_{h0l} = 11.5\%$ .  $R$  is defined throughout as  $\sum ||F_o|| - ||F_c|| / \sum ||F_o||$ , where the summation is over the unique, observed reflections

only. Consideration of the projected bond lengths made possible the estimation of approximate  $y$  coordinates. With these coordinates and an overall isotropic temperature factor, a series of four three-dimensional Fourier syntheses and two difference syntheses reduced  $R$  to 14.9%.

The refinement was continued with the Busing & Levy (1959) full matrix least-squares program. A modified Hughes weighing scheme was used, with  $\nu/w=0$  for unobserved reflections for which  $F_c \leq F_{\min}$ ,  $\nu/w=1$  for unobserved reflections for which  $F_c > F_{\min}$  and for observed reflections with  $F_o \leq 8$ , and  $\nu/w=8/F_o$  for reflections with  $F_o > 8$ . The function minimized was  $\sum w(|F_o| - |F_c|)^2$ . Individual atom anisotropic

temperature factors were used. Two cycles of refinement reduced  $R$  to 8.0%. At this point the hydrogen atoms were introduced in calculated positions and 20 reflections (marked E in Table 3) were omitted from subsequent calculations because of secondary extinction effects. Three cycles of least-squares refinement followed by adjustment of scale factor reduced  $R$  to the final value of 5.8%. During the last cycle no parameter shifted by more than  $0.1\sigma$ .

The final parameters and their estimated standard deviations are given in Tables 1 and 2. Final values of observed and calculated structure factors are given in Table 3.

Table 1. Atomic coordinates and their e.s.d.'s

 $(\times 10^4)$ 

Atom	$x/a$	$\sigma_x$	$y/b$	$\sigma_y$	$z/c$	$\sigma_z$
Cu	0000	0	0000	0	0000	0
O	-0036	3	-0256	4	1550	3
N	1008	3	-2042	5	0211	3
C(1)	0248	5	-3703	8	-1628	5
C(2)	0384	7	-4377	10	-2656	6
C(3)	1368	7	-4139	10	-2871	6
C(4)	2268	7	-3268	10	-2071	6
C(5)	2183	5	-2547	8	-1010	5
C(6)	1170	4	-2775	6	-0819	3
C(7)	1607	4	-2706	6	1257	3
C(8)	1531	4	-1478	7	4662	3
C(9)	2338	4	-2630	8	4576	4
C(10)	2351	4	-2985	8	3457	4
C(11)	1558	3	-2204	6	2393	3
C(12)	0735	3	-1032	6	2482	3
C(13)	0722	4	-0689	7	3646	3
H(1)	-0542		-3901		-1472	
H(2)	-0292		-5147		-3247	
H(3)	1449		-4571		-3677	
H(4)	3080		-3133		-2204	
H(5)	2889		-1832		-0398	
H(7)	2190		-3700		-1284	
H(8)	1513		-1189		5517	
H(9)	2927		-3239		5350	
H(10)	2976		-3847		3382	
H(13)	0103		0159		3744	

Table 2. Thermal parameters and their e.s.d.'s

(All  $\times 10^4$ )

Atom	$\beta_{11}$	$\beta_{22}$	$\beta_{33}$	$\beta_{12}$	$\beta_{13}$	$\beta_{23}$
Cu	66(1)	120(3)	57(1)	13(1)	22(1)	3(1)
O	71(2)	118(10)	43(2)	53(3)	28(2)	20(3)
N	70(5)	101(9)	53(2)	13(3)	27(2)	5(3)
C(1)	138(5)	165(17)	95(4)	-14(6)	62(4)	-42(6)
C(2)	244(10)	174(16)	108(6)	-16(10)	95(6)	-50(7)
C(3)	223(9)	187(18)	115(6)	11(10)	117(7)	-16(8)
C(4)	203(8)	227(17)	145(7)	77(10)	137(7)	63(9)
C(5)	115(5)	213(15)	107(4)	28(6)	74(4)	30(6)
C(6)	105(4)	61(11)	72(3)	32(4)	47(3)	15(4)
C(7)	80(3)	114(12)	71(3)	34(4)	36(3)	21(4)
C(8)	111(4)	162(13)	50(3)	8(5)	31(3)	12(4)
C(9)	94(4)	231(15)	61(3)	29(6)	21(3)	38(5)
C(10)	93(4)	213(15)	74(3)	48(5)	33(3)	39(5)
C(11)	62(3)	132(11)	57(3)	11(4)	25(2)	14(4)
C(12)	64(3)	112(12)	49(2)	1(4)	21(2)	7(4)
C(13)	92(4)	133(12)	59(3)	16(5)	33(3)	3(4)

