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Crystal Structure of *N*-Salicylideneglycinatoaquocopper(II) Tetrahydrate

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N-Salicylideneglycinatoaquocopper(II) tetrahydrate, [Cu($C_9H_7NO_3$).(H_2O)].4H_2O, crystallizes in the monoclinic space group $C2/c$, with eight formula units per unit cell, of dimensions, $a = 10.721$, $b = 17.769$, $c = 13.895$ Å, $\beta = 94.71°$. Intensity data were collected on a diffractometer with Mo $K\alpha$ radiation. The molecular structure of the complex is essentially the same as that found by other workers in *N*-salicylideneglycinatoaquocopper(II) hemihydrate. The environment of the copper(II) ion is a square pyramid, with four short and one long coordination bond. The crystal structure of the tetrahydrate is entirely different from that of the hemihydrate; the complexes are not bound together by coordination bonds, but are connected by nine hydrogen bonds to form a three-dimensional network. The bond distances of N–C(3) of the salicylaldimine residue and C(2)–N of the glycine residue are 1·302 Å and 1·461 Å respectively. A comparison on these bonds of the related compounds was also made in relation to the transamination reactions.

Introduction

Kishita, Nakahara & Kubo (1964) prepared complexes from copper(II) ion and *N*-salicylideneglycine at various temperatures. Below 10°C they obtained *N*-salicylideneglycinatoaquocopper(II) tetrahydrate [Cu($C_9H_7NO_3$).(H_2O)] . 4H_2O (SGCT) and above 30°C they obtained the hemihydrate (SGCH). The structures of the complexes were discussed on the basis of the magnetic susceptibility. The value of the magnetic moment obtained, 1·86 Bohr magnetons, suggested that the copper(II) ions were separated from each other so as not to permit appreciable spin interaction between them.

In this laboratory the crystal structure of SGCH was established (Ueki, Ashida, Sasada & Kakudo, 1967) and it was found that the complex had a five-coordinated square pyramid configuration. In the structure the fifth weak coordination bond is formed by the 'free' carboxyl oxygen atom of an adjacent complex. Therefore, the crystal structure of SGCT, especially the hydrogen bonding system of the free crystallization water molecules [water molecules which do not coordinate to the copper(II) ion] and the coordination configuration of the copper(II) ion, were of much interest.

Since this complex is expected to be a catalytic intermediate in the non-enzymatic transamination reactions (Eichhorn & Marchand, 1956: Longenecker & Snell, 1957), the bond distances concerning the nitrogen atom are also of interest.

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Experimental

The crystals of SGCT were supplied by Professor A. Nakahara of this University. They are bright-green needles, with the needle axis along the crystallographic c axis. A crystal with dimensions $0.12 \times 0.07 \times 0.22$ mm was used throughout the experiment. This was mounted with its b axis along the spindle axis. Oscillation and Weissenberg photographs were taken to determine the
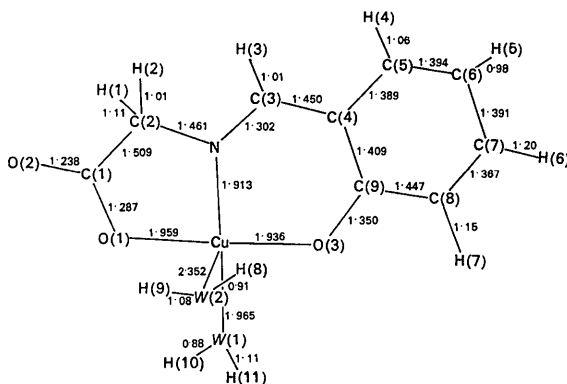

Fig. 1. Bond lengths in the complex, including $W(2)$.

cell dimensions and the space group. The more accurate cell dimensions were obtained with the use of a diffractometer with Mo $K\alpha$ radiation ($\lambda = 0.71069$ Å). The crystal data are: monoclinic with $a = 10.721 \pm 0.010$, $b = 17.769 \pm 0.006$, $c = 13.895 \pm 0.006$ Å, $\beta = 94.71 \pm 0.05°$, $D_x = 1.744$ g. cm^{-3} ($Z = 8$), $\mu = 17.5$ cm^{-1}, space group $C2/c$ or Cc.

Intensity data were collected on a General Electric XRD-5 diffractometer with Mo $K\alpha$ radiation within a sphere of radius $2 \sin \theta/\lambda = 0.962$. The measurement was carried out below 15°C. The stationary-crystal stationary-counter technique was used with a counting time of 10 seconds for each reflexion. A total of 1245 reflexions were measured, of which 164 were recorded as of zero intensity. Beyond the sphere the intensities dropped rapidly, indicating large thermal vibrations in the crystal.

The absorption correction was ignored. The extinction effect was found not to be appreciable at the final stage of the refinement.

Determination of the structure

The space group, $C2/c$, was first assumed for this crystal and used throughout the structure determination, and resulted in a reasonable structure.

Table 1. *Atomic positional parameters and their standard deviations* (e.s.d.'s in Å)

	x	y	z	$\sigma(x)$	$\sigma(y)$	$\sigma(z)$
Cu	0.12566	0.14374	0.09551	0.0011	0.0011	0.0011
O(1)	0.3028	0.1636	0.0806	0.0057	0.0061	0.0059
O(2)	0.4933	0.1116	0.1007	0.0060	0.0067	0.0074
O(3)	−0.0487	0.1172	0.1031	0.0057	0.0059	0.0056
N	0.1830	0.0441	0.1264	0.0068	0.0072	0.0065
C(1)	0.3782	0.1088	0.1028	0.0085	0.0097	0.0091
C(2)	0.3193	0.0375	0.1367	0.0088	0.0095	0.0096
C(3)	0.1167	−0.0167	0.1327	0.0087	0.0092	0.0087
C(4)	−0.0191	−0.0185	0.1261	0.0088	0.0083	0.0081
C(5)	−0.0771	−0.0878	0.1344	0.0097	0.0094	0.0090
C(6)	−0.2065	−0.0953	0.1325	0.0102	0.0099	0.0100
C(7)	−0.2790	−0.0306	0.1201	0.0098	0.0097	0.0087
C(8)	−0.2275	0.0388	0.1078	0.0091	0.0091	0.0087
C(9)	−0.0929	0.0468	0.1122	0.0085	0.0085	0.0078
W(1)	0.0749	0.2405	0.0361	0.0061	0.0062	0.0060
W(2)	0.1471	0.2020	0.2479	0.0061	0.0063	0.0059
W(3)	0.4018	0.2341	0.3115	0.0065	0.0069	0.0067
W(4)	0.2965	0.3127	0.4566	0.0063	0.0067	0.0063
W(5)	0.0550	0.3410	0.3606	0.0079	0.0088	0.0097
H(1)	0.355	0.036	0.213	0.08	0.08	0.08
H(2)	0.347	−0.013	0.116	0.10	0.10	0.10
H(3)	0.171	−0.061	0.146	0.12	0.12	0.12
H(4)	−0.023	−0.136	0.146	0.12	0.13	0.12
H(5)	−0.245	−0.143	0.137	0.08	0.09	0.08
H(6)	−0.390	−0.030	0.112	0.08	0.08	0.08
H(7)	−0.273	0.096	0.098	0.09	0.09	0.09
H(8)	0.230	0.212	0.251	0.08	0.08	0.08
H(9)	0.099	0.166	0.289	0.13	0.13	0.13
H(10)	0.042	0.276	0.068	0.12	0.12	0.12
H(11)	0.118	0.275	−0.016	0.09	0.09	0.09
H(12)	0.382	0.263	0.358	0.13	0.14	0.13
H(13)	0.425	0.205	0.354	0.12	0.13	0.12
H(14)	0.375	0.337	0.495	0.13	0.13	0.13
H(15)	0.244	0.364	0.466	0.14	0.14	0.13
H(16)	0.124	0.332	0.409	0.12	0.12	0.12
H(17)	0.073	0.280	0.323	0.12	0.12	0.12

