Table 4 (*cont.*)

O(2)–N(2)	3·16	1
O(8)–O(4)	3·34	1
N(3)–O(3)	3·37	1
N(6)–O(3)	3·11	1
O(2)–C(4)	3·37	1
O(2)–O(3)	3·22	1
O(1)–C(4)	3·27	2
O(3)–C(8)	3·38	2
O(1)–C(5)	3·13	2
O(1)–C(7)	3·46	2
O(3)–C(7)	3·47	2
O(7)–C(8)	3·29	3
O(6)–C(5)	3·43	3
O(4)–N(6)	3·25	4

Key to symmetry operations

1	$0·5+x, 0·5-y, -z$
2	$-x, 0·5+y, 0·5-z$
3	$0·5-x, -y, 0·5+z$
4	$x, y, 1·0+z$

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The Crystal and Molecular Structure of Copper(II) Chloride–Bis-(*N*,*N*-dimethylacetamido)thioether

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The crystal structure of copper(II) chloride–bis-(*N*,*N*-dimethylacetamido)thioether has been determined by three-dimensional X-ray analysis employing Patterson and Fourier techniques. The atomic parameters were refined by the full-matrix least-squares method to a final *R* index of 0·106 for 838 observed reflexions which were photographically recorded. The space group is $P\bar{1}$ with $Z=2$ and cell dimensions of $a=11·15\pm0·01$, $b=8·17\pm0·01$, $c=7·77\pm0·01$ Å, $\alpha=95·7\pm0·3$, $\beta=97·4\pm0·4$ and $\gamma=96·9\pm0·4°$. The central copper atom is pentacoordinated with the ligands arranged in a square-pyramidal configuration.

Pentacoordinated complexes of copper(II) are known in the trigonal-bipyramidal and square-pyramidal configurations (Barclay, Hoskins & Kennard, 1963; Gillard & Wilkinson, 1963). The molecule of copper(II) chloride–bis-(*N*,*N*-dimethylacetamido)thioether is an example of the latter type of fivefold coordination.

The brilliant green crystals of $CuCl_2.C_8H_{16}N_2O_2S$ crystallize in a triclinic lattice, space group $P\bar{1}$. The following unit-cell dimensions were obtained from measurements made on oscillation, precession and Weissenberg photographs:

$a=11·15\pm0·01$, $b=8·17\pm0·01$, $c=7·77\pm0·01$ Å
$\alpha=95·7\pm0·3$, $\beta=97·4\pm0·4$, $\gamma=96·9\pm0·4°$.

The crystal density measured by flotation is 1·63 g.cm^{-3} from which it follows that the unit cell contains two molecules (calculated density = 1·62 g.cm^{-3}). Using the multiple-film equi-inclination Weissenberg technique with Cu $K\alpha$ radiation, intensities were collected by visual comparison with a calibrated strip for 838 independent reflexions. Layer lines with $k=0$ to 4 were recorded with oscillation about the *b* axis.

A crystal of spherical shape (diameter ~0·2 mm) was used for the intensity measurements. The standard Lorentz and polarization corrections were made as well as absorption corrections according to *International Tables for X-ray Crystallography* (1962).

The structure was solved employing three-dimensional Patterson and Fourier syntheses. Refinement using equal weighting was carried out by means of a full-matrix least-squares program (Busing, Martin & Levy, 1962) which minimizes the function $\sum\omega(F_o-F_o)^2$. With individual isotropic thermal parameters for the

atoms the R index ($R=\sum||F_o|-|F_c||/\sum|F_o|$) was reduced to 0·106. The refined atomic parameters are listed in Table 1. The crystallographic program *ORFFE* of Busing, Martin & Levy (1964) was used to calculate interatomic distances and angles. A summary of these values appears in Table 2. The observed and calculated structure factors are given in Table 3. Unobserved reflexions were excluded from the refinement (Dunning & Vand, 1969).

