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The Crystal and Molecular Structure of Hydrated Dichlorodithiabendazolecobalt(II), $Co(tb)_2Cl_2.xH_2O$*

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The crystal and molecular structure of hydrated dichlorodithiabendazolecobalt(II) hydrate $Co(tb)_2Cl_2.xH_2O$ *has been determined by single crystal X-ray diffraction methods. The complex crystallizes in the monoclinic* $P2_1/c$ *space group with four molecules in a unit cell of dimensions* $a = 11.48$ (2), $b = 19.09$ (2), $c = 10.67$ (2) Å, $\beta = 98.20$ $(24)^{\circ}$. *The multiple film equi-inclination Weissenberg technique was used to measure the intensities of 2505 reflexions. Using the symbolic addition procedure for centro-symmetric crystals, the phases of 580 reflexions were obtained. Several cycles of electron density and difference maps revealed the complete structure. The conventional discrepancy factor after several cycles of full matrix least squares refinements was 0.140.*

Two bidentate chelate molecules in cis-*configuration and two chlorine atoms are coordinated to the Co atom to form an octahedron in which the thiazole rings are* trans *to each other. This octahedron is slightly distorted to relieve the strains in the two 5-membered chelate rings. The presence of an infinite tunnel running in the* a-*direction and the experimental observation that two moles of water of crystallisation can be removed mithout disturbing the structure indicate the crystal to be zeolitic in character.*

Introduction

Thiabendazole, a 2-(4-thiazolyl)benzimidazole is a well known anthelmintic and fungistatic agent but its potential efficacy is reduced by its virtual insolubility in water. Its structural similarity to such chelating agents as 2,2′-dipyridine and 1,10-phenanthroline prompted the preparation of complex with such « non-toxic » metals as cobalt, coper, iron, manganese, nickel and zinc, which would be more water soluble, yet retain the biological activity of the base.[1] Little structural information could be gained from spectroscopic and magnetic data due to the insolubility of the majority of the complexes in even the most polar solvents. Also the presence of three nitrogen and one sulphur atoms makes its mode of coordination less predictable. For these reasons it was decided to examine one of the complexes by X-ray diffraction. Dichlorodithiabendazolecobalt(II) hydrate was chosen for such an analysis because good crystals could be obtained from a mixture of methanol and ether.

Experimental Section

The preparation and analysis of the complex $Co(tb)_2Cl_2.2H_2O$ has been published elsewhere.[1] The complex crystallizes in the monoclinic system as pink diamond shaped plates with the *a* and *c* axes parallel to the diagonals of the plate and the *b* axis parallel to the thichness edge. The space group, obtained from systematic absences is $P2_1/c$. The unit cell parameters, measured at room temperature from Weissenberg patterns onto which had been superimposed the powder pattern of silicon ($a = 5.4305$ Å at 25°C), were found to be $a = 11.48$ (2)*, $b = 10.09$ (2), $c = 10.67$ (2) Å. $\beta = 98.20$ $(24)^{\circ}$, $V = 2314$ (16) $Å^3$.[3] The density of the crystals was determined from both relative density bottle and from flotation measurements, using water and a mixture bromo- and iodobenzene respectively. The experimental density $D_{obs} = 1.568$ (4), indicated 1 mole of water in the complex ($C_{20}H_{14}N_6S_2Cl_2Co.xH_2O$ requires ($Z = 4$), $D_{calc} = 1.53$, 1.58 and 1.63 when $x = 0.1$ and 2 respectively). The crystals are flat prisms with diamond shaped cross-sections, the long and short diagonals corresponding to the *b* and *c* axes respectively. The intensity data were collected from two crystals of approximate dimensions $0.25 \times 0.13 \times 0.08$ mm^3 at room temperature by the multiple film equi-inclination Weissenberg method using CoK_α radiation ($\lambda = 1.7902$ Å, $\mu = 74.6$ cm^{-1}). The intensities of 2505 reflexions were measured against a calibrated scale and corrected for the Lorentz and polarisation factors and α_1, α_2 splitting[2] but not for absorption nor for spot shape on the non-zero levels. In all, 805 (31.1%) reflections were too weak to be observed. Approximate correlation factors beween sets of photographs were determined and used to place the data on the absolute scale by a least fit of Wilson's plot.[3]

All computations were carried out on a one bank CDC3600 computer, using programs developed by

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(*) tb is used to indicate the ligand thiabendazole.

[1] C. Kowala, K.S. Murray, J.M. Swan, and B.O. West, *Austral. J. Chem.* 24. 1369 (1971).

(*) The figures in the parentheses here and in succeeding tables are the standard deviations of the least significant digits.

[2] A.J.M. Rae and W.W. Barker, *Acta Cryst.*, 14, 1208 (1961).

[3] A.J.C. Wilson, *Nature*, *150*, 151 (1942).