A three-dimensional Patterson function followed by a minimum function revealed all the atoms in the complex, though there were seven possible positions for four water molecules. Successive least-squares calculations by the block-diagonal approximation, with all the atoms, including the seven possible positions for free water molecules, resulted in large temperature factors for three of the seven possibilities. By excluding these three positions the R index was 0·071 with isotropic thermal parameters. Further refinement by the least-squares method, using all the intensity data with unit weight, gave $R = 0.061$ after three cycles, in which the thermal factors for all the atoms were anisotropic of the form $\exp[-(\beta_{11}h^2 + \beta_{22}k^2 + \beta_{33}l^2 + \beta_{12}hk + \beta_{13}hl + \beta_{23}kl)]$. The difference Fourier summation at this stage showed up all the hydrogen atoms. Atomic parameters of all atoms given by the final least-squares refinement with hydrogen atoms assumed as isotropic are listed in Tables 1 and 2, with their standard deviations. The observed and calculated structure factors are listed in Table 3. The final R index was 0·050. The block-diagonal least-squares program and Fourier summation program were written by one of the authors (T. Ashida) for the HITAC-5020 computer. The atomic scattering factors for copper(II) ion and neutral

C, N, O, H atoms were taken from *International Tables for X-Ray Crystallography* (1962). The anomalous dispersion terms were ignored.

Description of the structure and discussion

The molecular structure of the complex is substantially the same as that of SGCH. The bond lengths and angles in the complex of SGCT are shown in Figs. 1 and 2, and also tabulated in Tables 4, 5 and 6 with

Fig. 2. Bond angles in the complex.

Table 2. *The thermal parameters and their standard deviations* ($\times 10^4$)

The thermal parameters for hydrogen atoms are isotropic $B(\text{Å})$.

	β_{11}	$\sigma(\beta_{11})$	β_{22}	$\sigma(\beta_{22})$	β_{33}	$\sigma(\beta_{33})$	β_{12}	$\sigma(\beta_{12})$	β_{13}	$\sigma(\beta_{13})$	β_{23}	$\sigma(\beta_{23})$
Cu	61	1	26	0	44	1	2	1	15	1	7	1
O(1)	64	6	30	2	51	4	12	6	11	8	3	5
O(2)	58	7	34	3	97	6	17	7	34	10	0	6
O(3)	68	6	29	2	41	4	8	6	15	8	12	5
N	62	7	29	3	29	4	8	8	2	9	15	6
C(1)	52	9	34	4	49	6	−4	10	13	12	−15	8
C(2)	58	9	30	4	57	7	0	10	−4	12	16	9
C(3)	67	10	29	4	40	6	0	10	23	12	0	7
C(4)	83	10	19	3	27	5	11	9	6	11	5	7
C(5)	98	11	28	4	39	6	−13	11	5	13	−19	8
C(6)	107	12	28	4	59	7	−46	11	8	14	−8	8
C(7)	103	11	33	4	30	5	−11	11	7	12	−1	8
C(8)	81	10	26	4	39	6	5	10	19	12	8	7
C(9)	72	9	26	4	23	5	−24	9	13	11	0	7
W(1)	90	7	29	3	49	4	9	7	21	9	17	5
W(2)	87	7	34	3	44	4	−25	7	18	8	−1	5
W(3)	90	7	39	3	66	5	−12	8	14	9	−31	6
W(4)	86	7	37	3	55	4	2	7	−12	9	−18	6
W(5)	114	9	57	4	137	8	−2	10	24	14	55	9
H(1)	1·0											
H(2)	3·9											
H(3)	7·4											
H(4)	6·9											
H(5)	1·7											
H(6)	1·4											
H(7)	2·6											
H(8)	0·4											
H(9)	8·1											
H(10)	5·5											
H(11)	2·7											
H(12)	8·6											
H(13)	7·0											
H(14)	8·1											
H(15)	9·5											
H(16)	7·0											
H(17)	9·0											

