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The Crystal Structure of Copper(II) Chloride Bis(Dimethylsulphoxide)

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Received February 24, 1970

$[(CH_3)_2SO]_2CuCl_2$ belongs to the orthorhombic system, Pnma, with 4 formula groups in a unit cell. The dimensions of the unit cell at 23-24°C are $a = 8.0542 \pm 0.0013$, $b = 11.5464 \pm 0.0105$, $c = 11.3670 \pm 0.0082$A. The calculated density of 1.827 g/cc agrees well with the measured value of 1.83 g/cc. Intensities of 1609 independent reflections were measured by counter using θ–2θ can technique. Refinement of atomic parameters including hydrogen positional parameters has led to a R of 0.075. The crystal structure was determined by the heavy-atom method. It consists of a distorted square planar coordination for copper in which the Cl(1)–Cu–Cl(2) angle is $146.13 \pm 0.09°$ and the four bond lengths are: 2.283 ± 0.003A for Cu–Cl(1), 2.290 ± 0.002A for Cu–Cl(2), and 1.955 ± 0.004A for the two equivalent Cu–O bonds.

Introduction

As part of a study of the structural and spectral properties of copper(II) halide species, the crystal structure of the compound $[(CH_3)_2SO]_2CuCl_2$ or $CuCl_2$ $(DMSO)_2$ has been determined.

Preparation and Data Collection. Large, green crystals of $CuCl_2(DMSO)_2$ are easily grown by dissolving anhydrous $CuCl_2$ in an alcoholic solution dimethylsulphoxide.[1]

Examination of X-ray diffraction photographs revealed that the crystal was orthorhombic with mmm diffraction symmetry. The lattice constants, measured with Zr filtered MoKα radiation with a Picker diffractometer and G. E. single crystal orienter, were found to be $a = 8.054 \pm 0.001$, $b = 11.546 \pm 0.010$, and $c = 11.367 \pm 0.008$A. Systematic extinctions $[k+l = 2n+1$ for $\{okl\}$, $h = 2n+1$ for $\{hko\}]$ limited the choice of space group to Pnma or Pna2_1. The calculated density $(Z = 4)$ of 1.827 g/cc is in good agreement with the observed value of 1.83 g/cc.

A total of 1609 reflections were recorded from a crystal $(0.18 \times 0.18 \times 0.20$ mm) on a Picker diffractometer equipped with a G.E. single crystal orienter. A θ–2θ scan technique was used and the time intervals used in the scanning of a peak and its background on both sides are 100 and 10 seconds respectively. Of the reflections examined, 1274 had a net count greater than 5% above the background. Those with a net count of less than this were assigned a net count of 5% of the background and treated as unobserved reflections. The standard deviation for each reflection was calculated by

$$\sigma = F(TC+BG+0.01NC^2+0.01BG^2)^{1/2}/(2NC)$$

where TC = total counts, BG = background counts, and NC = net counts. The linear absorption coefficient was calculated to be 29.8 cm^{-1} which approximately corresponds to a μR of 0.3. Absorption corrections were neglected.

Structure Determination. The choice of Pnma was assumed since the statistical distribution of intensities[2] approached closer to that predicted for a centrosymmetric structure. From the 3-dimensional Patterson map the copper atoms were found to lie in the 4-fold special positions located at the mirror planes $y = 1/4$ and $y = 3/4$. The possible x and z values for copper atom were derived from the Harker lines at $x = 1/2$, $y = 0$ and at $y = 1/2$, $z = 1/2$. Thereby, the correct copper atomic positions were clearly indicated by the combination of x, y, and z values which gave the lowest R value. The resulting lowest R_1 value was 0.520 based on all the observed reflections and 0.437 based on the strongest 80% of the observed reflections. It was also observed from the Patterson map that all the chlorine atoms had to lie in the mirror planes. Nevertheless, the positions for the chlorine atoms were easily located from the difference map with contribtuions from the copper atom substracted out. These were in agreement with the peaks shown in the Patterson map.

With the positions of the chlorine atoms roughly located, three cycles of least square refinement[3] led the R_1 value to 0.397 on the basis of 80% of the observed reflections.

The remaining atoms, excluding the hydrogen atoms, were found from the examination of a difference Fourier map using only the largest 80% of the observed reflections. The Busing, Martin, and Levy Least square program[3] were used to refine the

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(1) J. Selbin, W. E. Bull, and L. H. Holmes, Jr., *J. Inorg. Nucl. Chem.*, *16*, 219 (1961).

(2) R. Dewar and A. Stone, *Fortran Symbolic Addition Programm*, University of Chicago, (1965).