All hydrogen atoms were given isotropic  $B = 3.50 \text{ \AA}^2$ 

### Discussion

The presence of only two molecules in the cell of space group  $P2_1/n$  requires that the molecule be centrosymmetric. Intramolecular distances and angles are

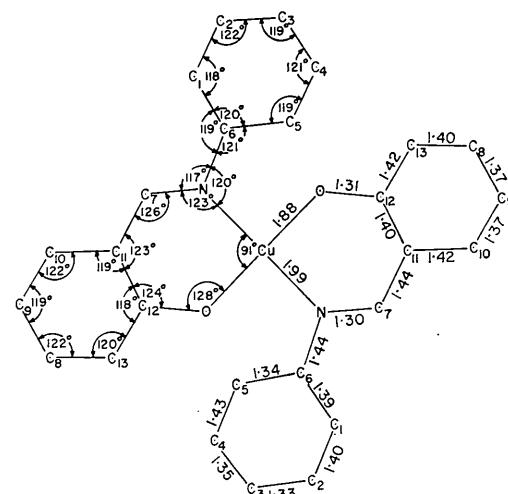


Fig. 1. Bond lengths and angles.

Table 3. Observed and calculated structure factors

The columns are  $h$ ,  $10F_o$  and  $10F_c$ . Unobserved reflections are marked with \*. Reflections omitted because of secondary extinction effects are marked with E.