Table 3. *The observed and calculated structure factors on absolute scale*

K	FO	FC
H,L= 0 0		
2	8	5
4	132	-128
6	126	123
8	124	123
10	129	-126
12	50	-46
14	16	-4
16	45	-48
H,L= 0 1		
2	214	-207
4	65	61
6	5	12
8	28	-29
10	85	-81
12	76	78
14	43	45
16	10	10
H,L= 0 2		
0	147	140
2	19	-14
4	117	-117
6	46	46
8	56	58
10	62	-61
12	8	11
14	0	0
16	0	4
H,L= 0 3		
2	267	-257
4	45	-41
6	223	221
8	142	-136
10	77	-78
12	113	109
14	16	20
16	0	8
H,L= 0 4		
0	492	-509
2	283	-282
4	192	183
6	92	-90
8	104	-100
10	100	101
12	31	34
14	0	0
16	53	53
H,L= 0 5		
2	97	-94
4	42	46
6	37	32
8	15	5
10	28	-15
12	13	-2
14	49	-47
H,L= 0 6		
0	244	-239
2	36	23
4	184	184
6	104	-102
8	54	-53
10	53	55
12	46	43
14	42	-38
H,L= 0 7		
2	225	226
4	62	-60
6	81	-79
8	78	77
10	18	21
12	34	-26
14	48	-53
H,L= 0 8		
0	163	155
2	134	125
4	23	6
6	17	17
8	18	-7
10	0	7
12	34	-39
H,L= 0 9		
2	149	145
4	32	-29
6	97	-94
8	56	55
10	17	22
12	21	-14
H,L= 0 10		
0	101	96
2	31	14
4	100	-102
6	36	32
8	71	69
10	70	-68
H,L= 0 11		
2	37	-36
4	19	-18
6	22	25
8	0	-14
H,L= 0 12		
0	30	-16
2	52	-55
4	66	-73
6	25	27
H,L= 0 13		
2	92	-96
4	24	25
H,L= 1 0		
1	181	185
3	18	-19
5	14	13
7	72	79
9	10	-9
11	64	-64
13	24	25
15	45	44
17	44	-44
H,L= 1 1		
1	185	-180
3	114	-111
5	190	189
7	34	-37
9	151	-149
11	82	87
13	82	82
15	54	-51
H,L= 1 2		
1	67	-62
3	138	143
5	45	-46
7	111	-117
9	62	64
11	0	6
13	0	-11
15	24	-31
H,L= 1 3		
1	69	-67
3	101	106
5	43	43
7	53	51
9	150	-153
11	90	93
13	58	58
15	0	-10
H,L= 1 4		
1	182	-181
3	139	141
5	19	20
7	143	-145
9	28	31
11	62	66
13	63	-65
15	25	-28
H,L= 1 5		
1	91	94
3	68	75
5	169	-168
7	56	58
9	50	54
11	53	-58
13	27	-31
15	18	21
H,L= 1 6		
1	56	-58
3	86	86
5	24	-24
7	8	2
9	15	10
11	24	23
13	0	3
15	0	-15
H,L= 1 7		
1	109	107
3	10	13
5	160	-164
7	41	41
9	88	83
11	46	-43
13	80	-79
H,L= 1 8		
1	88	86
3	84	-84
5	14	-15
7	71	68
9	0	1
11	30	-33
13	52	50
H,L= 1 9		
1	48	-45
3	53	49
5	9	-10
7	0	-2
9	0	12
11	10	10
H,L= 1 10		
1	49	50
3	66	-64
5	42	-41
7	87	86
9	43	-43
11	39	-43
H,L= 1 11		
1	45	-48
3	19	-18
5	96	96
7	14	-17
9	48	-46
H,L= 1 12		
1	0	-10
3	0	7
5	0	10
7	0	-8
H,L= 1 13		
1	56	-54
3	15	-21
H,L= 1 -1		
1	54	-51
3	114	-112
5	44	-46
7	88	86
9	59	-58
11	14	12
13	37	-43
15	37	-37
17	0	6
H,L= 1 -2		
1	121	115
3	219	-221
5	58	58
7	176	179
9	73	-74
11	99	-104
13	67	71
15	20	22
H,L= 1 -3		
1	127	128
3	123	128
5	96	-101
7	34	38
9	127	128
11	59	-61
13	72	-67
15	20	21
H,L= 1 -4		
1	55	-49
3	237	-237
5	62	54
7	23	-18
9	0	2
11	21	21
13	16	17
15	14	-12
H,L= 1 -5		
1	214	214
3	37	37
5	45	-52
7	40	-37
9	91	90
11	15	-17
13	9	-6
15	56	60
H,L= 1 -6		
1	56	-55
3	113	137
5	16	-12
7	117	-114
9	31	30
11	109	108
13	47	-48
15	40	-39
H,L= 1 -7		
1	53	-54
3	41	-41
5	22	-19
7	29	-32
9	17	-14
11	0	-8
13	39	41
H,L= 1 -8		
1	29	28
3	116	111
5	72	73
7	95	-96
9	21	20
11	22	19
13	38	-39
H,L= 1 -9		
1	60	-58
3	94	-91
5	96	97
7	16	-21
9	53	-51
11	0	-2
H,L= 1-10		
1	0	12
3	18	-17
5	9	1
7	41	40
9	20	-21
11	41	-44
H,L= 1-11		
1	23	-25
3	13	12
5	77	78
7	0	-4
9	0	1
H,L= 1-12		
1	0	-6
3	83	-88
5	31	-36
7	50	52
H,L= 1-13		
1	28	27
3	21	26
H,L= 2 0		
0	11	-6
2	64	-58
4	62	-56
6	75	-81
8	131	133
10	22	23
12	17	16
14	0	10
16	18	20
H,L= 2 1		
2	85	-85
4	62	64
6	176	181
8	24	20
10	44	-49
12	107	107
14	9	-14