(3) W. R. Busing, K. O. Martin, and H. A. Levy, *A Fortran Crystallographic Loast Square Programm*, U. S. Atomic Energy Commission Report ORNL-TM-305 (1962).

Table I. Final Parameters for $[(CH_3)_2SO]_2CuCl_2$ [a, b]

Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Cu(1)	0.3209(1)	0.2500	0.3614(1)	0.0084(1)	0.0060(5)	0.0061(5)	−0.0987(1)	−0.2839(7)	−1.7890(4)
Cl(2)	0.4984(3)	0.2500	0.2040(2)	0.0090(3)	0.0022(1)	0.0037(1)	0.0	−0.0010(1)	0.0
Cl(3)	0.2974(3)	0.2500	0.5616(2)	0.0156(4)	0.0042(1)	0.0057(2)	0.0	0.0030(2)	0.0
S(4)	0.1807(2)	0.4826(1)	0.4237(1)	0.0081(2)	0.0048(1)	0.0035(1)	0.0	−0.0003(2)	0.0
O(5)	0.3135(5)	0.4190(3)	0.3523(4)	0.0104(6)	0.0029(1)	0.0046(1)	0.0000(1)	0.0013(1)	0.0000 1
C(6)	0.2932(10)	0.5823(7)	0.5112(8)	0.0149(13)	0.0030(2)	0.0059(3)	0.0004(3)	0.0029(4)	−0.0006(2)
C(7)	0.0890(10)	0.5777(7)	0.3213(6)	0.0163(13)	0.0062(5)	0.0090(7)	−0.0003(7)	−0.0016(8)	−0.0038(5)
H(8)	0.204(13)	0.639(10)	0.542(10)	0.0308 [b]	0.0060(5)	0.0061(6)	0.0039(7)	0.0001(7)	0.0007(4)
H(9)	0.355(14)	0.648(11)	0.464(10)	—	—	—	—	—	—
H(10)	0.369(15)	0.550(11)	0.553(9)	—	—	—	—	—	—
H(11)	0.166(14)	0.169(10)	0.292(11)	—	—	—	—	—	—
H(12)	0.035(14)	0.546(10)	0.270(10)	—	—	—	—	—	—
H(13)	0.007(14)	0.653(9)	0.374(9)	—	—	—	—	—	—

$$R_1 = \frac{\Sigma||F_{obs}|-|F_{calc}||}{\Sigma|F_{obs}|} = 0.075 \qquad R_3 = \left[\frac{\Sigma(|F_{obs}|-|F_{calc}|)^2 w}{\Sigma|F_{obs}|^2 w}\right]^{1/2} = 0.077$$

[a] Standard deviations on the least significant digit are given in parenthesis. [b] The thermal parameters for H are assumed the same for all H atoms and correspond to an isotropic value of B = 8.

atomic parameters. The scattering factor for hydrogen atoms of Stewart[4] was used while those for the rest of the atoms were taken from the Inte rnational Tables for X-ray Crystallography.[5] The fact that the copper and chlorine atoms are in special positions at the mirror planes,y = 1/4 and y = 3/4, has fixed their y-positional parameters and the β_{12} and β_{23} anisotropic thermal parameters. The other atomic parameters were then refined to R_1 of 0.079 using the 1274 observed reflections before the hydrogen atoms were located. At this stage, it was possible to find positions of the hydrogen atoms from the difference Fourier map generated by all the 1609 reflections. These positional parameters were refined further but attempts to refine the temperature factors for the hydrogen atoms yielded unreasonable values. The final R_1 value converged at 0.075 for 1274 observed reflections and at 0.098 with all reflections included. The final parameters are listed in Table I, observed and calculated structure factors are tabulated in Table II, and principal interatomic distances and angles[6] are given in Table III and IV. The geometry of the unit formula, $CuCl_2(DMSO)_2$ is shown in Figure 1 and Figure 2 shows how a pair of $CuCl_2(DMSO)_2$ molecules are linked through long Cu—Cl interactions which may be continued to form a chain structure. These stereoscopic illustrations were made on the Washington State University CalComp plotter using the Oak Ridge Fortran Thermal-Ellipsoid Plot Program (ORTEP).[7]

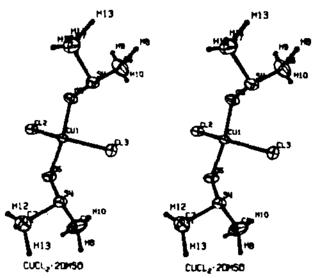

Figure 1. A Stereoscopic Illustration of the $CuCl_2(SMSO)_2$ Molecule.