-15,C,L		14	119	126	5	149	-5	12	135	135	7	7C	-6	11,1,L	4	172	181	C,2,L	S,2,L	-8,3,L								
3	32	31	-1,C,L	7	149	-17	-6,1,L	9	31C	32C	C	174	192	6	344	357	1	652E	SC2	C	115	-113						
7	97	95	E,6	65	61	IC	102	100	1	6C	57	7	221	221	2	125	247	1	225	247	2	34	35					
7	33	30	3	495	487	6	62	-6C	1	4C1	414	111	7	58	50	8	276	266	3	214	263	3	122	132				
6	28	37	5	385	367	3	2	354	4C4	12	110	3	33	29	9	100	-179	4	27C	275	3	46	4C					
-14,0,L	9	595	581	-14,1,L	7	43	6	14	47	45	4	57	57	1C	153	145	5	235	2C5	4	259	17	223	234				
4	83	77	11	282	193	1	62	62	5	216	283	2	1,L	12	126	124	7	250	-2	6	25	5	7	141	135			
6	41	36	12	155	177	3	47	46	7	246	233	C	83CE	1353	6	57	-65	14	93	95	6	144	145	10	200			
8	71	76	0,C,L	4	27	-32	E	58	-56	1	14	20	1	166	1C6	3	17	111	1C7	10,2,L	10	56	52					
IC	51	52	5	55	56	5	96	5	225	240	2	31B	289	2	52	52	-7,2,L	11	25*	11	165	165	11	165	174			
-13,C,L	4	475	448	7	74	17	4C	47	3	45C	473	3	47	42	1	212	224	12	126	126	C	206	205	1	3C0	0		
8	436	439	8	44	-46	12	45	-78	5	275	216	13,1,L	2	234	6	2	250	-17	1	280	19	3	254	-17	-7,3,L			
1	55	55	1C	45	45	9	56	52	13	157	161	6	33	40	3	226	233	12,1,L	4	58	51	5	32	-27	1	155	-144	
3	73	75	12	112	123	1C	149	-2	14	170	-16	7	249	249	C	115	123	4	27	-12	4	155	157	4	234	229		
5	114	126	14	24	36	11	72	74	EC	73	9	77	76	2	4C	37	6	98	-94	1	322E	372	6	76	74			
7	144	132	1,C,L	-13,1,L	-5,1,L	10	224	-23	7	642	642	2	344	346	1	184	-176	5	32	28	1	155	144	3	37	37		
11	117	122	1	476E	782	1	51	56	1	5C	77	12	184	12	5	211	211	4	156	134	C	56	-90	6	324	316		
-12,C,L	3	112	12	2	45	45	2	465	445	13	67	69	C	53	57	1C	87	-87	5	41C	411	C	56	-90	6	324	316	
5	362	318	3	2C0	-5	140	1	6	55	45	4	125	162	3,1,L	12	286	-6	7	344	352	2	27	29	8	234	229		
2	91	92	7	293	270	4	55	55	4	125	162	3,1,L	13	12C	105	6	92	-44	6	116	116	3	28	38	7	255	249	
4	158	166	5	142	-143	9	210	-9	5	17C	-149	1	76	76	2	130	-2	-6,2,L	10	125	125	4	155	157	1	155	157	
6	2C0	196	11	182	170	6	9C	55	6	555	521	C	562E	61C	-15,2,L	12	126	126	10	125	125	4	155	157	1	155	157	
8	237	246	15	115	119	7	5C	-53	7	52	55	1	76	76	2	130	-2	-6,2,L	10	125	125	4	155	157	1	155	157	
1C	1C9	129	2,C,L	1	6	131	128	7	178	185	2	415	448	3	57	54	6	116	116	3	28	38	7	255	249			
-11,C,L	1	376	4C8	1	45	11	56	52	12	167	165	7	41	49	5	49	52	2	437	481	7	67	76	12,2,L	12,2,L			
2	271	26C	12	1C1	1	3	2C9	-3	7	214	-6	7	67	77	4	230	262	2,2,L	C	66	68	-6,3,L	-6,3,L					
3	126	134	6	328	318	-12,1,L	14	1C5	111	9	151	180	-14,2,L	6	43C	483	C	1046E	1486	1	32	32	1	417	460			
5	197	201	6	32C	311	IC	32E	11	1	83	83	-4,1,L	10	12C	126	1	33	28	8	104	104	3	210	5				
6	51	54	12	147	151	2	226	1	11	15	15	11	15	11	15	11	15	11	15	11	15	11	15	11	15	11		
11	110	1C8	3,C,L	4	22	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11		
13	72	85	3,C,L	4	22	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11		
-10,C,L	1	385	42C	6	64	-65	4	57	52	5	11C	293	4,1,L	5	23	17	11	163	175	6	251	242	1	51	1C8	7	41C	406