The molecular geometry and atomic numbering are illustrated in Fig. 1. The central copper atom is surrounded by five ligands in a distorted square-pyramidal configuration. The two chlorine, the sulphur and one of the oxygen atoms lie within the square plane, separated from the copper atom by distances of 2·267 ± 0·004, 2·277 ± 0·004, 2·410 ± 0·005 and 2·031 ± 0·003 Å respectively. The least-squares plane through these four ligands is given by the equation

$$0{\cdot}4447\ X+0{\cdot}8509\ Y-0{\cdot}2796\ Z=1{\cdot}4226^*$$

and shows them to be coplanar to within 0·04 Å. The

Table 1. *Refined atomic parameters (fractional coordinates and isotropic temperature factors*

Standard deviations are given in parentheses.

	x	y	z	B
Cu	0·2079 (3)	0·1546 (3)	0·1272 (5)	3·41 (7) Å^2
Cl(1)	0·1784 (6)	0·2828 (7)	0·3846 (10)	3·45 (13)
Cl(2)	0·3737 (6)	0·0427 (7)	0·2257 (10)	3·37 (13)
S	0·2000 (5)	−0·0094 (7)	−0·1468 (9)	2·20 (12)
O(1)	0·0409 (12)	0·1944 (17)	0·0230 (25)	2·76 (32)
O(2)	0·2775 (13)	0·3417 (17)	−0·0442 (23)	2·90 (32)
N(1)	−0·0780 (16)	0·2604 (22)	−0·2028 (29)	2·83 (39)
N(2)	0·4125 (16)	0·3956 (21)	−0·2282 (27)	2·66 (38)
C(1)	0·0127 (19)	0·1846 (26)	−0·1427 (38)	2·29 (45)
C(2)	0·3401 (18)	0·2923 (24)	−0·1557 (33)	1·99 (43)
C(3)	0·0797 (19)	0·0771 (25)	−0·2682 (33)	2·44 (46)
C(4)	0·3302 (19)	0·1038 (25)	−0·2239 (33)	2·41 (46)
C(5)	−0·1255 (23)	0·2473 (32)	−0·4002 (42)	4·27 (61)
C(6)	−0·1474 (20)	0·3629 (27)	−0·0903 (35)	2·97 (51)
C(7)	0·4116 (23)	0·5735 (31)	−0·1887 (39)	3·96 (58)
C(8)	0·4911 (23)	0·3354 (31)	−0·3561 (39)	4·17 (60)

Table 2. *Interatomic distances and angles*

Standard deviations are given in parentheses.

Cu–Cl(1)	2·267 (4) Å	C(1)–C(3)	1·60 (1) Å
Cu–Cl(2)	2·277 (4)	C(2)–C(4)	1·58 (1)
Cu–S	2·410 (5)		
Cu–O(1)	2·031 (3)	C(3)–S	1·83 (2)
Cu–O(2)	2·284 (3)	C(4)–S	1·86 (2)
Cl(1)···Cl(2)	3·417 (2)	C(1)–N(1)	1·31 (1)
S·····Cl(1)	4·654 (2)	C(2)–N(2)	1·33 (1)
S·····Cl(2)	3·269 (2)		
		N(1)–C(5)	1·57 (3)
O(1)–C(1)	1·30 (2)	N(1)–C(6)	1·51 (2)
O(2)–C(2)	1·27 (2)	N(2)–C(7)	1·45 (3)
		N(2)–C(8)	1·52 (2)
Cl(1)–Cu–Cl(2)	97·5 (3)°	Cu–O(1)–C(1)	121·0 (3)°
S–Cu–Cl(1)	168·7 (4)	Cu–O(2)–C(2)	116·6 (3)
S–Cu–Cl(2)	88·4 (3)		
S–Cu–O(1)	82·9 (3)	S–C(3)–C(1)	110·4 (2)
S–Cu–O(2)	77·2 (3)	S–C(4)–C(2)	108·1 (2)
Cl(1)–Cu–O(1)	89·3 (4)		
Cl(2)–Cu–O(2)	110·4 (4)	O(1)–C(1)–C(3)	119·9 (2)
O(1)–Cu–O(2)	85·7 (3)	O(2)–C(2)–C(4)	121·8 (2)
Cl(2)–Cu–O(1)	165·5 (5)		
Cl(1)–Cu–O(2)	103·7 (4)	O(1)–C(1)–N(1)	118·4 (1)
		C(3)–C(1)–N(1)	121·6 (2)
Cu–S–C(3)	98·8 (2)		
Cu–S–C(4)	99·0 (2)	O(2)–C(2)–N(2)	121·2 (2)
C(3)–S–C(4)	99·3 (2)	C(4)–C(2)–N(2)	117·0 (2)
		C(1)–N(1)–C(5)	122·2 (5)
		C(1)–N(1)–C(6)	124·5 (6)
		C(2)–N(2)–C(7)	119·2 (5)
		C(2)–N(2)–C(8)	121·4 (5)