16	43	-41
H,L= 2 2		
0	99	-88
2	118	110
4	13	-4
6	148	-155
8	44	-50
10	118	117
12	0	-2
14	88	-83
16	0	6
H,L= 2 3		
2	30	33
4	70	-65
6	18	21
8	76	76
10	46	-45
12	63	-61
14	42	42
16	21	21
H,L= 2 4		
0	107	-107
2	79	75
4	162	157
6	92	-88
8	60	-60
10	0	5
12	0	2
14	63	-58
H,L= 2 5		
2	66	67
4	72	-71
6	150	-144
8	72	74
10	0	-3
12	96	-86
14	0	0
H,L= 2 6		
0	27	-25
2	10	5
4	0	-2
6	130	127
8	17	-16
10	55	-56
12	0	8
14	51	49
H,L= 2 7		
2	17	17
4	21	18
6	85	-84
8	17	21
10	55	51
12	24	-24
14	15	-17
H,L= 2 8		
0	51	50
2	32	-29
4	129	-128
6	95	92
8	48	47
10	53	-48
12	10	14
H,L= 2 9		
2	34	-34
4	71	71
6	39	38
8	41	-41
10	23	26
12	46	41
H,L= 2 10		
0	41	40
2	0	-5
4	53	-56
6	13	-15
8	10	13
10	10	9
H,L= 2 11		
2	62	-62
4	50	53
6	32	34
8	33	-41
H,L= 2 12		
0	44	-39
2	39	40
4	28	26
6	21	-27
H,L= 2 -1		
2	93	-96
4	90	93
6	39	38
8	115	-121
10	0	-10
12	120	127
14	32	-37
16	65	-65
H,L= 2 -2		
0	72	63
2	93	-96
4	36	34
6	31	37
8	128	131
10	106	-109
12	25	-24
14	90	84
16	0	1
H,L= 2 -3		
2	129	130
4	89	-90
6	80	-80
8	90	-92
10	0	0
12	0	-1
14	17	-17
16	0	5
H,L= 2 -4		
0	50	49
2	25	21
4	0	-2
6	50	50
8	0	0
10	122	-121
12	0	-5
14	34	32
16	24	-24
H,L= 2 -5		
2	119	126
4	69	-70
6	79	-82
8	128	127
10	0	0
12	80	-76
14	0	2
H,L= 2 -6		
0	79	80
2	80	-79
4	72	76
6	51	-50
8	43	-44
10	15	15
12	32	34
14	43	-39
H,L= 2 -7		
2	13	14
4	48	-54
6	51	53
8	68	67
10	37	35
12	44	-42
14	0	6
H,L= 2 -8		
0	55	-60
2	8	3
4	60	58
6	42	-40
8	29	-28
10	84	80
12	27	25
H,L= 2 -9		
2	49	-54
4	17	24
6	37	40
8	44	-42
10	0	-8
12	26	31
H,L= 2-10		
0	9	4
2	15	-10
4	16	13
6	0	1
8	10	-9
10	23	28
H,L= 2-11		
2	23	-24
4	27	27
6	22	20
8	67	-67
H,L= 2-12		
0	50	47
2	17	-17
4	36	-37
6	18	20
H,L= 2-13		
2	0	0
H,L= 3 0		
1	104	-98
3	175	178
5	9	8
7	33	-43
9	32	28
11	48	48
13	16	-12
15	43	-44
H,L= 3 1		
1	42	-44
3	42	43
5	25	28
7	73	73
9	0	-3
11	42	38
13	16	-19
15	0	0
H,L= 3 2		
1	99	-101
3	77	83
5	33	35
7	161	-166
9	27	28
11	71	69
13	49	-45
15	17	-21
H,L= 3 3		
1	109	-103
3	160	158
5	96	-99
7	13	-12
9	94	92
11	25	-27
13	62	-59
15	57	53
H,L= 3 4		
1	11	8
3	11	-11
5	53	-53
7	34	36
9	50	-52
11	0	8
13	0	0
15	0	1
H,L= 3 5		
1	79	77
3	12	9
5	83	-83
7	52	-50
9	42	45
11	16	-18
13	47	-44
H,L= 3 6		
1	89	89
3	120	-121
5	32	30
7	82	83
9	0	-10
11	61	-56
13	29	26
H,L= 3 7		
1	67	-67
3	21	20
5	0	0
7	12	-17
9	0	-6
11	0	5
13	0	10
H,L= 3 8		
1	25	26
3	24	-20
5	18	-17
7	59	61
9	0	-2
11	14	-17
H,L= 3 9		
1	42	-39
3	34	-34
5	88	85
7	9	16
9	51	-48
11	28	28
H,L= 3 10		
1	13	-16
3	0	11
5	9	5
7	43	-42
9	0	6
H,L= 3 11		
1	0	-5
3	14	-15
5	32	36
7	0	6
H,L= 3 12		
1	30	-29
3	37	35
H,L= 3 -1		
1	131	-132
3	8	-11
5	68	78
7	10	14
9	78	-78
11	17	18
13	67	67
15	48	-46
H,L= 3 -2		
1	65	60
3	65	-69
5	13	18
7	84	86
9	0	-2
11	23	-25
13	28	30
15	0	8
H,L= 3 -3		
1	102	-109
3	37	-28
5	37	-36
7	7	4
9	151	-150
11	34	31
13	25	25
15	18	-14
H,L= 3 -4		
1	77	75
3	75	-79
5	98	-98
7	91	96
9	0	-6
11	123	-123
13	80	77
15	10	10
H,L= 3 -5		
1	46	50
3	14	14
5	47	-58
7	0	-2
9	63	56
11	43	-43
13	14	-15
15	26	27
H,L= 3 -6		
1	7	4
3	10	-6
5	22	-22
7	22	-20
9	12	15
11	50	-50
13	0	1
H,L= 3 -7		
1	142	144
3	44	46
5	57	-61
7	72	72
9	96	92
11	0	-2
13	49	-48
H,L= 3 -8		
1	66	-64
3	91	90
5	12	10
7	37	-38
9	28	29
11	42	39
13	18	-17
H,L= 3 -9		
1	0	3
3	21	18