[4] W.R. Busing, K.O. Martin, and H. A. Levy, Oak Ridge National Laboratory Report No. ORNL-TM-305 (1962).

Busing, Martin and Levy[4] (least squares refinement), J.F. Blount (Fourier syntheses), Norment[5] (derivation of normalized structure factors and least squares planes) and by one of us (J.A.W.) (data processing routines, and symbolic addition procedure).

Structure Determination

Patterson function. A three-dimensional sharpened Patterson function was computed. Probable sites for the cobalt atom and for six octahedrally coordinated ligand atoms were determined and used as the basis for a number of electron density, difference and β-modified[6] maps. Only one ligand molecule eventually became evident and perhaps because the chlorine atoms had been incorrectly identified as being in *trans* coordination sites, no further progress with this partial structure was made.

Symbolic Addition Procedure. The absolute scale and overall temperature factors were redetermined by the K-curve method of Karle and Hauptmann[7] and found to be in satisfactory agreement with those determined earlier by Wilson's method. The statistical averages and distribution of magnitudes of the normalized structure factors are given in Table 1.

Table 1. Statistical Averages and Distributions of $|E_H|$.

	Experimental	Centro-symmetric
$<\lvert E_H\rvert>$	0.851	0.798
$<\lvert E_H^2-1\rvert>$	0.892	0.968
$<E_H^2>-1$	0.023	0.000
$\lvert E_H\rvert>3$	0.3%	0.3%
$\lvert E_H\rvert>2$	3.3%	5.0%
$\lvert E_H\rvert>1$	29.6%	32.0%

In the initial stage, the 95 reflexions with $|E_H|$ values greater than 2.0 were taken and all triplet index relationships found manually. A symbol was given to the phase of each reflexion and these were gradually equated to one another as coincidences were found in the list of triplets. Ninety consistent signs were found of which 9 were considered to be in doubt and for 5 reflexion, no relationship could be found. At this stage, a symbolic addition computer program was written in which a set of mutually consistent signs and symbols is gradually built up as the lower limit of acceptable $|E_H|$ values is allowed to decrease. The ninety reflexions for which signs and symbols had just been found were used as input. The phases of 580 reflexiones out of a possible 704 with $|E_H|$ greater than 1.1 were determined in terms of two symbols a and b. At an early stage of the procedure, it had become clear that $a = -b$ and towards the end, a number of relationships consistently indicated that $a = +1$.

Electron Density Calculations. The first electron density map based on the 580 reflexions, the phases of which had been determined by the symbolic addition procedure, revealed the sites of all but four