Table 3. *Observed and calculated structure factors*

The columns are h, k, $10F_{obs}$ and $10F_{calc}$.

		L = 0		9	-7	179	159	-1	-2	995	-966	3	5	115	-89
1	0	303	320	10	-1	181	136	-1	-3	667	-630	3	6	170	180
2	0	498	-593	10	-2	181	155	-1	-5	101	122	4	1	85	-108
3	0	381	-395	10	-4	207	-196	-2	-1	1060	-1145	4	3	249	-203
4	0	104	-87	11	-1	229	173	-2	-2	1270	-1347	4	4	273	-251
5	0	730	720	11	-2	144	121	-2	-3	332	-295	4	5	118	150
6	0	191	178	11	-3	201	156	-2	-4	387	366	5	1	298	-343
7	0	442	-439	11	-5	157	-158	-2	-5	104	59	5	2	267	-289
8	0	233	-227			L = 1		-2	-6	283	-235	5	3	266	-254
10	0	256	237	1	0	115	-130	-3	-1	258	-266	6	2	154	136
11	0	102	66	2	0	724	-708	-3	-2	445	-389	6	3	305	348
12	0	131	-101	3	0	252	228	-3	-3	724	716	6	4	293	336
0	1	605	691	4	0	495	496	-3	-4	544	528	7	1	336	366
0	2	321	-332	5	0	504	478	-3	-5	269	-165	7	2	201	180
0	3	305	219	6	0	319	-332	-4	-2	495	502	7	3	316	349
0	5	171	126	7	0	176	-146	-4	-3	223	179	8	1	118	-120
0	6	256	242	10	0	207	205	-4	-4	102	-110	8	3	120	-97
0	7	232	236	11	0	161	-100	-5	-1	516	542	8	4	202	-259
1	1	577	-633	12	0	101	-105	-5	-2	221	241	9	3	115	-165
1	2	9835	9835	0	-1	321	389	-5	-3	261	-284	-1	1	269	267
1	3	434	-422	0	-2	588	541	-5	-5	202	261	-1	2	427	-366
1	5	276	269	0	-3	68	-97	-6	-1	132	159	-1	3	768	-825
1	6	240	230	0	-4	342	-310	-6	-2	329	-292	-1	4	485	-473
1	8	101	-116	0	-5	336	300	-7	-1	565	-561	-1	5	150	132
2	1	321	-379	0	-6	290	301	-7	-2	458	-463	-2	1	290	351
2	2	239	-233	0	-7	237	276	-8	-1	112	-95	-2	2	644	625
2	3	116	100	0	-8	203	241	-8	-2	115	119	-2	3	269	-258
2	4	409	360	1	1	266	-306	-9	-1	118	125	-2	4	479	-499
2	5	238	250	1	2	151	141	-9	-2	269	268	-2	6	165	184
2	7	256	-245	1	3	130	67	0	1	455	373	-2	7	120	123
2	8	140	116	1	4	218	240	0	2	268	-348	-3	1	93	69
3	1	386	344	1	5	580	654	0	3	337	-342	-3	2	398	437
3	2	154	171	1	6	197	203	0	4	199	-167	-3	3	207	243
3	3	218	-217	2	1	887	830	0	5	251	244	-3	4	166	-155
3	4	220	180	2	2	352	390	0	6	280	293	-3	5	152	-177
3	5	248	-246	2	3	113	127	-1	0	458	522	-4	2	113	129
3	6	354	-373	2	4	526	570	-2	0	120	68	-4	3	447	454
3	7	255	-253	2	5	105	90	-3	0	147	71	-4	4	399	363
3	8	95	-100	2	6	201	-169	-5	0	139	153	-4	5	110	135
4	1	246	324	3	1	66	101	-6	0	181	203	-5	1	167	97
4	2	140	-74	3	2	238	-208	-7	0	246	-233	-5	2	648	-697
4	3	410	-445	3	3	172	-174	-8	0	155	-156	-5	3	403	-402
4	4	265	-286	3	4	295	-299	-9	0	117	173	-5	4	276	302
4	8	128	143	3	5	453	-453	-1	1	536	551	-6	1	185	197
5	1	361	351	3	6	312	-344	-1	3	299	-283	-6	2	192	-214
5	2	156	99	4	2	236	-212	-1	4	279	-291	-6	3	623	-600
5	3	210	-164	4	3	187	-208	-1	6	254	283	-6	4	329	-363
5	4	231	244	4	4	313	-251	-2	1	323	-288	-7	1	367	384
5	5	161	-164	4	5	161	-164	-2	2	273	-235	-7	2	314	319
5	6	148	119	4	6	169	159	-2	3	342	-283	-7	3	154	115
5	7	222	213	5	1	284	-312	-2	4	389	374	-7	4	230	-208
6	1	333	-341	5	5	235	251	-2	5	368	-369	-7	5	119	-137
6	2	487	-499	5	6	168	146	-2	6	301	-293	-8	2	297	338
6	4	244	199	6	1	287	-252					-8	3	306	326
6	6	145	86	6	4	232	210	-3	1	257	221	-9	3	317	333
7	1	704	-726	6	5	207	187	-3	2	70	-22	-9	4	170	150
7	2	132	-119	6	6	132	96	-3	3	240	265	-1	0	184	257
7	3	243	246	7	1	105	104	-3	4	469	465	-2	0	74	-28
8	2	266	256	7	2	155	185	-3	6	304	-262	-3	0	199	-227
8	3	179	149	7	3	231	263	-4	1	124	53	-4	0	381	383
9	1	252	212	8	3	168	-188	-4	2	218	-199	-6	0	174	246