5	0	-2
7	0	-10
9	18	21
11	0	0
H,L= 3-10		
1	24	-26
3	21	26
5	45	48
7	63	-62
9	29	32
H,L= 3-11		
1	19	-17
3	57	-68
5	49	50
7	40	-45
9	63	-72
H,L= 3-12		
1	0	9
3	10	-14
5	0	-12
H,L= 3-13		
1	32	-31
H,L= 4 0		
0	177	-188
2	96	105
4	59	54
6	52	-55
8	62	-64
10	100	103
12	0	8
14	86	-81
H,L= 4 1		
2	69	77
4	15	13
6	59	-60
8	8	10
10	54	50
12	47	-45
14	24	-26
H,L= 4 2		
0	83	82
2	34	29
4	7	7
6	7	-9
8	51	-50
10	62	61
12	31	-30
14	25	-28
H,L= 4 3		
2	107	108
4	31	-35
6	83	-88
8	133	126
10	23	28
12	88	-84
14	20	28
H,L= 4 4		
0	58	54
2	12	9
4	87	-87
6	42	42
8	32	32
10	43	-42
12	24	-22
14	46	44
H,L= 4 5		
2	0	2
4	50	-52
6	8	7
8	28	33
10	18	-22
12	0	0
14	0	3
H,L= 4 6		
0	21	18
2	39	-37
4	106	-104
6	94	96
8	0	-4
10	16	-16
12	14	-16
H,L= 4 7		
2	84	-81
4	19	18
6	49	48
8	57	-59
10	26	-29
12	38	36
H,L= 4 8		
0	15	-17
2	0	-2
4	16	6
6	13	18
8	9	-11
10	0	-1
H,L= 4 9		
2	13	-11
4	9	9
6	49	52
8	41	-40
10	10	-17
H,L= 4 10		
0	26	-23
2	29	32
4	58	57
6	10	-17
8	40	-45
H,L= 4 11		
2	29	31
4	0	2
6	0	-9
H,L= 4 12		
0	32	-31
H,L= 4 -1		
2	155	-156
4	158	163
6	53	-51
8	80	-79
10	0	-8
12	59	59
14	35	-36
H,L= 4 -2		
0	57	-58
2	79	-76
4	120	120
6	33	-38
8	28	-28
10	38	40
12	18	18
14	20	-21
H,L= 4 -3		
2	118	-122
4	43	42
6	101	101
8	94	-91
10	23	-23
12	80	77
14	0	7
H,L= 4 -4		
0	36	37
2	22	-24
4	83	-82
6	70	73
8	37	37
10	105	-103
12	38	32
14	54	56
H,L= 4 -5		
2	47	-47
4	13	18
6	0	1
8	55	52
10	30	-33
12	0	3
14	23	30
H,L= 4 -6		
0	175	178
2	35	-34
4	84	-84
6	42	42
8	63	61
10	93	-93
12	17	-13
14	56	53
H,L= 4 -7		
2	91	91
4	50	-53
6	47	-44
8	78	77
10	0	3
12	54	-54
H,L= 4 -8		
0	8	3
2	15	19
4	26	22
6	58	-59
8	56	58
10	0	-8
12	10	-14
H,L= 4 -9		
2	82	81
4	26	-28
6	59	-59
8	33	34
10	18	20
H,L= 4-10		
0	105	-102
2	16	12
4	80	74
6	62	-59
8	14	-16
H,L= 4-11		
2	10	-8
4	0	0
6	0	5
8	28	-28
H,L= 4-12		
0	49	-52
2	0	-4
4	38	41
H,L= 5 0		
1	85	-90
3	77	79
5	46	42
7	111	-115
9	30	32
11	57	58
13	46	-40
H,L= 5 1		
1	139	144
3	131	131
5	203	-209
7	33	32
9	86	89
11	25	-25
13	60	-60
H,L= 5 2		
1	140	138
3	10	9
5	11	-13
7	43	44
9	0	-4
11	16	-23
13	22	-31
H,L= 5 3		
1	91	94
3	20	19
5	87	-86
7	0	-2
9	22	26
11	27	-22
13	0	0
H,L= 5 4		
1	112	113
3	131	-129
5	22	-22
7	116	118
9	32	-36
11	58	-55
13	25	22
H,L= 5 5		
1	36	-32
3	79	-76
5	81	77
7	21	21
9	61	-64
11	0	6
13	37	37
H,L= 5 6		
1	28	-30
3	87	-87
5	0	-4
7	21	30
9	14	-16
11	0	-10
H,L= 5 7		
1	77	-70
3	48	-50
5	85	82
7	21	23
9	60	-60
11	15	17
H,L= 5 8		
1	59	-62
3	73	70
5	0	-1
7	44	-43
9	0	0
H,L= 5 9		
1	19	22
3	9	-15
5	24	22
7	23	-22
H,L= 5 10		
1	0	-7
3	84	83
5	10	13
H,L= 5 11		
1	41	43
3	21	24
H,L= 5 -1		
1	30	31
3	31	34
5	15	-15
7	0	6
9	35	37
11	0	3
13	22	-29
H,L= 5 -2		
1	203	-202
3	63	70
5	45	45
7	100	-110
9	0	-4
11	98	99
13	35	-29
H,L= 5 -3		
1	212	-217
3	23	-26
5	130	134
7	0	-4
9	100	-100
11	63	60
13	30	31
H,L= 5 -4		
1	12	11
3	7	3
5	19	22
7	8	-4
9	12	-11
11	0	4
13	0	5
H,L= 5 -5		
1	171	-169
3	39	-41
5	9	91
7	0	0
9	91	-89
11	31	32
13	35	35
H,L= 5 -6		
1	155	156
3	101	-98
5	15	-14
7	87	86
9	9	-10
11	74	-72
13	30	28
H,L= 5 -7		
1	17	19
3	0	6
5	37	-38
7	0	-2
9	24	25
11	23	-26
H,L= 5 -8		
1	59	58
3	82	-81
5	29	-30
7	66	70
9	21	-11
11	35	-37
H,L= 5 -9		
1	75	72
3	75	76
5	97	-95
7	0	10
9	74	67
H,L= 5-10		
1	54	-59
3	22	20