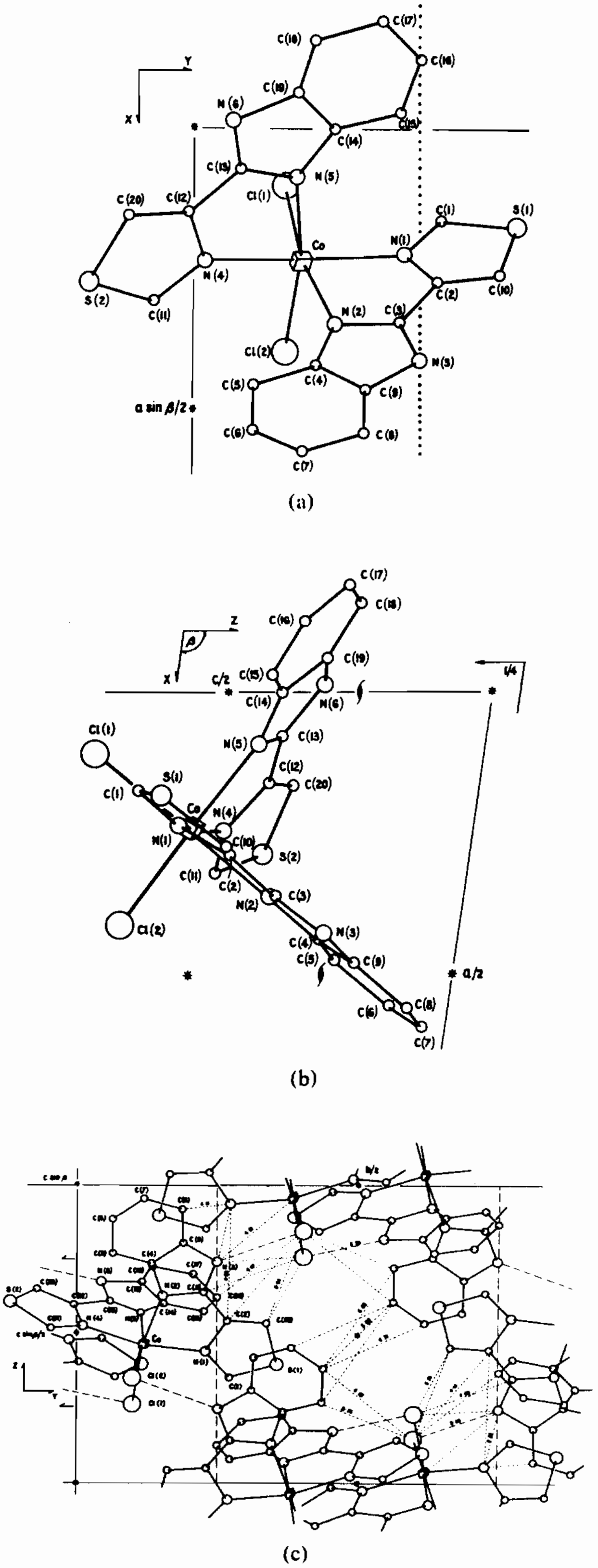

Figure 1. Projections of the structure of the dichlorodithiabendazolecobalt(II) complex viewed (a) along the *c* axis, (b) along the *b* axis, (c) along the *a* axis.

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(5) H.G. Norment, Naval Research Laboratories Reports 5739 and 5739 (Addenda) (1962).

(6) G.N. Ramachandran, and S. Raman, *Acta Cryst.*, *12*, 957 (1959).

(7) J. Karle and H. Hauptman, *Acta Cryst.*, 6, 473 (1953).

Table II. Observed and Calculated Structure Factors (Columns are h,k,F_o and F_c unobserved reflection are starred).