9	3	181	-166	8	4	205	-198	-4	4	535	589	0	-1	339	-322
10	1	181	139	8	5	111	-144	-4	5	567	602	0	-2	168	200
12	1	199	-235	9	2	239	-249	-4	6	233	215	0	-3	205	169
1	-1	1014	1184	9	3	167	-154	-5	2	340	-293	0	-4	421	-387
1	-3	236	-192	11	1	157	-142	-5	3	514	-544	0	-5	236	-193
1	-4	292	207	1	-1	278	301	-5	4	336	-323	0	-6	188	197
1	-5	255	-195	1	-2	553	501	-5	6	291	280	1	-1	303	-270
1	-6	96	-85	1	-3	169	149	-6	1	362	362	1	-2	167	166
1	-7	232	170	1	-4	275	-281	-6	2	363	338	1	-3	485	517
1	-8	178	190	1	-5	255	-262	-6	3	141	-120	1	-4	248	258
2	-1	442	-401	1	-6	109	-44	-6	4	468	473	1	-5	96	-98
2	-2	210	228	2	-1	146	-188	-6	5	282	-270	1	-6	188	-186
2	-3	274	-241	2	-2	612	557	-7	1	300	-309	2	-1	502	424
2	-4	332	-265	2	-3	216	223	-7	2	145	175	2	92	360	-290
2	-5	210	-168	2	-4	207	181	-7	3	186	215	2	-4	926	900
2	-6	502	-501	2	-5	97	77	-7	4	358	-407	2	-5	425	386
2	-7	274	-250	2	-6	155	-118	-7	5	291	-282	3	-1	430	-413
2	-8	102	-89	2	-7	290	-267	-8	2	111	-81	3	-2	601	-552
3	-1	299	-367	2	-8	235	-264	-8	3	114	135	3	-3	851	-866
3	-2	344	233	3	-1	924	-947	-8	5	242	-230	3	-4	295	-279
3	-3	211	173	3	-2	735	-720	-9	1	202	183	3	-5	266	295
3	-4	203	179	3	-3	231	-209	-9	2	204	162	4	-1	452	464
3	-5	277	249	3	-4	124	-48	-9	4	242	246	4	-2	110	-109
3	-7	255	-213	3	-5	200	173	-9	5	294	342	4	-3	450	-432
3	-8	228	-169	3	-6	193	145	-10	1	221	143	4	-4	517	-546
4	-1	264	-283	3	-8	202	-249	-10	3	242	-251	4	-5	276	-238
4	-2	331	-328	4	-1	535	514	-10	4	119	-109	5	-1	238	262
4	-3	101	-112	4	-2	703	-739	-10	5	115	121	5	-2	389	435
4	-5	272	243	4	-3	657	-657	-11	1	119	126	5	-3	160	151
4	-6	445	502	4	-4	247	-199	-11	2	118	135	5	-4	174	-181
4	-7	147	90	4	-5	208	-184	-11	3	116	-86	5	-5	188	-144
4	-8	175	-170	4	-6	114	68	-11	4	195	-254	6	-1	283	-296
5	-1	493	493	4	-8	115	-97	-11	5	148	-158	6	-2	136	186
5	-2	191	157	5	-1	935	998			L = 2		6	-3	334	324
5	-3	110	-112	5	-2	548	498	1	0	569	436	7	-1	103	22
5	-4	258	-233	5	-5	188	165	2	0	161	-156	7	-2	105	-99
5	-6	380	344	5	-6	116	101	3	0	173	-101	7	-3	187	213
5	-7	296	298	5	-7	207	185	4	0	267	336	7	-4	318	334
5	-8	99	-66	5	-8	113	133	5	0	300	-335	7	-5	201	174
6	-1	555	564	6	-1	182	174	6	0	100	-82	8	-2	275	-281
6	-2	266	273	6	-2	450	461	7	0	267	321	8	-3	280	-301
6	-3	208	121	6	-3	171	121	8	0	116	148	9	-1	165	142
6	-5	220	-177	6	-8	188	184	0	1	441	-376	9	-3	235	-240
6	-6	146	88	7	-1	248	-211	0	2	983	-980	9	-4	203	-187
6	-7	207	175	7	-2	103	110	0	3	532	-477	10	-2	201	203
6	-8	165	148	7	-3	151	168	0	4	250	221	10	-3	163	139
7	-1	211	-180	7	-6	119	-105	0	5	151	163	11	-1	155	-165
7	-2	88	-32	7	-7	231	-260	0	7	120	-174	11	-3	185	212
7	-3	206	-147	7	-8	145	-159	1	1	59	-44	-1	-1	55	104
7	-4	194	-148	8	-1	270	-327	1	2	124	128	-1	-2	532	441
7	-5	102	-68	8	-2	157	-174	1	3	734	753	-1	-3	432	-360
7	-6	331	-335	8	-5	169	161	1	4	514	559	-1	-4	519	-512
7	-7	269	-199	8	-8	162	-156	1	5	219	182	-1	-5	169	186
8	-1	189	-141	9	-2	287	-332	2	1	202	229	-1	-6	155	160
8	-5	208	145	9	-3	290	-282	2	2	484	524	-2	-1	155	-209
8	-7	216	-191	9	-4	169	-112	2	3	281	245	-2	-2	798	-754
8	-8	117	-98	9	-5	167	-147	2	5	194	-215	-2	-3	664	-652
9	-3	253	-220	9	-7	174	-156	3	1	131	140	-2	-4	87	-82
9	-5	255	196	10	-1	316	324	3	3	164	-147	-2	-5	100	106
9	-6	244	186	10	-2	239	209	3	4	260	-226	-3	-1	309	-293