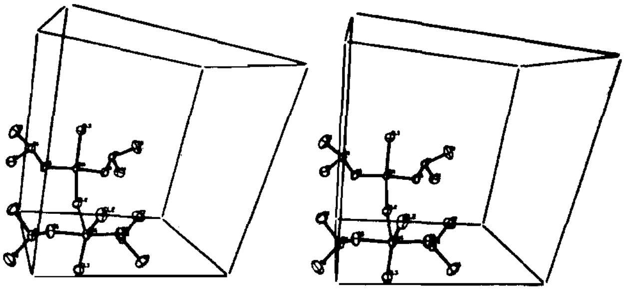

Figure 2. A Stereoscopic Illustration of the Packing in $CuCl_2(DMSO)_2$.

Discussion

The crystal structure consists of $CuCl_2(DMSO)_2$ molecules which, by virtue of long Cu—Cl interactions, are tied together to form chains parallel to the a-axis. Within the $CuCl_2(DMSO)_2$ molecules, the sulphoxide molecule bonds to the copper atoms through the oxygen atoms. A mirror plane passes through each $CuCl_2(DMSO)_2$ molecule, the copper and both chlorine atoms lying on the mirror plane. The coordination sphere around the copper atom has approximately C_{2v} symmetry. Each copper atom has five neighbors, four with normal Cu-ligand distances and a fifth at a considerable longer distance. The Cu—O bond lengths are 1.955(4)A and the O—Cu—O bond angle is 173.0(3)°. The Cu—Cl(2) and Cu—Cl(3) bond distances are 2.290(2) and 2.284(2)A respectively, while the Cl(2)—Cu—Cl(3) bond angle is 146.1-

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(4) R. F. Stewart, E. R. Davidson, and W. T. Simpson, *J. Chem. Phys.*, 42, 3178 (1965).
(5) C. H. McGillavry, G. D. Rieck, and K. Lonsdale, « International Tables for X-ray Crystallography », Vol. III, The Kynoch Press, Birmingham, Englanr, 1962.
(6) W. R. Busing, K. O. Martin, and H. A. Levy, *A Fortran Crystallographic Function and Error Program*, U .S. Atomic Energy Commission Report ORNL-TM-306, (1964).
(7) C. K. Johnson, *A Fortran Thermal Ellipsoid Plot Program for Crystal Structure Illustrations*, Oak Ridge National Laboratory, Oak Ridge, Tennessee (1965).

Table II. Observed and Calculated Structure Factors for CuCl$_2$. DMSO[a]