L = 0			
0	2	304	-404
0	4	2529	-2261
0	6	1556	-1250
0	8	2598	1865
0	10	374	303
0	12	632	-533
0	14	559	-424
0	16	198	128
0	18	487	394
0	20	143	123
1	0	297	140
1	1	1957	-1742
1	2	557	340
1	3	371	-376
1	4	186	-71
1	5	804	609
1	6	75	75
1	7	1056	867
1	8	507	315
1	9	766	-547
1	10	182	-155
1	11	125	-147
1	12	134	-157
1	13	58*	-61
1	14	149	117
1	15	61*	-94
1	16	125	-95
1	17	144	130
1	18	58*	54
1	19	88	-22
1	20	43*	21
2	0	857	-940
2	1	343	299
2	2	303	238
2	3	990	-1023
2	4	748	504
2	5	491	418
2	6	394	-270
2	7	39*	-33
2	8	1393	-1225
2	9	46*	6
2	10	249	-177
2	11	422	-332
2	12	467	408
2	13	216	177
2	14	61*	-82
2	15	240	159
2	16	196	-196
2	17	63*	55
2	18	174	-167
2	19	50*	-3
2	20	210	199
3	0	823	-779
3	1	103	92
3	2	107	117
3	3	683	-739
3	4	125	157
3	5	193	-218
3	6	39*	49
3	7	509	358
3	8	158	-131
3	9	669	554
3	10	188	-117
3	11	55*	-6
3	12	155	-120
3	13	422	-368
3	14	379	-295
3	15	63*	-15
3	16	251	-199
3	17	288	289
3	18	260	220
3	19	234	255
4	0	388	417
4	1	575	607
4	2	72	-67
4	3	412	373
4	4	136	-50
4	5	199	-214
4	6	413	368
4	7	731	-656
4	8	247	219
4	9	431	423
4	10	55*	-70
4	11	267	203
4	12	481	-483
4	13	61*	9
4	14	63*	-52
4	15	66*	-83
4	16	312	320
4	17	58*	-46
4	18	127	157
4	19	79	-78
5	0	331	313
5	1	477	-431
5	2	305	-318
5	3	378	-421
5	4	120	74
5	5	103	-79
5	6	308	283
5	7	387	429
5	8	118	125
5	9	295	-256
5	10	269	-282
5	11	279	-276
5	12	61*	40
5	13	63*	-64
5	14	361	331
5	15	248	278
5	16	100	-107
5	17	120	-114
5	18	120	-173
6	0	807	-798
6	1	135	-100
6	2	213	-179
6	3	27*	-84
6	4	743	794
6	5	198	220
6	6	553	648
6	7	55*	31
6	8	548	-674
6	9	217	-250
6	10	520	-632
6	11	61*	-16
6	12	185	203
6	13	137	122
6	14	420	540
6	15	58*	33
6	16	127	-135
6	17	46*	-71
7	0	594	525
7	1	541	545
7	2	32*	61
7	3	668	732
7	4	164	-138
7	5	124	112
7	6	205	-217
7	7	332	-483
7	8	197	192
7	9	110	-119
7	10	63*	98
7	11	398	485
7	12	134	146
7	13	196	217
7	14	182	-176
7	15	173	-191
7	16	46*	-31
8	0	126	166
8	1	275	314
8	2	35*	65
8	3	278	341
8	4	118	-120
8	5	61*	-50
8	6	61*	-15
8	7	139	-169
8	8	134	150
8	9	68*	111
8	10	146	158
8	11	186	223
8	12	58*	7
8	13	131	-118
8	14	91	-100
8	15	123	-172
9	0	61*	32
9	1	104	-66
9	2	61*	32
9	3	103	-58
9	4	63*	0
9	5	139	161
9	6	131	-111
9	7	72*	-22
9	8	63*	-17
9	9	61*	8
9	10	58*	5
9	11	123	-154
9	12	50*	-23
9	13	43*	54
10	0	66*	-10
10	1	66*	-18
10	2	39*	30
10	3	227	-250
10	4	142	-119
10	5	116	91
10	6	118	-120
10	7	230	370
10	8	55*	-112
10	9	53*	87
10	10	50*	55
10	11	193	-227
11	0	141	113
11	1	116	135
11	2	33*	-60
11	3	100	61
11	4	89	-64
11	5	53*	-35
11	6	101	134
11	7	100	-150
11	8	43*	-9
12	0	166	232
12	1	58	-65
12	2	81	115
12	3	65	-30
L = 1			
0	1	1506	-2136
0	2	421	434
0	3	166	-47
0	4	1205	-1106
0	5	1364	1034
0	6	1180	899
0	7	130	-156
0	8	1349	1045
0	9	1472	-1256
0	10	118	50
0	11	51*	1
0	12	993	-839
0	13	613	592
0	14	239	-213
0	15	245	245
0	16	414	327
0	17	458	-429
0	18	60*	70
0	19	229	-244
0	20	130	-141
-1	1	428	-621
1	1	530	-522
-1	2	369	-235
1	2	383	311
-1	3	75	-124
1	3	413	200
-1	4	272	-197
1	4	425	405
-1	5	598	-656
1	5	188	89
-1	6	220	222
1	6	572	-529
-1	7	121	-158
1	7	628	561
-1	8	583	508
1	8	464	-348
-1	9	501	403
1	9	230	-200
-1	10	47*	28
1	10	673	608
-1	11	477	329
1	11	245	-236
-1	12	530	-414
1	12	425	399
-1	13	174	-169
1	13	252	263
-1	14	183	154
1	14	167	-126
-1	15	324	-272
1	15	117	99
-1	16	67*	67
1	16	352	-305
-1	17	179	-154
1	17	134	-118
-1	18	282	-251
1	18	60*	5
-1	19	54*	61
1	19	54*	-21
-1	20	142	-135
1	20	128	129
-2	1	1067	936
2	1	686	683
-2	2	1376	1456
2	2	213	182
-2	3	438	-418
2	3	647	600
-2	4	31*	3
2	4	840	667
-2	5	628	-605
2	5	235	-228
-2	6	36*	21
2	6	414	305
-2	7	273	222
2	7	40*	93
-2	8	44*	22
2	8	153	79
-2	9	1063	972
2	9	526	482
-2	10	51*	51
2	10	149	98
-2	11	54*	81
2	11	191	154
-2	12	217	-140
2	12	244	171
-2	13	828	-707
2	13	439	-402
-2	14	62*	-73
2	14	433	-392
-2	15	62*	71
2	15	208	232
-2	16	67*	2
2	16	348	-351
-2	17	458	416
2	17	360	350
-2	18	121	94
2	18	208	199
-2	19	51*	9
2	19	51*	-37
-2	20	40*	20
2	20	120	139
-3	1	88	134
3	1	1088	-1147
-3	2	968	-953
3	2	427	316
-3	3	488	469
3	3	702	701
-3	4	384	346
3	4	492	433
-3	5	901	-811
3	5	850	879
-3	6	178	149
3	6	189	158
-3	7	250	-224
3	7	44*	-26
-3	8	94	-32
3	8	79	-24
-3	9	700	628
3	9	301	-286
-3	10	185	236
3	10	440	-427
-3	11	888	739
3	11	104	-69
-3	12	132	128
3	12	60*	38
-3	13	217	-176
3	13	219	195
-3	14	62*	63
3	14	295	303
-3	15	228	-228
3	15	292	299
-3	16	67*	-79
3	16	181	-158
-3	17	62*	42
3	17	126	138
-3	18	141	151
3	18	237	-282
-3	19	99	115
3	19	140	-149
-4	1	560	-465
4	1	416	-427
-4	2	641	656
4	2	78	-112
-4	3	348	314
4	3	236	250
-4	4	664	723
4	4	370	296
-4	5	530	526
4	5	181	194
-4	6	244	214
4	6	284	249
-4	7	179	-175
4	7	602	-539
-4	8	651	-596
4	8	164	176
-4	9	757	-723
4	9	506	-432
-4	10	205	-184
4	10	389	-434
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4	11	371	417
-4	12	562	562
4	12	62*	-76
-4	13	591	571
4	13	105	111
-4	14	62*	122
4	14	157	138
-4	15	67*	60
4	15	220	-199
-4	16	276	-277
4	16	358	308
-4	17	276	-293
4	17	159	-185
-4	18	108	-122
4	18	139	-166
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4	19	123	118
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5	1	59	-69
-5	2	196	-241
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-5	3	183	-188
5	3	101	92
-5	4	482	-528
5	4	150	122
-5	5	216	-275
5	5	380	-403
-5	6	129	99
5	6	522	-494
-5	7	207	206
5	7	316	276
-5	8	145	155
5	8	54*	-36
-5	9	189	161
5	9	222	-109
-5	10	60*	-66
5	10	593	602