3	41C	388	7	151	15C	5	247	274	C	152	-165	7	224	-17	14	119	118	8	3C2	295	14,2,L	9	131	133				
2	126	123	5	4C1	368	8	219	-15	6	2C3	-172	1	32C	323	8	64	86	15	34	4C	12C	1C4	10	66	65			
4	120	126	7	4C4	381	9	4C	45	7	274	3C9	2	264	-242	9	31	24	1	32	4C	12C	1C4	10	66	65			
8	131	146	11	96	47	11	27	89	6	2C4	281	4	165	154	-5,2,L	11	12C	112	C	75	87	11	81	87				
1C	2C4	216	15	17	27	15	1C	56	52	5	231	225	-12,2,L	11	12C	112	12,2,L	12	12,2,L	12	12,2,L	12	12,2,L	12				
12	147	151	4,C,L	13	1C7	115	11	74	61	6	151	180	-14,2,L	6	43C	483	C	1046E	1486	1	32	32	-5,3,L	-5,3,L				
14	45	54	C	533	540	-11,1,L	13	12C	126	12	166	166	-14,2,L	10	12C	126	1	33	28	8	104	104	3	210	5			
-9,0,L	2	296	3C1	14	22	11	22	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11		
1	242	247	6	23C	226	2	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12		
3	246	244	10	1C6	1C2	3	41	-31	-3,1,L	11	1C	46	46	9	104	104	7	223	241	4,1,L	62	55	43	4	343	343		
5	172	162	12	27	4C	5	25	25	2	154	-549	5	1,1,L	5	23	7	12C	1C4	8	4C	-33	4	32	12	12	12		
11	196	199	5,C,L	7	42	-37	3	256	-251	1	153	-130	11,1,L	9	40	40	29	15	9	115	115	5	287	277	1	41C	406	
13	111	113	1	385	369	9	229	13	13	141	-131	3	157	131	-11,1,L	11	12C	114	142	5	152	152	1	313	313			
-8,C,L	3	138	-56	10	84	9C	6	431	438	4	175	177	12,2,L	14	51	-46	1C	555	573	1	655	666	11	133	142			
5	265	2C0	11	2C0	21	2	171	-186	5	31	26	1	20*	15	15	35	33	11	12C	13	3	174	174	11	120	120		
2	490	468	7	205	192	5	25	25	27	7	205	-293	2	246	-25	8	224	239	7	255	-54	1	55	56	11	17	19	
4	124	129	13	91	117	1C5	12	15C	12	7	25	25	1	31	60	-54	7	224	239	2	245	251	1	55	56	11	17	19
6	285	285	11	91	87	14	9C	66	1C	114	114	7	27	77	4	55	42	1	31	60	5	250	-19	3	31	31		
8	194	-103	1	321	329	12	11C	-2	11C	11C	11	11	11	11	11	11	11	11	11	11	11	11	11	11	11			
1C	219	231	6,C,L	-1C1	1L	13	1C5	151	12	166	166	12	166	166	-11,1,L	11	12C	113	142	5	152	152	1	333	359			
12	209	211	11,C,L	5	274	274	1	1C5	152	6	152	236	7,1,L	5	128	126	1	356E	72C	3	315	317	11	82	-3,3,L			
-7,C,L	4	231	216	2	12	12	217	217	1	212	212	12,2,L	6	205	224	12	125	-125	1	313	313	1	481	526				
3	314	334	C	387	363	1	54	-42	23C	13	13C	13	13	1	3C	-31	27	3	252	294	3	1352	4C9					
6	165	172	2	125	159	14	67	67	14	5C	47	3	112	-111	11,1,L	11	12C	116	146	7	255	283	1	3C2	-1C5			
10	1C3	1C1	6	216	266	5	152	152	4	172	171	1	100	94	1	3C0	-5	13	1C5	1C4	0	424	435					
14	90	9C	6	65	74	7	2C7	247	5	31	325	C	54	-54	5	125	137	-2,2,L	7	20*	22	1	41C	406				
-5,C,L	9	88	27	-6,1,L	1C	220	17	2	142	-138	7	30*	8	30*	8	17C	227	6	217	214	1	115	111	1	343	387		
1	202	319	1	256	303	1C	14	74	74	1	212	212	1	137	97	7	30*	8	318	318	1	115	111	1	343	387		
3	118	-93	114	125	11	44	-27	5	3C8	275	12,2,L	6	114	114	3	21	21	1	32	27	1	22	22					
5	172	210	5,C,L	97	97	12	123	126	4	464	467	8,1,L	2	193	193	1	214	214	1	32	27	1	22	22				
7	177	175	7	72	76	13</td																						