K	L	FO	FC
H = 0			
0	2	412	438
0	4	964	-1048
0	6	98	57
0	8	312	-323
0	10	346	-342
0	12	-56	21
0	14	526	541
1	1	1651	-1227
1	3	83	96
1	5	1377	1115
1	7	145	152
1	9	461	-462
1	11	241	-219
1	13	213	211
1	15	193	-214
2	0	427	-381
2	2	803	761
2	4	319	300
2	6	537	-517
2	8	338	-361
2	10	294	302
2	12	530	548
2	14	171	-151
3	1	891	869
3	3	894	-899
3	5	1001	-1033
3	7	79	-65
3	9	290	281
3	11	342	357
3	13	115	-131
3	15	-61	41
4	0	2686	2175
4	2	199	193
4	4	745	-752
4	6	544	-531
4	8	344	-346
4	10	225	-242
4	12	-59	-90
4	14	452	449
5	1	1171	-1158
5	3	396	-367
5	5	753	720
5	7	124	152
5	9	-56	-283
5	11	108	-92
5	13	174	189
5	15	227	-251
6	0	1540	-1607
6	2	531	525
6	4	470	467
6	6	856	-854
6	8	314	-307
6	10	318	310
6	12	336	345
6	14	161	-178
7	1	586	570
7	3	469	-458
7	5	1013	-1028
7	7	-73	-53
7	9	548	557
7	11	345	338
7	13	188	-167
8	0	1236	1233
8	2	79	91
8	4	487	-474
8	6	297	-284
8	8	140	-149
8	10	186	-170
8	12	132	-110
9	1	683	-677
9	3	757	-229
9	5	284	277
9	7	112	124
9	9	131	100
9	11	-54	-11
9	13	174	119
10	0	584	-592
10	2	241	242
10	4	257	258
10	6	186	-193
10	8	-55	-83
10	10	212	186
10	12	283	264
11	1	318	300
11	3	344	-347
11	5	598	-697
11	7	-53	13
11	9	521	493
11	11	270	268
12	0	950	997
12	2	-53	-47
12	4	353	-344
12	6	129	153
12	8	-53	11
12	10	194	-165
13	1	504	-509
13	3	262	-277
13	5	195	202
13	7	84	107
13	9	-52	-1
14	0	371	-397
14	2	-51	42
14	4	165	177
14	6	-50	-16
14	8	-60	-44
15	1	142	110
15	3	287	-277
15	5	341	-377
16	0	290	316
16	2	55	-86
H = 1			
0	1	102	-60
0	2	2118	1879
0	3	321	354
0	4	469	-472
0	5	423	-437
0	6	778	-847
0	7	745	789
0	8	143	151
0	9	104	-49
0	10	-56	-14
0	11	334	-337
0	12	290	-286
0	13	-59	41
0	14	98	106
0	15	109	15
1	1	1338	1060
1	2	247	-203
1	3	820	-813
1	4	69	41
1	5	625	-612
1	6	701	690
1	7	326	306
1	8	369	-373
1	9	261	-260
H = 1			
1	10	102	-119
1	11	452	-447
1	12	71	88
1	13	193	170
1	14	59	-56
1	15	248	243
2	1	645	-593
2	2	498	512
2	3	-56	-39
2	4	1059	1105
2	5	653	664
2	6	797	824
2	7	135	-141
2	8	494	-507
2	9	223	237
2	10	717	-744
2	11	62	62
2	12	75	-83
2	13	165	-174
2	14	-54	40
2	15	-56	-63
3	1	951	-946
3	2	321	-293
3	3	79	65
3	4	491	474
3	5	92	-48
3	6	589	-600
3	7	323	-331
3	8	160	154
3	9	-61	64
3	10	114	104
3	11	310	317
3	12	95	-122
3	13	-57	-14
3	14	-62	59
3	15	166	-187
4	1	-55	-73
4	2	820	816
4	3	78	-47
4	4	86	93
4	5	261	-259
4	6	517	-527
4	7	519	528
4	8	98	-16
4	9	84	-113
4	10	71	78
4	11	210	-213
4	12	180	-165
4	13	-58	-6
4	14	69	84
4	15	-62	-10
5	1	1137	1154
5	2	109	-95
5	3	619	-594
5	4	130	127
5	5	621	-593
5	6	549	527
5	7	114	104
5	8	385	-385
5	9	283	-274
5	10	175	-155
5	11	326	-328
5	12	-61	51
5	13	245	243
5	14	84	-34
5	15	253	253
6	1	485	-473
6	2	381	-365
6	3	86	-87
6	4	1089	1096
6	5	587	580
6	6	813	825
6	7	281	-275
6	8	516	-516
6	9	98	124
6	10	489	-489
6	11	145	151
6	12	-56	46
6	13	187	-183
6	14	56	27
7	1	311	-306
7	2	268	270
7	3	560	551
7	4	169	177
7	5	-61	107
7	6	432	-438
7	7	481	-498
7	8	177	177
7	9	112	96
7	10	-57	-2
7	11	426	446
7	12	130	-113
7	13	-59	21
7	14	81	66
8	1	-58	12
8	2	519	506
8	3	-61	-51
8	4	-57	12
8	5	205	-177
8	6	371	-364
8	7	339	345
8	8	-61	48
8	9	108	-93
8	10	160	149
8	11	148	-133
8	12	128	-96
8	13	-60	4
9	1	833	838
9	2	205	197
9	3	119	-95
9	4	-61	1
9	5	346	-334
9	6	411	394
9	7	112	-114
9	8	208	-208
9	9	151	-153
9	10	197	-185
9	11	118	-98
9	12	122	42
9	13	167	182
10	1	195	-189