-5	11	197	-239
5	11	62*	-64
-5	12	233	-268
5	12	62*	89
-5	13	164	-134
5	13	273	-301
-5	14	223	204
5	14	202	-175
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5	15	210	231
-5	16	60*	20
5	16	57*	-57
-5	17	113	81
5	17	54*	-24
-5	18	184	-167
5	18	44*	63
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6	1	516	466
-6	2	454	460
6	2	760	867
-6	3	332	-338
6	3	422	-446
-6	4	108	-82
6	4	113	-66
-6	5	541	-632
6	5	581	-623
-6	6	105	-148
6	6	311	-350
-6	7	181	188
6	7	195	245
-6	8	130	-131
6	8	276	-283
-6	9	565	703
6	9	473	538
-6	10	62*	48
6	10	232	300
-6	11	120	-122
6	11	62*	-46
-6	12	65*	11
6	12	107	137
-6	13	383	-460
6	13	138	-132
-6	14	65*	54
6	14	107	116
-6	15	60*	56
6	15	60*	-96
-6	16	54*	35
6	16	254	-241
-6	17	246	247
6	17	44*	55
-7	1	447	-515
7	1	260	311
-7	2	451	504
7	2	955	-1147
-7	3	149	157
7	3	266	307
-7	4	57*	42
7	4	246	-238
-7	5	598	653
7	5	126	-154
-7	6	182	-227
7	6	417	437
-7	7	101	-118
7	7	126	-104
-7	8	114	98
7	8	387	420
-7	9	280	-323
7	9	130	120
-7	10	402	445
7	10	472	-486
-7	11	244	-280
7	11	67*	-1
-7	12	132	-87
7	12	215	-212
-7	13	125	98
7	13	116	100
-7	14	110	-134
7	14	57*	24
-7	15	54*	70
7	15	51*	-86
-7	16	47*	-6
7	16	138	180
-8	1	253	-281
8	1	284	-325
-8	2	125	80
8	2	424	-497
-8	3	257	315
8	3	262	313
-8	4	110	-73
8	4	62*	60
-8	5	133	135
8	5	62*	11
-8	6	162	146
8	6	206	193
-8	7	282	-330
8	7	142	-144
8	8	62*	65
8	8	116	103
-8	9	306	-338
8	9	67*	-62
-8	10	124	122
8	10	282	-297
-8	11	126	131
8	11	188	197
-8	12	126	-86
8	12	110	105
-8	13	57*	19
8	13	54*	-47
-8	14	87	36
8	14	47*	50
-8	15	83	-96
8	15	40*	-35
-9	1	164	-77
9	1	105	-20
-9	2	269	-325
9	2	188	165
-9	3	164	171
9	3	123	110
-9	4	136	107
9	4	70*	-52
-9	5	114	-58
9	5	67*	-18
-9	6	294	300
9	6	145	-131
-9	7	67*	40
9	7	148	-155
-9	8	111	73
9	8	138	136
-9	9	65*	-32
9	9	62*	65
-9	10	262	-302
9	10	174	194
-9	11	57*	-29
9	11	232	290
-9	12	54*	-3
9	12	83	-76
-9	13	87	-81
9	13	44*	-16
-10	1	395	420
10	1	147	-155
10	2	430	-434
10	2	133	126
-10	3	196	-181
10	3	35*	16
-10	4	65*	-37
10	4	105	-114
-10	5	126	-137
10	5	147	127
-10	6	362	330
10	6	107	-83
-10	7	60*	63
10	7	206	215
-10	8	254	256
10	8	54*	58
-10	9	272	279
10	9	85	76
-10	10	108	-106
10	10	47*	83
-10	11	85	-82
10	11	95	-119
-11	1	81	90
11	1	54	47
-11	2	442	422
11	2	143	-108
11	3	57*	42
11	3	95	-124
-11	4	57*	33
11	4	51*	-11
-11	5	54*	36
11	5	51*	-64
11	6	138	-128
11	6	85	111
-11	7	47*	-60
11	7	44*	40
-11	8	44*	-88
-11	9	192	32
-12	1	196	-162
-12	2	77	68
-12	3	107	79
-12	4	40*	-31
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2	6	72*	-104
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3	2	142	122
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3	4	161	120
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3	5	179	-327
-3	6	326	-297
3	6	73*	-81
-3	7	89	-58
3	7	57*	37
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4	1	35*	22
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4	2	387	-394
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4	4	177	-142
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4	5	61*	29
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4	6	333	414
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4	7	111	95
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5	2	318	-265
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5	4	187	189
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5	5	499	537
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6	1	129	-109
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6	2	161	146
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6	3	113	76
-6	4	124	90
6	4	50	15
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6	5	55*	102
-6	6	79*	61
6	6	69*	15
-6	7	56*	-25
6	7	47*	6
-7	1	38*	-47
7	1	32*	-25
-7	2	40*	15
7	2	145	94
-7	3	77	121
7	3	83	-73
-7	4	248	196
7	4	44*	76
-7	5	228	216
7	5	47*	12
-7	6	76*	-11
7	6	99	-74
-7	7	119	132
7	7	40*	23
-8	1	246	235
8	1	26*	-45
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8	2	67	55
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8	3	25*	9
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8	4	34*	73
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-9	2	34*	10
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-9	4	120	92
-9	5	226	-206
-9	6	60*	-20
-9	7	41*	-3
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-10	2	198	217
-10	3	26*	17
-10	4	36*	2
L = 8			
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0	2	120	114
0	3	133	104
0	4	123	-127
0	6	150	-108
0	7	187	-198
-1	0	189	-175
1	0	41	-59
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1	1	87	-16
-1	2	90	-68
1	2	37*	48
-1	3	213	-166
1	3	215	-203
-1	4	211	192
1	4	176	-171
-1	6	196	258
1	6	79*	-67
-1	7	225	224
1	7	138	86
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2	1	35*	71
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2	2	97	-61
-2	3	34*	0
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-2	4	364	-345
2	4	214	272
-2	6	215	-236
2	6	78*	-14
-2	7	161	134
2	7	55*	20
-3	0	41*	-52
3	0	191	-128
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3	1	259*	-293
-3	2	115	-97
3	2	40*	-23
-3	3	303	284
3	3	110	-63
-3	4	279	-291
3	4	158	181
3	6	73*	-20
3	6	170	209
-3	7	195	-172
3	7	232	271
-4	0	346	-367
4	0	360	-375
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4	1	209	171
-4	2	37*	66
4	2	127	121
-4	3	91	68
4	3	36*	2
-4	4	214	164
4	4	116	-126
-4	6	79*	28