Table 3 (cont.)

0,3,L	6	255	257	2	68	65	7	26	-24	13	95	1C2	6	74	-75	11,4,L	3	63	66	12	123	115	4,5,L				
	7	2C	22	3	11*	15	6	16C	175	7	171	162	8	19*	28	C 43	-67	5	175	184	C 36	-24					
1	538E	568	8	162	170	4	41	25	9	15*	-2	-2,4,L	5	19*	1C7	1 1C4	114	6	175	184	1	347	357				
2	159	146	5	36	-26	5	12*	12	1C	65	24	1C	6	17*	1C7	1 1C4	114	6	155	156	2	24	26				
3	11	56	10	66	58	6	66	71	11*	28	1	2C5	220	1C	16*	-13	2	16*	5	7	156	154	-2,5,L				
4	55	55	7	11*	21	12	133	135	2	317	334	11	46	55	3	81	84	5	155	155	1	2C4	239				
5	322	295	6,3,L	8	52	48				3	78	-79							9	1C2	51	3	22C	246			
6	125	115								4	274	289							1C	17	16	5	126	116			
7	225	214	C	BC	55	-13,4,L				5	71	67							11	16*	-17	4	65	76			
8	1C3	-114	1	354	4C8		1	315	342	6	328	313	C	363	349	C 1C5	1C3	12	14*	-8	5	315	330				
9	119	127	2	1C5	-57	1	112	1C3	2	54	58	7	67	61	1	6C	-59	1	14*	-2	13	1C7	51				
1C	82	-85	3	115	112	2	14*	2C	3	155	163	8	246	247	6	21	234	2	45	49	7	24C	245				
11	116	118	4	19*		3	64	62	4	14*	-21	9	34	36	3	82	73				8	62	78*				
12	17*	-2C	5	121	135	4	45	45	5	217	211	10	233	243	4	165	186	13,4,L				1C	46	-54			
13	66	69	6	57	58	6	67	66	1C	129	111	38	-20	5	57	37											
7	164	156	7	23	25	7	EC	7C	12	1C7	1C8	6	2C8	210	C	38	-39	1	48	42	1C	27	-34				
1,3,L			8	36	35	9	25	27	5	65	78	-1,4,L		E	65	78	-13,5,L	4	167	166	-1,5,L	C 264	250				
9	35	28				9	35	28	8	55	1C4		9	31	26			5	71	-62	1	96	-5C				
C	5C1	531	1C	22	-18	9	1C8	55	1C	15*	60	66	1	52	48	6	124	127	2	374	352	3	18*	21			
1	339	-333				11	18*	-22	1	497E	620	1C	60	66				3	21	251	5	14	-3				
2	410	419	7,3,L			-12,4,L	12	36	25	2	34	-23						4	121	114	6	114	1C6				
3	3C2	285				3	5C	1C1	3	153	204	5,4,L		2	61	62	4,4	128	117	6	246	251	5	18*	18		
4	179	-154	C	224	222	1	47	42						4	65	62	9	156	-16	5	115	6	114	1C6			
5	36	35	1	14*	-17	2	75	76	-t,6,L		5	155	156	C	152	144	5	130	-4	1C	25	6	312	413			
6	400	386	2	1C5	111	3	65	65		6	113	-105	1	296	286	6	7C	7C	11	1C6	6	8	6C	63			
7	18*	-19	2	112	1C1	4	63	66	1	24	2C	7	242	245	2	16*	7	7	12*	12	77	8	142	13C			
8	123	116	4	82	73	5	17	4	21	45	8	77	76	3	3C	25	8	5C	52	13	9C	9	26	32			
9	114	-108	5	2C*	-13	6	15C	152	3	22	-5	9	215	239	4	62	62			1C	12C	122	6,5,L				
10	104	1C3	6	12C	1C8	7	17	8	4	111	1C9	1C	44	-48	5	137	132	-12,5,L									
11	52	-56	7	68	68	8	116	113	5	1C0	-57	11	95	99	6	2C2	-11			11	46	-47	C 42	-41			
12	79	79	8	66	66	9	47	38	6	167	160	12	16*	-50	9	89	95	3	91	93	2	174	179				
2,3,L			8,3,L			-11,4,L	5	1C7	-166	0,4,L		1C	23	-24	4	16*	2	4	21	-18	1	358	4C6				
						1C	15*	3						5	86	84	5	143	139	2	64	61	6	32	40		
C	74	-75												6	15*	23	5	12	131	C,5,L	3	12	16	4,15*	-2		