10	2	75	-82
10	3	-53	-8
10	4	426	431
10	5	317	302
10	6	437	426
10	7	125	-154
10	8	229	-210
10	9	150	114
10	10	312	-509
10	11	79	82
10	12	-55	17
11	1	122	-91
11	2	258	249
11	3	377	375
11	4	139	132
11	5	-54	-12
H = 1			
11	6	214	-254
11	7	440	-441
11	8	129	116
11	9	-59	29
11	10	-55	-31
11	11	319	322
12	1	-54	88
12	2	404	413
12	3	-50	3
12	4	224	-238
12	5	186	-186
12	6	368	-354
12	7	276	248
12	8	153	149
12	9	61	-38
12	10	129	109
13	1	533	550
13	2	-54	54
13	3	201	-202
13	4	-53	82
13	5	304	-333
13	6	258	263
13	7	-56	-71
13	8	146	-184
13	9	131	-153
14	1	117	-72
14	2	97	-130
14	3	-51	18
14	4	130	121
14	5	69	132
14	6	204	211
14	7	133	-121
15	1	93	-19
15	2	-53	79
15	3	111	117
15	4	160	140
15	5	87	-81
16	1	90	65
16	2	61	101
H = 2			
0	0	1401	-1689
0	1	78	34
0	2	1172	-1327
0	3	344	-353
0	4	746	788
0	5	1126	-1254
0	6	185	174
0	7	146	-154
0	8	76	-82
0	9	773	809
0	10	521	530
0	11	226	216
0	12	198	-184
0	13	165	-168
0	14	298	-307
0	15	-58	16
1	0	1148	1241
1	1	70	33
1	2	231	-216
1	3	403	373
1	4	779	-779
1	5	840	-840
1	6	281	287
1	7	210	-210
1	8	181	166
1	9	547	538
1	10	363	-347
1	11	76	-88
1	12	135	-142
1	13	73	54
1	14	172	161
1	15	116	94
2	0	321	-324
2	1	839	-822
2	2	92	118
2	3	707	-683
2	4	451	-437
2	5	304	301
2	6	262	251
2	7	170	164
2	8	334	353
2	9	-60	-32
2	10	428	-443
2	11	93	106
2	12	137	-122
2	13	99	62
2	14	-56	-1
2	15	145	-150
3	0	754	-766
3	1	647	638
3	2	615	-575
3	3	64	52
3	4	301	310
3	5	610	617
3	6	173	155
3	7	335	355
3	8	136	-134
3	9	482	-475
3	10	195	198
3	11	83	-29
3	12	-59	79
3	13	-56	-32
3	14	183	-217
3	15	74	-21
4	0	675	-695
4	1	162	153
4	2	672	-656
4	3	479	-439
4	4	710	701
4	5	886	-899
4	6	371	378
4	7	-58	-19
4	8	100	79
4	9	510	540
4	10	401	423
4	11	212	228
4	12	125	-126
4	13	-57	-69
4	14	201	-202
4	15	-60	-31
5	0	727	712
5	1	215	209
5	2	284	-271
5	3	428	422
5	4	573	-555
5	5	564	-554
5	6	425	419
5	7	184	-159
5	8	262	240
5	9	381	378
5	10	299	-310
5	11	154	-139
5	12	196	-186
5	13	128	48
5	14	81	97
H = 2			
6	0	346	334
6	1	581	-573
6	2	281	260
6	3	595	-558
6	4	420	-413
6	5	477	463
6	6	359	367
6	7	264	255
6	8	416	421
6	9	200	-202
6	10	422	-426
6	11	101	119
6	12	104	-63
6	13	127	143
6	14	86	79
7	0	1054	-1066
7	1	140	105
7	2	130	-130
7	3	-56	42
7	4	594	606
7	5	729	722
7	6	109	79
7	7	126	148
7	8	73	30
7	9	526	-540
7	10	229	244
7	11	-60	-39
7	12	-64	3
7	13	-59	-36
7	14	235	-211
8	0	455	-447
8	1	186	174
8	2	377	-346
8	3	175	-153
8	4	421	428
8	5	540	-547
8	6	213	195
8	7	-56	-1
8	8	-55	16
8	9	357	363
8	10	293	297
8	11	185	161
8	12	88	-80
8	13	-61	-51
9	0	136	68
9	1	-61	-31
9	2	124	-37
9	3	334	334
9	4	131	-106
9	5	187	-176
9	6	250	248
9	7	266	-249
9	8	297	288
9	9	132	133
9	10	166	-158
9	11	106	-126
9	12	173	-197
9	13	57	-6
10	0	-55	44
10	1	289	-295
10	2	110	125
10	3	221	-211
10	4	281	-272
10	5	261	275
10	6	97	59
10	7	126	93
10	8	134	151
10	9	123	-111
10	10	265	-279
10	11	-55	32
10	12	-55	-48
11	0	754	-769
11	1	-58	43
11	2	91	-104
11	3	90	83
11	4	429	426
11	5	506	501
11	6	-55	84
11	7	72	36
11	8	105	60
11	9	404	-417
11	10	144	159
11	11	-56	-58
12	0	372	-348
12	1	156	179
12	2	202	-220
12	3	-53	42
12	4	278	272
12	5	369	-372
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7	10	-59	-28
8	1	-57	-83
8	2	356	347
8	3	111	121
8	4	79	62
8	5	90	-104
8	6	156	-159
8	7	123	138
8	8	-54	-2
8	9	-58	11
9	1	387	356
9	2	63	-38
9	3	-55	-57
9	4	164	-177