-3	-2	364	-318	3	-1	344	351	-2	6	216	218				
-3	-3	481	489	3	-2	194	135	-3	1	229	243				
-3	-4	654	630	3	-3	337	-310	-3	2	91	131				
-3	-5	331	314	3	-4	368	-318	-3	3	178	157				
-3	-6	161	146	3	-6	223	210	-3	4	197	-185				
-4	-1	197	181	4	-2	184	146	-3	6	176	176				
-4	-2	476	432	4	-3	267	227	-3	7	116	134				
-4	-3	617	644	4	-4	292	-290	-4	1	219	134				
-4	-4	511	495	4	-5	281	-235	-4	2	97	-87				
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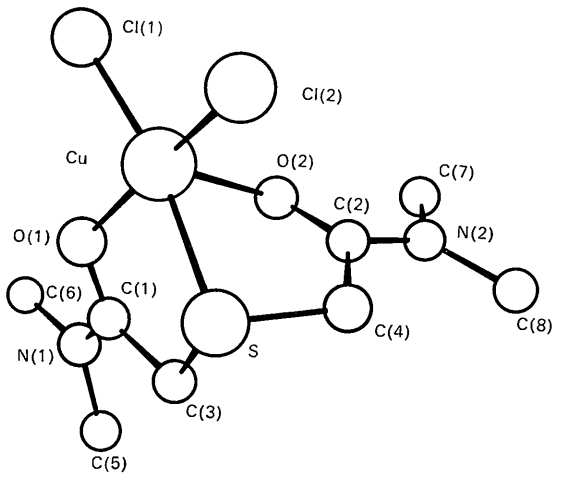