1	563	593	C	15*	16	1	65*	1C6	11	71	67	1	245	236	6,4,L	6	15*	-3	6	18*	-6	2	247	267	7	55	62
2	438	-424	1	218	225	2	19	28	12	1C5	1C4	2	45C	492	C	236	255	8	25	27	6	4	184	19C	8	31	40
3	124	127	2	205	2C4	3	51	52	12	1C4	14	3	51	-50	C	236	255	8	25	27	6	4	271	279	6,5,L		
4	14*	-4	3	54	89	4	54	-66	14	75	8C	4	88	89	1	85	-97	9	98	92	5	43	27	6	55	62	
5	446	436	4	2C*	6	5	147	146		5	225	-214	6	216	198	3	60	-94	-11,5,L	1C	165	162	6,5,L				
6	18*	16	5	1C1	95	6	75	76	-5,4,L		6	216	198	3	60	-94			1C	165	162	C 261	293				
7	3C5	310	6	18*	5	7	2C3	2CC	1	127	140	8	192	200	9	19*	14	1	35	4C	12	74	6,5,L				
8	56	-62	7	1C2	1C3	6	41	35	12	1C7	1C6	10	1C7	-26	4	160	157	11	17	51	3	24	22				
9	98	88	8	24	-23	6	4C	32	2	155	156	9	61	71	6	1C3	94	2	112	123	11	17	51	3	24	-22	
1C	36	-35	1C	44	-32	3	2C4	3C2	1C	111	118	7	18*	18	10	2C7	21	-5,5,L									
11	107	1C7	9,3,L	11	43	41	4	15*	5	11	69	78	8	144	148	4	115	112	5	17*	18	1	24C	234			
12	32	-26	C	257	264	6	61	65	5	161	165	12	84	88	5	17*	18	1	24C	234	6	78	81				
3,3,L			1	68	60	-1C,4,L	7	454	444	7	154	154	1,4,L	C	85	-8C	7C	174	11	2C4	-52	1	165	158	8,5,L		
			2	76	77		8	74	65				1	182	152	5	31	19	15	16*	17	3	54	56	8,5,L		
C	6C0	617	2	2C*	11	1	15*	4	5	144	144	1,4,L		2	172	162	6	31	19	15	16*	17	3	54	56	8,5,L	
11	118	111	4	67	63	2	14C	1C6	11	75	76	C	54	89	2	172	162	6	31	19	15	16*	17	3	54	56	
2	340	337	5	34	-29	3	32	32	-24	11	1C7	112	1C	44C	492	3	132	133	11	26	-28	7	88	82	2C1	48	-50
3	180	177	6	66	67	6	66	66	53	12	23	37	2	153	-139	4	19*	15	8	216	213	6,224	1,123	117			
4	366	376	7	13	-16	5	15*	7	13	8C	79	3	372	372	5	164	16C	-1C,5,L	9	15*	-16	1C	67	19*			
5	8C	8C	6	188	177	14	32	35	5	236	-217	6	18*	-11	1C	121	116	5	167	161	6,4	55	56	1,13	146		
6	302	305	1C,3,L	7	65	65			5	261	251	7	127	126	1	132	145	11	124	-122	5	65	58	4	22	-38	
7	62	-68	8	124	115	-t,4,L	6	69	-67	E	46	5C	5	2C	18*	3	121	116				2,5,L	7	93	1CC		
8	154	148	9	86	-56	5	45	-53						7	158	154	8,4,L	5	167	175							
9	88	8C	1	89	84	10	8C	77	1	154	2C1	5	21	-28	11	66	65	6	51	-43	5	145	133	3	17*	-16	
1C	74	69	2	2C*	9	11	21	-24	1C	45	43	2	28	21	7	33	36				1C	167	161	3	125	138	
11	41	39	6	61	54	12	66	65	13	111	125	1C	47	-50	C	271	287	6	8C	7	212	222	C 167	161			
12	94	96	4	17*	-18	4	237	281	11	65	63	1	46	46	7	95	91	2	26	43	2	25	31	1	31	-34	
3	5	48	46			5	74	66	5	14	55	45	6	276	257	C	49	-57	2	126	126	12	15*	-15			
4	2C6	209	9	132	13C	8	61	55	14	55	45	6	276	257	1	15*	-3	11	159	152	1C	16*	-22	1C,5,L			
5	155	159	12,3,L	1C	53	-5C	-3,4,L	8	52	40	2	19*	2	4	97	85	11	15*	154	-15	11	EC	67	C 42	-36		
6	115	115	12,3,L	1C	66	1C8	1C5	2	65	66	11	15*	1	5	7C	11											