Table 3 (*cont.*)

K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC
5	0	0	4	78	75	4	22	19	2	30	-27	1	27	-25	7	106	103	2	89	-88	2	9	13	3	10	-6
7	29	-32	6	81	78	6	19	-10	4	27	-33	3	97	98	9	30	-31	4	38	42	4	14	15	5	29	34
H,L= 5-11			8	75	-72	8	0	0	6	0	4	5	0	-6	11	28	34	6	93	92	6	61	58	7	14	16
1	38	42	10	25	-27	10	32	-28	H,L= 6-11			7	67	-65	H,L= 7 -6			8	0	1	8	55	52	H,L= 9 -2		
3	23	25	12	53	50	12	30	29	2	65	64	9	0	-9	1	13	-16	H,L= 8 4			H,L= 8 -6			1	38	33
5	15	-23	H,L= 6 6			H,L= 6 -4			4	10	-9	H,L= 7 7			3	18	19	0	52	-50	0	103	-102	3	69	-64
H,L= 5-12			0	112	-114	0	63	-61	H,L= 7 0			1	20	17	5	19	-15	2	13	13	2	32	30	5	27	-25
1	51	-50	2	43	44	2	11	-7	1	17	19	3	42	-45	7	0	-1	4	26	28	4	58	55	7	42	38
H,L= 6 0			4	46	45	4	90	89	3	66	-67	5	40	-42	9	57	52	6	29	-34	6	0	1	H,L= 9 -3		
0	23	-12	6	49	-42	6	51	-50	5	56	53	7	21	-21	H,L= 7 -7			8	46	-46	8	15	-19	1	34	31
2	32	32	8	22	-25	8	73	-73	7	91	92	H,L= 7 8			1	59	-54	H,L= 8 5			H,L= 8 -7			3	14	-16
4	34	-35	10	0	-2	10	65	68	9	40	-41	1	31	-32	3	9	-12	2	0	-4	2	63	-61	5	31	-29
6	49	51	H,L= 6 7			12	0	8	11	41	-45	3	46	46	5	49	48	4	0	0	4	17	18	7	18	17
8	30	-20	2	56	-54	H,L= 6 -5			H,L= 7 1			5	51	49	7	14	-4	6	0	8	6	52	47	H,L= 9 -4		
10	25	28	4	0	5	2	133	-134	1	8	5	H,L= 7 9			9	53	-52	H,L= 8 6			H,L= 8 -8			1	0	-6
12	20	-23	6	34	33	4	33	33	3	29	29	1	40	40	H,L= 7 -8			0	53	-52	0	10	-2	3	10	4
H,L= 6 1			8	47	-46	6	82	83	5	40	-45	H,L= 7 -1			1	31	31	2	0	-7	2	14	-5	5	49	-48
2	79	84	10	0	-2	8	96	-92	7	36	-35	1	86	93	3	61	-61	4	51	53	4	10	-12	7	0	2
4	81	-83	H,L= 6 8			10	30	-29	9	28	30	3	8	-1	5	0	13	6	37	-40	H,L= 8 -9			H,L= 9 -5		
6	65	-63	0	73	-76	12	64	66	11	0	9	5	146	-145	7	54	55	H,L= 8 7			2	37	-40	1	34	30
8	65	69	2	22	24	H,L= 6 -6			H,L= 7 2			7	33	-39	H,L= 7 -9			2	58	56	H,L= 9 0			3	29	32
10	31	32	4	89	87	0	61	62	1	17	14	9	9	11	1	0	-1	4	18	-26	1	31	28	5	56	-54
12	63	-61	6	48	-49	2	35	31	3	55	-59	11	40	-43	3	0	7	H,L= 8 -1			3	24	-21	H,L= 9 -6		
H,L= 6 2			8	21	-20	4	43	-37	5	69	-69	H,L= 7 -2			5	14	-22	2	51	56	5	23	22	1	25	-22
0	176	179	H,L= 6 9			6	48	45	7	125	123	1	17	-15	H,L= 7-10			4	32	-35	7	51	49	3	64	56
2	16	-14	2	20	20	8	19	21	9	19	16	3	67	65	1	18	23	6	87	-86	H,L= 9 1			5	0	7
4	142	-140	4	25	-26	10	25	-25	11	14	-21	5	0	11	3	37	-37	8	46	-42	1	22	-18	H,L= 9 -7		
6	91	91	6	52	-49	12	0	-5	H,L= 7 3			7	37	-34	H,L= 8 0			10	0	5	3	28	-24	1	0	-2
8	82	81	H,L= 6 10			H,L= 6 -7			1	21	-20	9	66	-65	0	56	62	H,L= 8 -2			5	62	59	H,L= 10 0		
10	61	-66	0	32	-33	2	115	-112	3	22	-21	11	0	-2	2	9	-3	0	12	-10	7	21	-21	0	30	34
12	0	12	2	0	9	4	57	55	5	157	155	H,L= 7 -3			4	65	-71	2	32	33	H,L= 9 2			2	0	10
H,L= 6 3			H,L= 6 -1			6	25	24	7	0	4	1	34	32	6	43	43	4	60	-62	1	14	-18	4	0	10
2	22	-16	2	164	168	8	17	-17	9	0	-9	3	8	6	8	67	66	6	0	6	3	27	26	H,L= 10 1		
4	0	-3	4	82	-83	10	10	-15	11	65	68	5	36	-32	10	26	-28	8	14	-9	5	44	43	2	41	-36
6	42	44	6	61	-65	H,L= 6 -8			H,L= 7 4			7	36	37	H,L= 8 1			10	28	-30	7	18	-20	H,L= 10 2		
8	13	-14	8	87	86	0	125	125	1	20	16	9	32	32	2	68	-71	H,L= 8 -3			H,L= 9 3			0	40	-35
10	14	-18	10	0	6	2	59	-58	3	9	-6	11	40	-42	4	39	42	2	83	83	1	0	-4	2	0	2
12	29	35	12	33	-37	4	51	-55	5	54	-55	H,L= 7 -4			6	22	25	4	23	-20	3	0	-16	H,L= 10 -1		
H,L= 6 4			H,L= 6 -2			6	52	51	7	38	-37	1	36	-38	8	45	-41	6	79	-79	5	0	12	2	37	-30
0	53	52	0	215	-216	8	43	48	9	34	39	3	80	80	10	0	-2	8	63	59	H,L= 9 4			4	32	34
2	0	1	2	26	26	10	49	-53	11	0	-4	5	18	-18	H,L= 8 2			10	21	22	1	33	-34	H,L= 10 -2		
4	98	-99	4	101	102	H,L= 6 -9			H,L= 7 5			7	108	-105	0	24	24	H,L= 8 -4			3	21	22	0	74	69
6	55	53	6	76	-81	2	56	55	1	82	-78	9	14	19	2	9	8	0	55	-50	5	0	0	2	18	-19
8	0	11	8	81	-78	4	9	-6	3	9	-12	11	75	71	4	25	-24	2	13	13	H,L= 9 5			4	50	-48
10	41	-40	10	69	72	6	23	-20	5	93	95	H,L= 7 -5			6	17	21	4	57	54	1	23	22	H,L= 10 -3		
12	0	-10	12	0	2	8	33	33	7	0	-5	1	37	-34	8	46	44	6	33	-29	3	0	10	2	21	17
H,L= 6 5			H,L= 6 -3			H,L= 6-10			9	41	-39	3	9	-7	10	0	-5	8	57	-52	H,L= 9 -1					
2	100	-95	2	31	29	0	10	13	H,L= 7 6			5	54	52	H,L= 8 3			H,L= 8 -5			1	38	-36			

their standard deviations, in comparison with those in SGCH. The least-squares planes of various parts of the complex are listed in Table 7 with the normal distances of atoms from them.

Table 4. *Bond distances in N-salicylideneglycinatoaquocopper*(II) *tetrahydrate, in comparison with hemihydrate*

The estimated standard deviations for the bond distances are in parentheses (in 10^{-3} Å).

Bonds	SGCT	SGCH
Cu—*W*(1)	1·965 (6)	2·016 (6)
-O(1)	1·959 (6)	1·953 (6)
-N	1·913 (7)	1·949 (7)
-O(3)	1·936 (6)	1·928 (6)
C(1)-O(1)	1·287 (11)	1·284 (10)
-O(2)	1·238 (12)	1·249 (10)
-C(2)	1·509 (14)	1·533 (12)
N—C(2)	1·461 (12)	1·446 (11)
-C(3)	1·302 (12)	1·282 (11)
C(4)-C(3)	1·450 (13)	1·457 (11)
-C(5)	1·389 (13)	1·420 (12)
-C(9)	1·409 (12)	1·409 (11)
C(6)-C(5)	1·394 (14)	1·389 (13)
-C(7)	1·391 (14)	1·379 (13)
C(8)-C(7)	1·367 (13)	1·409 (12)
-C(9)	1·447 (13)	1·412 (11)
C(9)-O(3)	1·350 (10)	1·337 (10)

The largest deviation of any atom from the plane, *P*(1), through the complex is 0·25 Å for the *W*(1) atom. Thus, the planarity of the complex is better than that in SGCH in which several atoms deviate by more than 0·3 Å from the plane. The plane through the glycine residue [*P*(3)] and the one containing the salicylaldimine residue [*P*(5)] make a dihedral angle of 9·5°, and this is seven degrees smaller than that in SGCH. The glycine residue is mostly normal in its bond distances and angles as in the usual amino acids. The shift of the nitrogen atom from the carboxyl plane, 0·12 Å, is considerably smaller than 0·35 Å in SGCH, and 0·44 Å, 0·58 Å, 0·31 Å in α-, β-, γ-glycine respectively (Marsh, 1958: Iitaka, 1960: Iitaka, 1961).

The bond distances in the benzene ring fluctuate significantly over a range of 0·05 Å from the mean value 1·400 Å, and the angles in it have an average value of 120·0°.