Table II. (Continued).

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4	7	165	-202
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5	2	129	-106
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5	3	142	79
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5	7	160	-197
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6	0	37*	11
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6	2	32*	-10
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6	3	126	-88
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6	4	42*	-41
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6	7	84	88
-7	0	383	386
7	0	31*	-25
-7	1	106	85
7	1	25*	-31
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7	2	26*	-2
-7	3	78	-87
7	3	85	79
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7	4	33*	78
-7	6	202	-205
-7	7	47*	-50
-8	0	164	-200
-8	1	81	105
-8	2	122	-123
-8	3	31*	45
-8	4	45*	57
-8	6	124	90
-8	7	92	-102
-9	0	33*	15
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-9	2	29*	3
-9	3	27*	-29
-9	4	37*	83
-9	6	48*	-109
L = 9			
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0	2	415	-438
0	3	37*	-12
0	4	109	-89
0	6	220	192
0	7	52*	-29
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-1	2	119	69
1	2	284	-281
-1	3	293	-279
1	3	170	117
-1	4	53*	-52
1	4	52*	2
-1	6	139	-103
1	6	215	228
-1	7	237	232
1	7	88	-68
-2	1	38*	77
2	1	36*	-68
-2	2	40*	37
2	2	149	120
-2	3	110	91
2	3	165	159
-2	4	144	-152
2	4	149	175
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2	6	144	-111
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2	7	152	-189
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3	1	35*	-35
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3	2	276	277
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3	3	33*	-40
-3	4	119	-110
3	4	48*	16
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3	7	45*	33
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4	1	152	165
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4	2	34*	29
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4	3	31*	29
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4	4	44*	107
-4	6	72*	38
4	6	59	-2
-4	7	50*	-60
4	7	40*	35
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5	1	28*	69
-5	2	38*	17
5	2	29*	-32
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5	3	66	82
-5	4	50*	-1
5	4	38*	-25
-5	6	69*	-30
5	6	49*	69
-5	7	48*	-51
-6	1	101	-90
6	1	22*	39
-6	2	259	268
6	2	84	78
-6	3	97	102
-6	4	47*	11
-6	6	208	-243
-6	7	44*	30
-7	1	235	-257
-7	2	81	-55
-7	3	205	246
-7	4	42*	-15
-7	6	57*	-56
-7	7	38*	-10
-8	1	27*	46
-8	2	28*	8
-8	3	26*	36
-8	4	36*	13
L = 10			
0	0	186	-178
0	1	93	56
0	2	35*	74
0	3	279	272
0	4	77	62
0	6	168	257
0	7	177	-191
-1	0	41*	90
1	0	162	142
-1	1	84	-91
1	1	254	310
-1	2	36*	-11
1	2	34*	-26
-1	3	33*	-34
1	3	31*	39
-1	4	138	167
1	4	187	-158
-1	6	64*	103
1	6	59*	-53
-1	7	137	152
1	7	216	-214
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2	0	202	204
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2	1	91	-79
-2	2	36*	-24
2	2	95	-82
-2	3	33*	10
2	3	29*	-52
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2	4	41*	-40
-2	6	64*	29
2	6	55*	-33
-2	7	76	30
2	7	36*	40
-3	0	39*	-15
3	0	33*	-9
-3	1	34*	18
3	1	28*	-9
-3	2	35*	17
3	2	29*	44
-3	3	32*	-66
3	3	26*	4
-3	4	46*	-95
3	4	37*	-3
-3	6	63*	-111
3	6	47*	-86
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-4	0	180	169
4	0	29*	-46
-4	1	33*	37
4	1	24*	48
-4	2	34*	-4
4	2	97	-10
-4	3	31*	-20
4	3	22*	46
-4	4	44*	-57
-4	6	60*	-55
-4	7	64	-34
-5	0	37*	-4
-5	1	122	-166
-5	2	32*	-30
-5	3	175	-192
-5	4	69	119
-5	6	55*	104
-5	7	129	215
-6	0	346	406
-6	1	28*	-14
-6	2	104	-11
-6	3	26*	-33
-6	4	110	-178
-6	6	89	-59
-7	0	101	111
-7	1	104	133
-7	2	74	33
-7	3	141	184
L = 11			
0	1	110	107
0	2	26*	18
0	3	125	-151
-1	1	101	-99
1	1	23*	33
-1	2	149	225
1	2	136	-148
-1	3	25*	-14
1	3	22*	84
-2	1	79	-106
-2	2	130	82
-2	3	25*	17
-3	1	112	-149
-3	2	27*	-42
-3	3	96	147
-4	1	55	-69
-4	2	109	-152
-4	3	23*	-7