Table 4. Bond distances and angles and their e.s.d.'s

Bond	(Å)	(Å)	Angle	(°)	(°)
Cu–O	1.878 (0.003)	O–Cu–N		91.4 (0.2)	
Cu–N	1.993 (0.004)	Cu–O–C(12)		128.0 (0.4)	
O–C(12)	1.313 (0.004)	Cu–N–C(7)		123.4 (0.3)	
N–C(7)	1.302 (0.005)	Cu–N–C(6)		119.6 (0.3)	
N–C(6)	1.438 (0.006)	C(6)–N–C(7)		116.8 (0.5)	
C(1)–C(2)	1.404 (0.010)	N–C(6)–C(1)		118.6 (0.6)	
C(2)–C(3)	1.326 (0.014)	N–C(6)–C(5)		120.9 (0.6)	
C(3)–C(4)	1.347 (0.010)	C(6)–C(1)–C(2)		119.0 (0.8)	
C(4)–C(5)	1.429 (0.010)	C(1)–C(2)–C(3)		121.4 (1.0)	
C(5)–C(6)	1.343 (0.008)	C(2)–C(3)–C(4)		119.3 (1.0)	
C(6)–C(1)	1.389 (0.007)	C(3)–C(4)–C(5)		121.9 (1.0)	
C(7)–C(11)	1.436 (0.006)	C(4)–C(5)–C(6)		117.9 (0.8)	
C(8)–C(9)	1.373 (0.008)	N–C(7)–C(11)		126.1 (0.5)	
C(9)–C(10)	1.371 (0.007)	C(7)–C(11)–C(10)		118.1 (0.5)	
C(10)–C(11)	1.421 (0.005)	C(7)–C(11)–C(12)		122.5 (0.5)	
C(11)–C(12)	1.399 (0.006)	C(10)–C(11)–C(12)		119.4 (0.5)	
C(12)–C(13)	1.422 (0.006)	O–C(12)–C(11)		123.7 (0.5)	
C(13)–C(8)	1.396 (0.006)	O–C(12)–C(13)		118.3 (0.5)	
C(1)–O'	3.164				
C(5)–O'	3.308	C(11)–C(12)–C(13)		118.0 (0.5)	
C(2)–C(13')	3.261	C(8)–C(13)–C(12)		120.3 (0.5)	
C(3)–C(13')	3.619	C(9)–C(8)–C(13)		121.9 (0.6)	
C(4)–C(13')	3.984	C(8)–C(9)–C(10)		118.5 (0.6)	
		C(9)–C(10)–C(11)		122.1 (0.6)	

Table 5. Equations for least-squares planes

Coordination	$-0.0823x - 0.0634y - 0.0424z = 0$
Salicylaldimine No. 1	$-0.0871x - 0.0954y - 0.0140z = 0.0581$
Salicylaldimine No. 2	$-0.0871x - 0.0954y - 0.0140z = -0.0581$
Phenyl No. 1	$-0.0481x + 0.1976y - 0.1188z = -0.4158$
Phenyl No. 2	$-0.0481x + 0.1976y - 0.1188z = 0.4158$

The bond distances and angles within the salicylaldimine group appear to be normal.