9	5	247	-245
9	6	-54	19
9	7	71	-47
9	8	128	-92
10	1	-55	80
10	2	78	-92
10	3	72	-53
10	4	160	201
10	5	-53	62
10	6	200	202
10	7	137	-143
11	1	52	3
11	2	60	-59
H = 7			
11	3	212	225
11	4	173	145
11	5	113	-51
11	6	103	-91
12	1	81	-91
12	2	231	236
12	3	-52	41
12	4	65	-34
H = 8			
0	0	642	-662
0	1	103	122
0	2	302	-312
0	3	-55	55
0	4	412	440
0	5	119	-125
0	6	65	99
0	7	84	99
0	8	-56	-18
0	9	123	118
0	10	283	276
0	11	-59	28
1	0	85	59
1	1	109	90
1	2	-56	-37
1	3	219	216
1	4	134	-115
1	5	342	-332
1	6	78	115
1	7	77	-103
1	8	155	135
1	9	291	276
1	10	-60	12
1	11	105	-100
2	0	178	-175
2	1	173	-163
2	2	109	-34
2	3	248	-240
2	4	199	-187
2	5	-56	18
2	6	248	245
2	7	87	46
2	8	318	307
2	9	-57	49
2	10	215	-225
2	11	98	52
3	0	-54	-102
3	1	-52	70
3	2	-56	115
3	3	65	-35
3	4	161	179
3	5	290	297
3	6	-58	-92
3	7	83	100
3	8	-55	-25
3	9	270	-262
3	10	-65	-18
4	0	406	-412
4	1	92	61
4	2	247	-272
4	3	-58	41
4	4	314	336
4	5	-58	-95
4	6	183	172
4	7	82	53
4	8	93	20
4	9	94	94
4	10	182	212
5	0	-55	12
5	1	121	126
5	2	89	-47
5	3	310	303
5	4	105	-85
5	5	211	-217
5	6	158	131
5	7	-64	-105
5	8	151	134
5	9	213	193
5	10	-63	-14
6	0	-56	64
6	1	170	-186
6	2	-57	-16
6	3	205	-203
6	4	213	-231
6	5	-54	39
6	6	254	279
6	7	113	-3
6	8	294	279
6	9	-57	13
7	0	80	-120
7	1	-54	11
7	2	-52	-5
7	3	-58	25
7	4	117	124
7	5	379	385
7	6	-56	-29
7	7	65	53
7	8	125	-82
8	0	207	-235
8	1	-57	45
8	2	175	-189
8	3	-55	44
8	4	231	239
8	5	-59	-70
8	6	91	109
8	7	-57	18
8	8	89	-34
9	0	65	-10
9	1	131	69
9	2	138	-115
9	3	244	261
9	4	61	-77
9	5	82	-55
9	6	135	137
9	7	66	-99
10	0	-52	24
10	1	94	-92
10	2	-54	11
10	3	121	-116
10	4	170	-151
10	5	-52	31
11	0	64	-103
11	1	-56	27
11	2	-52	-16
11	3	74	47
H = 9			
0	1	-56	36
0	2	353	-357
0	3	311	325
0	4	-52	41
0	5	131	-166
0	6	93	102
0	7	202	-218
0	8	77	-77
H = 9			
0	9	121	-100
1	1	225	-192
1	2	259	266
1	3	193	155
1	4	180	-142
1	5	119	72
1	6	85	-35
1	7	99	-75
1	8	-62	8
1	9	94	109
2	1	293	288
2	2	74	-65
2	3	206	-217
2	4	274	-270
2	5	-55	-60
2	6	192	-189
2	7	-58	-69
2	8	133	139
2	9	81	62
3	1	107	117
3	2	274	-299
3	3	88	-85
3	4	-57	67
3	5	-55	33
3	6	-59	-31
3	7	121	96
3	8	-61	30
3	9	116	-42
4	1	103	23
4	2	205	-211
4	3	211	218
4	4	109	-33
4	5	165	-173
4	6	64	69
4	7	170	-176
4	8	-58	-17
5	1	226	-229
5	2	189	185
5	3	137	121
5	4	189	-195
5	5	124	107
5	6	70	-45
5	7	-59	-19
5	8	69	50
6	1	221	225
6	2	-59	71
6	3	265	-253
6	4	291	-289
6	5	-56	-65
6	6	194	-179
6	7	-55	-16
7	1	-56	41
7	2	314	-301
7	3	163	-150
7	4	54	-2
7	5	-54	18
7	6	-58	20
8	1	-59	-15
8	2	94	-131
8	3	176	175
8	4	-58	-18
8	5	104	-110
9	1	218	-213
9	2	82	86
9	3	71	35
H = 10			
0	0	765	363
0	1	81	-59
0	2	-56	-14
0	3	-57	75
0	4	-57	-6
0	5	230	249
0	6	-54	21
0	7	-57	27
1	0	148	-174
1	1	113	-129
1	2	-56	46
1	3	103	85
1	4	138	147
1	5	123	76
1	6	125	-78
1	7	-62	-33
2	0	-56	-92
2	1	219	217
2	2	146	113
2	3	270	261
2	4	-55	-12
2	5	66	3
2	6	-58	-39
2	7	112	-97
3	0	171	160
3	1	-54	92
3	2	-52	9
3	3	142	-128
3	4	171	-131
3	5	-61	-76
3	6	-56	-39
4	0	216	218
4	1	88	-34
4	2	91	-14
4	3	61	86
4	4	-58	4
4	5	211	194
4	6	88	-55
5	0	87	-92
5	1	100	-128
5	2	75	89
5	3	-57	46
5	4	157	113
5	5	-63	44
6	0	186	-183
6	1	184	197
6	2	98	92
6	3	215	230
6	4	-58	0
7	0	249	261
7	1	94	78
7	2	-54	41
7	3	109	-108
H = 11			
0	1	68	-64
0	2	-57	-75
0	3	103	-101
1	1	-57	-2
1	2	-61	-100
1	3	-60	34
2	1	203	-210
2	2	-60	50
2	3	62	26
3	1	-54	-19
3	2	86	88