The coordination configuration of the copper(II) ion is not an octahedron, but a square pyramid (Fig. 3). The bond distances and angles around the copper(II) ion are tabulated in Tables 4 and 5 in comparison with the values in SGCH, and they are in fairly good agreement with each other except for those such as the Cu–*W*(1) distance. The fifth coordination atom *W*(2) lies at the apex of the square pyramid at a distance, 2·352 Å, from the copper(II) ion. The copper(II) ion is shifted toward this apical water molecule by 0·135 Å from the plane *P*(2). This is a common feature of the square pyramid configuration of the copper(II) ion observed in the crystalline state.

In spite of the similarity in the structures of the complexes in SGCH and SGCT, their crystal structures are completely different from one another. In SGCT, the approximate plane of the complex [*P*(1)] is nearly perpendicular to the *c* axis. A part of the crystal structure viewed along the *c* axis is shown in Fig. 4. The packing of the complexes and the hydrogen bonding system are shown in Fig. 5, together with water mol-

ecules and the schematically drawn complex molecules. In SGCT, the fifth coordination bond is formed by one of the water molecules, while that in SGCH is the 'free' carboxyl oxygen atom of the adjacent complex. Therefore, in SGCH the complexes are joined together strongly by the fifth coordination bond to form an infinite chain of the complexes along the b axis. In SGCT no coordination bonds are involved in constructing the crystal structure, and there are nine hydrogen bonds in the asymmetric unit. Some of them are used to connect the complexes *via* water molecules to form a three-dimensional network, and the others connect the water molecules to each other.

Since this crystal was prepared below 10 °C while the SGCH crystal was obtained above 30 °C, the behaviour of the SGCT crystal in the intermediate temperature

Table 5. *Bond angles in N-salicylideneglycinatoaquocopper*(II) *tetrahydrate and hemihydrate*

The standard deviations for the angles are listed in parentheses.

Atoms	SGCT	SGCH	
$W(1)$–Cu—O(1)	92·0 (3)	88·0	angles around C(2) with H(1), H(2):102, 121, 99, 111, 112;
$W(1)$–Cu—O(3)	89·8 (3)	91·0	angles around C(3) with H(3):111, 124;
O(1)–Cu—N	83·9 (3)	83·4	angles around C(5) with H(4):120, 118;
O(3)–Cu—N	93·4 (3)	94·6	angles around C(6) with H(5):121, 121;
$W(1)$–Cu—N	168·0 (3)	165·3	angles around C(7) with H(6):125, 113;
O(1)–Cu—O(3)	174·8 (3)	166·3	angles around C(8) with H(7):131, 109;
Cu—O(1)-C(1)	115·7 (6)	116·5	
O(1)–C(1)-O(2)	124·8 (9)	125·3	H(10)–$W(1)$–H(11) 99
O(2)–C(1)-C(2)	119·1 (8)	119·5	H(8)—$W(2)$–H(9) 127
O(1)–C(1)-C(2)	116·1 (8)	115·2	H(12)–$W(3)$–H(13) 139
C(1)–C(2)-N	110·0 (8)	109·8	H(14)–$W(4)$–H(15) 89
C(2)–N—Cu	113·4 (6)	112·3	H(16)–$W(5)$–H(17) 86
C(3)–N—Cu	128·1 (6)	125·5	
C(2)–N—C(3)	118·3 (8)	121·8	
N—C(3)-C(4)	124·3 (8)	125·1	
C(3)–C(4)-C(5)	117·7 (8)	116·1	
C(3)–C(4)-C(9)	122·9 (8)	124·3	
C(5)–C(4)-C(9)	119·4 (8)	119·6	
C(4)–C(5)-C(6)	122·4 (9)	120·7	
C(5)–C(6)-C(7)	117·9 (9)	120·2	
C(6)–C(7)-C(8)	122·3 (9)	120·0	
C(7)–C(8)-C(9)	119·7 (8)	121·1	
C(8)–C(9)-O(3)	116·4 (8)	117·4	
C(4)–C(9)-O(3)	125·4 (8)	124·3	
C(8)–C(9)-C(4)	118·2 (8)	118·4	
C(9)–O(3)-Cu	125·4 (5)	125·8	

Table 6. *Hydrogen bonds and close intermolecular atomic contacts*

Hydrogen bonds

$W(2)$–$W(3)$	2·86 Å	(within the original set)
$W(2)$–$W(5)$	3·13	(within the original set)
$W(3)$–$W(4)$	2·77	(within the original set)
$W(4)$–$W(5)$	2·86	(within the original set)
$W(3)$–O(2)	2·70	(within the original set)
$W(1)$–$W(5^{ii})$	2·74	
$W(2)$–O(3^{ii})	2·85	
$W(1)$–O(1^{iii})	2·76	
$W(4)$–O(3^{v})	2·79	

Close contacts less than 3·5 Å

Cu—C(5^{i})	3·35 Å	C(5)–C(5^{ii})	3·49
Cu—C(6^{i})	3·46	O(2)–$W(1^{iii})$	3·29
C(3)–C(9^{i})	3·43	$W(1)$–C(1^{iii})	3·36
C(7)–C(1^{i})	3·48	$W(4)$–C(3^{iv})	3·43
O(1)–C(6^{i})	3·29	$W(4)$–C(8^{v})	3·40
C(4)–C(4^{ii})	3·44	$W(4)$–C(9^{v})	3·45
$W(5)$–$W(5^{ii})$	3·20	$W(4)$–$W(1^{v})$	3·24
$W(2)$–C(9^{ii})	3·45	O(2)–C(8^{vi})	3·26

Code for superscripts

i	$-x$,	$-y$,	$-z$
ii	$-x$,	y,	$\frac{1}{2}-z$
iii	$\frac{1}{2}-x$,	$\frac{1}{2}-y$,	$-z$
iv	$\frac{1}{2}-x$,	$\frac{1}{2}+y$,	$\frac{1}{2}-z$
v	$\frac{1}{2}+x$,	$\frac{1}{2}-y$,	$\frac{1}{2}+z$
vi	$1+x$,	y,	z

range is also of interest. The present structure analysis of SGCT indicated a large thermal parameter of about 7·5 Å² for the *W*(5) oxygen atom. This high value of the temperature factor, compared with normal values for the other four water oxygen atoms, implies a large thermal vibration or a disorder on this site. The crystal used in the experiment was kept between 15°C and 25°C in air. After six months the crystal became non-transparent and gave a powder pattern corresponding to neither SGCH nor SGCT. Kishita, Nakahara & Kubo (1964) prepared a complex in this temperature range and found that the complex was a mixture of SGCH and SGCT. However, the powder pattern in our case did not correspond to such a mixture. The

Fig. 3. The distances in the square pyramid.

quantitative elemental analysis of the crystals suggested that the crystals are *N*-salicylideneglycinato-copper(II) hemihydrate. Since this crystal has only a half of the water molecule per complex, this will have a molecular structure different from both SGCH and SGCT.