The phenyl group shows no significant deviation from planarity (maximum distance of any atom from the least-squares plane, 0.010 Å). The several bond distances and angles in the phenyl group appear to be significantly different, but we are unable to suggest any interpretation of the differences.

The phenyl groups are roughly perpendicular to the remainder of the molecule, making an angle of 82.3° with the coordination group and 64.9° with the salicylaldimine group.

The shortest intermolecular contact distance of each atom is given in Table 6.

Dobler (1962) has recently reported the cell dimensions and space group of the corresponding nickel(II) compound. After making the appropriate transforma-

Table 6. Shortest intermolecular distances

Atom	Distance	Neighbor
C(1)	3.77 Å	C(7) at $-x, -1-y, -z$
C(2)	3.69	C(11) at $-x, -1-y, -z$
C(3)	3.69	C(4) at $\frac{1}{2}-x, -\frac{1}{2}+y, -\frac{1}{2}-z$
	3.69	C(8) at $x, y, -1+z$
C(4)	3.69	C(3) at $\frac{1}{2}-x, \frac{1}{2}+y, -\frac{1}{2}-z$
C(5)	3.33	C(13) at $\frac{1}{2}-x, -\frac{1}{2}+y, \frac{1}{2}-z$
C(6)	3.90	C(13) at $\frac{1}{2}-x, -\frac{1}{2}+y, \frac{1}{2}-z$
C(7)	3.45	C(13) at $\frac{1}{2}-x, -\frac{1}{2}+y, \frac{1}{2}-z$
C(8)	3.60	C(5) at $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$
C(9)	3.60	O at $\frac{1}{2}+x, -\frac{1}{2}-y, \frac{1}{2}+z$
C(10)	3.45	Cu at $\frac{1}{2}+x, -\frac{1}{2}-y, \frac{1}{2}+z$
C(11)	3.69	C(2) at $-x, -1-y, -z$
C(12)	3.80	C(10) at $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$
C(13)	3.33	C(5) at $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$
N	3.82	C(10) at $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$
O	3.60	C(9) at $-\frac{1}{2}+x, -\frac{1}{2}-y, -\frac{1}{2}+z$
Cu	3.45	C(10) at $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$

tion of axes, a comparison of the two cells:

$$\text{Cu: } a=12.15, b=7.96, c=11.94 \text{ Å}, \\ \beta=111^\circ 44', V=1073 \text{ Å}^3,$$

$$\text{Ni: } a=12.64, b=7.63, c=11.81 \text{ Å}, \\ \beta=112^\circ 13', V=1054 \text{ Å}^3,$$

indicates that the two molecules are nearly, but not completely, identical in structure.

This investigation was supported in part by the U.S. Public Health Service under Research Grant GM 10842.

#### References

- BERGHUIS, J., HAANAPPEL, IJ. M., POTTERS, M., LOOPSTRA, B. O., MACGILLAVRY, C. H. & VEENENDAAL, A. L. (1955). *Acta Cryst.* **8**, 478.
- BLOCK, B. P. (1958). Amer. Chem. Soc. Abstracts of Papers, 134th Meeting, p. 35S.
- BUSING, W. R. & LEVY, H. A. (1959). *A Crystallographic Least Squares Refinement Program for the IBM 704*. ORNL Central Files No. 59-4-37. Chem. Div. ORNL, Oak Ridge, Tennessee.
- DOBLER, M. (1962). *Helv. Chim. Acta* **45**, 1628.
- LINGAFELTER, E. C., SIMMONS, G. L., MOROSIN, B., SCHERINGER, C. & FREIBURG, C. (1961). *Acta Cryst.* **14**, 1222.
- MCWEENEY, R. (1951). *Acta Cryst.* **4**, 513.
- STACKELBERG, M. v. (1947). *Z. anorg. Chem.* **253**, 136.
- VIERVOLL, H. & ØGRIM, O. (1949). *Acta Cryst.* **2**, 277.