Table III. Atomic Positional and Temperature Parameters.

Atom	x	y	z	$B(\text{Å}^2)$
N(1)	0.2340(12)	0.2288(11)	0.4417(7)	4.30(37)
N(2)	0.3625(12)	0.1550(7)	0.6319(14)	4.09(36)
N(3)	0.4308(12)	0.2502(8)	0.7451(13)	4.26(36)
C(1)	0.1750(17)	0.2721(11)	0.3572(20)	5.23(54)
C(2)	0.2876(14)	0.2692(9)	0.5469(17)	4.20(43)
C(3)	0.3604(14)	0.2249(9)	0.6431(17)	4.47(42)
C(4)	0.4399(15)	0.1340(10)	0.7394(18)	4.88(48)
C(5)	0.4756(20)	0.0660(12)	0.7756(22)	5.58(54)
C(6)	0.5541(22)	0.0645(13)	0.8855(27)	7.44(67)
C(7)	0.5960(23)	0.1202(14)	0.9573(27)	7.38(67)
C(8)	0.5610(24)	0.1877(16)	0.9214(27)	6.02(56)
C(9)	0.4826(16)	0.1898(10)	0.8117(18)	4.85(48)
C(10)	0.2728(15)	0.3381(10)	0.5350(18)	4.46(46)
N(4)	0.2467(10)	0.0119(7)	0.5290(12)	4.02(34)
N(5)	0.0932(12)	0.1130(8)	0.5724(4)	4.65(38)
N(6)	—0.0151(16)	0.0442(10)	0.6798(17)	4.25(34)
C(11)	0.3175(20)	—0.0417(14)	0.5195(23)	4.89(47)
C(12)	0.1592(16)	—0.0069(11)	0.5968(19)	3.44(35)
C(13)	0.0802(13)	0.0503(8)	0.6122(15)	3.76(39)
C(14)	0.0018(12)	0.1545(8)	0.6000(15)	4.38(44)
C(15)	—0.0294(14)	0.2263(9)	0.5766(17)	4.65(43)
C(16)	—0.1270(17)	0.2500(10)	0.6241(19)	6.01(51)
C(17)	—0.1963(18)	0.2060(12)	0.6992(21)	6.57(60)
C(18)	—0.1615(19)	0.1353(12)	0.7250(22)	6.25(63)
C(19)	—0.0620(16)	0.1126(11)	0.6765(19)	5.07(47)
C(20)	0.1648(17)	—0.0709(11)	0.6506(20)	5.38(53)
Co	0.24491(20)	0.11914(15)	0.46278(25)	
C1(1)	0.1085(4)	0.1015(2)	0.2639(5)	
C1(2)	0.4146(4)	0.1004(2)	0.3542(4)	
S(1)	0.1845(4)	0.3581(3)	0.3996(4)	
S(2)	0.2859(4)	—0.1142(3)	0.6042(5)	