A remark on the non-enzymatic transamination reactions

As stated in the introduction the complex of SGCT is considered to be a catalytic intermediate in the non-enzymatic transamination reactions. This type of complex is called 'Type I' in this paper. On the other hand, there are complexes which are similarly prepared from a ketone (aldehyde)–amino acids–copper(II) ion system but not through transamination reactions. This type is called 'Type II'. The mechanism of the reactions proposed so far (Metzler, Ikawa & Snell, 1954) was concerned with the migration of the double bond around the nitrogen atom. Therefore, the bond distances concerning the nitrogen atom may give a clue to the reaction mechanism. The part of the structure in question is:
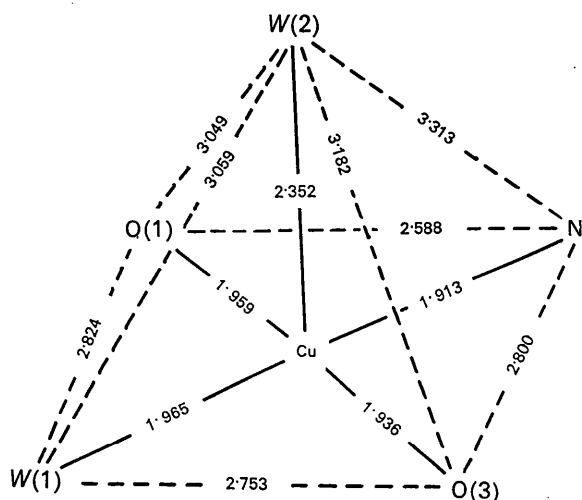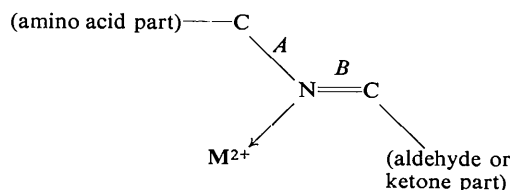

The distances of these bonds established by the X-ray diffraction method are:

Table 7. *Equations of least-squares planes and normal distances from the planes*

P(1)	$0·04803x - 0·22700y - 0·97271z + 1·67327 = 0·0$	(all the atoms)
P(2)	$0·00044x - 0·33939y - 0·94064z + 1·97517 = 0·0$	(square coordination atoms)
P(3)	$-0·01480x - 0·29621y - 0·95501z + 1·99813 = 0·0$	(Cu-glycinato)
P(4)	$0·04121x - 0·13172y - 0·99043z + 1·69070 = 0·0$	(benzene ring)
P(5)	$0·05017x - 0·14785y - 0·98774z + 1·69929 = 0·0$	(Cu-salicylaldimine)

Normal distances from the planes (× 10³ Å)

	P(1)	P(2)	P(3)	P(4)	P(5)
Cu	−134	−135 (−227)*	−40 (24)		77 (−34)
O(1)	79	−60 (−5)	24 (16)		
O(2)	115		2 (−60)		
O(3)	−195	−52 (−5)	51*	1*	−26 (−21)
N	−120	63 (5)	67 (142)		−55 (−65)
C(1)	39		8 (−19)		
C(2)	−162		−55 (−127)		−105*
C(3)	6		315*	−45*	−17 (−6)
C(4)	33			−9 (6)	6 (−18)
C(5)	170			13 (3)	43 (−27)
C(6)	159			−1 (−10)	19 (−19)
C(7)	29			−14 (8)	−20 (29)
C(8)	−58			16 (2)	−6 (29)
C(9)	−81			−4 (−9)	−15 (−3)
W(1)	253	54 (5)	243		611*

* Not included in the least-squares calculations.
A distance in parentheses indicates that of *N*-salicyldeneglycinatoaquocopper(II) hemihydrate. The coordinates (*x*,*y*,*z*) (in Å units) are referred to the orthogonal axes, *a*, *b* and *c**.

		Bond A	Bond B
Type I	SGCT	1·461 Å	1·302 Å
	SGCH	1·446	1·282
	MPV*	1·45	1·27
	mean value	1·453	1·285
Type II	PACD†	1·480	1·247

From the structural point of view, the difference between Type I and II is significant. In Type I, the bond B has the normal C=N bond dimensions, and the bond A is rather shorter than the normal single bond (1·47–1·49 Å). On the other hand, in Type II, the bond A is normal, while the bond B is much shorter than the usual (1·29–1·30 Å).

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* Manganese(II) pyridoxylidenevaline (Willstadter, Hamor & Hoard, 1963).

† Pyruvidene-β-alaninatoaquocopper(II) dihydrate (Ueki, Ashida, Sasada & Kakudo, 1968).

Fig. 4. A part of the crystal structure, looking down along the c axis.

In view of the fact that in both types, one bond, A or B, is shorter than normal, it may be considered that the nitrogen atom carries more electrons than usual and that either bond is electron-rich. This effect is common to both types, and may be one of the characteristics of the complexes derived from Schiff bases and the copper(II) ion.

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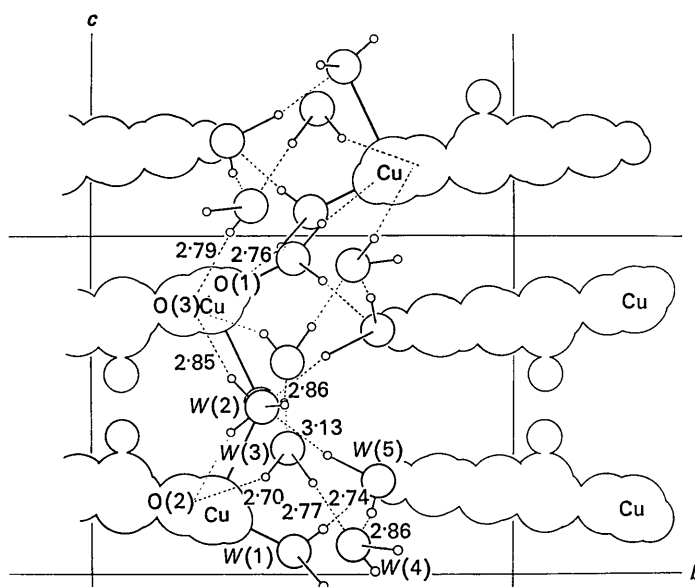

Fig. 5. The crystal structure with the hydrogen bonds, the complex molecules are drawn schematically.