[a] Unobserved reflections are designed by a minus sign preceeding the value for F_{obs}.

Table III. Interatomic Bond Distances and Bond Angles in CuCl$_2$. 2DMSO

Bond Distances		Bond Angles			
Bond	Distance (A)	Angle	Value (°)	Angle	Value (°)
Cu(1)—Cl(2)	2.290(2)	Cl(2)—Cu(1)—Cl(3)	146.13(9)	Cu(1)—Cl(2)—Cu(1′)	144.58(10)
Cu(1)—Cl(3)	2.284(2)	Cl(2)—Cu(1)—Cl(2′)	112.67(5)	Cu(1)—O(5)—S(4)	118.2 (2)
Cu(1)—O(5)	1.955(4)	Cl(2′)—Cu(1)—Cl(3)	101.20(8)	O(5)—S(4)—C(6)	104.7 (3)
Cu(1)—Cl(2′)	2.702(2)	Cl(2)—Cu(1)—O(5)	88.73(12)	O(5)—S(4)—C(7	103.9 (3)
O(5)—S(4)	1.531(4)	Cl(3)—Cu(1)—O(5)	92.87(12)	C(6)—S(4)—C(7)	100.4 (3)
S(4)—C(6)	1.771(7)	Cl(2′)—Cu(1)—O(5)	87.49(13)		
S(4)—C(7)	1.765(7)	O(5)—Cu(1)—O(5′)	173.01(26)		

Table IV. C—H Distances and Associated Bond Angles in $CuCl_2 . 2DMSO$

Bond Distances		Bond Angles			
Bond	Distance (A)	Angle	Value (°)	Angle	Value (°)
C(6)—H(8)	1.07(11)	S(4)—C(6)—H(8)	105(7)	H(8)—C(6)—H(9)	92(8)
C(6)—H(9)	1.04(12)	S(4)—C(6)—H(9)	115(6)	H(8)—C(6)—H(10)	124(10)
C(6)—H(10)	0.85(12)	S(4)—C(6)—H(10)	114(8)	H(9)—C(6)—H(10)	105(10)
C(7)—H(11)	0.85(12)	S(4)—C(7)—H(11)	108(7)	H(11)—C(7)—H(12)	110(10)
C(7)—H(12)	0.83(11)	S(4)—C(7)—H(12)	114(8)	H(11)—C(7)—H(13)	104(9)
C(7)—H(13)	1.18(11)	S(4)—C(7)—H(13	108(5)	H(12)—C(7)—H(13)	113(9)

Table V. Observed d—d Transition of the Various Cu^{II} Complexes[a]

$CuCl_2(DMSO)_2$	$K_2CuCl_4 . 2H_2O$ (square planar)	Cs_2CuCl_4 (tetrahedral)	$[Cr(NH_3)_6][CuCl_5]$ (trigonal bipyramidal)
12.9	12.5	4.80	8.3
14.9	13.1	5.55	10.0
		7.90	
		9.50	

[a] All numbers are in kK units (1 kK = 1000 cm^{-1}).

(1)°. The long Cu—Cl(2) distance arises from the packing which places one chlorine atom from one complex 2.70(2)A from the copper atom of the complex adjacent to it along the a-axis.