Fig. 1. Molecular geometry and atomic numbering.

copper atom is located above this plane at a distance of 0·21 Å. The second oxygen atom lies at the apex of the square pyramid. Since both oxygen atoms and the sulphur atom are involved in chemical bonding with the copper atom, the thioacetyl chains form part of two five-membered rings, perpendicular to each other. The equations of the best planes through the trigonal carbonyl carbon atoms C(1) and C(2) and their bonded neighbours are

$$0{\cdot}5710\ X+0{\cdot}8200\ Y-0{\cdot}0389\ Z=1{\cdot}432^{*} \text{ and}$$
$$0{\cdot}6762\ X-0{\cdot}1741\ Y+0{\cdot}7159\ Z=1{\cdot}199^{*}$$

respectively. For both sets of atoms, the maximum perpendicular deviation from the corresponding plane is less than 0·018 Å.

The distorted square-pyramid is best described in terms of the interatomic bonding angles. The Cl(1)–Cu–Cl(2) bond angle (97·5°) is increased at the expense of the bonding angles involving the other ligands in the square-planar arrangement. Thus, the O(1)–Cu–S bond angle is only 82·9°. Mutual repulsion by the two chlorine atoms complexed in a cisoid configuration is probably the major contributor to this distortion. Chlorine–oxygen repulsive forces also cause the Cu–O(1) bond to tend toward the ligands O(2) and S in the square plane. This is apparent from the O(2)–Cu–Cl(1) and O(2)–CuCl(2) bonding angles of 103·7 and 110·4° respectively, compared with the O(1)–Cu–O(2) and S–Cu–O(2) interatomic angles of 85·7 and 77·2°.

The shortest distance between the copper atoms in different molecules is $5{\cdot}14\pm0{\cdot}01$ Å, and these are related by a centre of symmetry. The smallest contact distance of $3{\cdot}20\pm0{\cdot}01$ Å is observed between two oxygen atoms [O(1)] also related by a centre of symmetry.

This analysis was undertaken at the request of Professor J. G. H. du Preez of the University of Port Elizabeth, who also provided the crystals.

* X, Y and Z are the orthogonalized coordinates with the X axis in the direction of **a** and the Y axis in the plane of **a** and **b**.

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