The complex assumes neither idealized planar nor trigonalbipyramidal geometry. The principle deviations are the Cl—Cu—Cl bond angle of 146° intermediate between the idealized values of 180°and 120° respectively, and the 2.7A Cu—Cl distance, 0.4A longer than the normal Cu—Cl bond distance. However, a number of experimental data point very strongly to the fact that the complex can be better described by considering it to be a distorted planar complex. These arguments will be enumerated in the following three paragraphs.

First, the bond distances are more consistant with a planar geometry than a trigonal-bipyramidal structure. The square-planar $CuCl_4^{2-}$ ion in $(C_2H_5NH_3)_2CuCl_4$ has bond distances of 2.30A,[8] in very good agreement with those observed in this structure. However, the equitorial Cu—Cl bond lengths in the $CuCl_5^{3-}$ ion in $Co(NH_3)_6CuCl_5$ are 2.39A.[9] This length is incompatible with the results presented here. Similarly, it can be concluded that the 2.7A Cu—Cl distance is too long to be normal covalent bond. If only van der Waals interactions are assumed between adjacent molecules, an intermolecular Cu—Cl distance of 2.5A is calculated. The observed distance is 0.2A longer than this and so it must be concluded that this is merely a convenient packing site for the location of the Cl(2) atom of the adjacent molecule.

The single crystal polarized spectrum is also consistent with this view. Langs[10] has measured the polarized spectra of $K_2CuCl_4 . 2H_2O$ and $CuCl_2 . 2DMSO$ among others. The former compound contains the *trans* planar $CuCl_2 . (H_2O)_2$ group. The spectra of both compounds shows two absorption bands in the d—d region, ranging from 12,500 to 15,000 cm^{-1}. On the other hand the d—d bands for the tetrahedral[11] and the bipyramidal[12] copper complexes occur at values below 10,000 cm^{-1}. These are summarized in Table V.

Table VI. Comparison of Bond Angles and Bond Distances in Gaseous DMSO itspresence in $CuCl_2 . 2DMSO$.

	Gaseous DMSO	DMSO in $CuCl_2 . 2DMSO$
C—S—C	100°±5°	100.4°±0.3°
O—S—C	107°±5°	104°—105°
S—C	1.82A	1.77A
S=O	1.47A	1.53A
C—H	1.08A	0.83—1.18A

The elongation of the S=O bond correlates well with the shift of the S=O stretching frequency toward a lower value.

The EPR data is also consistent with this interpretation. Reddy *et al.*[13] have assumed a strict planar grouping in interpreting their EPR data on $CuCl_2 . 2DMSO$ and concluded that the normal to the plane made an angle of 32° 19′ with the a-axis. This is close to the value of 22° found for the angle made by the bisector of the Cl—Cu—Cl bond angle with the a-axis. Knowing the geometry of the species, it is possible to calculate the principal g-values and so we have obtained $g_1 = 2.347$, $g_2 = 2.021$, and $g_3 = 2.107$, with g_1 being parallel to the bisector of the Cl—Cu—Cl bond angle, and g_3 parallel to the b-axis. It is interesting to compare these values with those found for the square-planar coordinated compound $CuCl_2(H_2O)_2$[14] where $g_1 = 2.352$, $g_2 = 2.037$, and $g_3 = 2.080$, and those found for the trigonal-bipyramidal $CuCl_5^3$ ion[15] where $g_1 = 2.234$ and $g_{11} =$

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(11) J. Ferguson, *J. Chem. Phys.*, *40*, 3406 (1964).

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(13) T. R. Reddy and R. Srinivasan, *J. Chem. Phys.*, *45*, 2714 (1966).

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2.0023. Since the g values depend on the nature of the distribution of the unpaired electron density through spin-orbit coupling terms in the Hamiltonian, the EPR data presents conclusive evidence that the electron distribution in the complex is basically the same as in a planar complex.

The existence of the oxygen coordinated dimethylsulphoxide molecule in $CuCl_2(DMSO)_2$ was predicted by Selvin *et al.*, based on the S=O stretching frequency of 1053 cm^{-1} to 980 cm^{-1} for DMSO and $CuCl_5(DMSO)_2$ respectively.

The structure of DMSO in gas phase has been determined[16] by the electron diffraction sector method as described by Viervoll.[17] It is interesting to observe that there is little change in the geometry of the gaseous DMSO molecule as compared to the DMSO ligand in the solid state. This may be best appreciated in Table VI. The elongation of the S=O bond correlates well with the shift of the S=O stretching frequency toward a lower value.

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(16) O. Bastiansen and H. Viervoll, *Acta Chem. Scand.*, *2*, 702 (1948).

(17) H. Viervoll, *Acta Chem. Scand.*, *1*, 120 (1947).