Anisotropic Thermal Parameters

	$U_{11}(\text{Å}^2)$	$U_{22}(\text{Å}^2)$	$U_{33}(\text{Å}^2)$	$U_{12}(\text{Å}^2)$	$U_{13}\text{Å}^2)$	$U_{23}(\text{Å}^2)$
Co	0.0464(20)	0.0393(22)	0.0634(27)	—0.0014(15)	0.0144(16)	—0.0024(10)
C1(1)	0.0622(32)	0.0636(37)	0.0673(42)	—0.0126(28)	0.0113(27)	0.0030(31)
C1(2)	0.0518(29)	0.0477(34)	0.0821(41)	0.0122(24)	0.0223(26)	0.0099(31)
S(1)	0.0832(38)	0.0481(35)	0.0793(45)	0.0103(31)	0.0157(33)	0.0102(29)
S(2)	0.0677(33)	0.0484(35)	0.1053(52)	0.0066(29)	0.0183(34)	0.0104(36)

atoms and one strong peak, interpreted as being a water molecule, later proved to be spurious. A structure factor calculation based on all these real and false atoms gave $R = \Sigma||F_o|-|F_c||/|F_o| = 0.304$. A second electron density map was calculated in which the contribution from the Co atom only had been removed from each structure factor. The remaining four atoms were readily apparent and all belonged to the aromatic ring of that molecule which had not become apparent in the earlier attempts by the « heavy atom » method. A second peak, also shown later to be spurious, was identified at this stage as the second expected water molecule.

Refinement. Four cycles of full matrix least squares refinement in which $\Sigma\omega(|F_o|-|F_c|)^2$ was minimised

Table IV. Interatomic Distances.

$C_{arom} - C_{arom}$ (Characteristic value = 1.394 (5)Å)[25]		$C(sp^2) - C(sp^2)$ (Characteristic value 1.44 — 1.49Å)[25]	
C(4)-C(5)	1.40±0.03	C(2)-C(3)	1.49±0.03 Å
C(5)-C(6)	1.41±0.04		
C(6)-C(7)	1.35±0.04	C(12)-C(13)	1.45±0.03
C(7)-C(8)	1.39±0.04		
C(8)-C(9)	1.37±0.03		
C(9)-C(4)	1.36±0.03	$C(sp^2) = C(sp^2)$	
C(14)-C(15)	1.43±0.03	(characteristic value = 1.335 (5) Å)[25]	
C(15)-C(16)	1.37±0.03		
C(16)-C(17)	1.43±0.04	C(2)-C(10)	1.33±0.03
C(17)-C(18)	1.45±0.04		
C(18)-C(19)	1.39±0.03	C(12)-C(20)	1.35±0.03
C(19)-C(14)	1.42±0.03		
$C(sp^2)-\{N(sp^2)$ and $= N(sp^2)\}$ resonance forms (Corresponding values in imidazole[21] and N-benzyl-4-methylthiazolium bromide[23] = 1.38 and 1.40Å respectively)		$C(sp^2) = N(sp^2)$ (Corresponding value in imidazole[21] = 1.33 Å)	
C(2)-N(1)	1.40±0.03	C(1)-N(1)	1.35±0.03
C(4)-N(2)	1.41±0.03	C(3)-N(2)	1.34±0.03
C(12)-N(4)	1.39±0.02	C(11)-N(4)	1.32±0.03
C(14)-N(5)	1.38±0.03	C(13)-N(5)	1.29±0.03
$C(sp^2)-\{NH(sp^3)$ and $= NH^+(sp^3)\}$ resonance forms. (Characteristic value = 1.43(1) Å)[25]		$C(sp^2)-S-$ (Characteristic value in conjugated heterocyclic rings = 1.718(5) Å)[25]	
C(3)-N(3)	1.35±0.03	C(1)-S(1)	1.70±0.03
C(9)-N(3)	1.46±0.03	C(10)-S(1)	1.69±0.02
C(13)-N(6)	1.40±0.03	C(11)-S(2)	1.71±0.03
C(19)-N(6)	1.43±0.03	C(20)-S(2)	1.73±0.03
$Co^{II}-Cl$ (Characteristic values in cobaltous complexes = 2.46 Å)[17,18]		$Co^{II} \leftarrow N(sp^2)$ (Value in $Co(NH_3)_6I_2$ = 2.11 Å)[15]	
Co-Cl(1)	2.47±0.008	Co-N(1)	2.14±0.02
Co-Cl(2)	2.43±0.007	Co-N(2)	2.20±0.02
		Co-N(4)	2.16±0.02
		Co-N(5)	2.22±0.02

with all atoms isotropic decreased R to 0.175. Clear indications of anisotropic vibrations of the Co and both pairs of Cl and S atoms were apparent on a difference map and two least squares cycles in which only these 5 atoms were given anisotropic temperature factors reduced R to 0.140. At this stage the sharp peaks and troughs around the Co, Cl and S atoms were reduced to less than ±1eÅ^{-3}. Several broad maxima however, appeared consistently in difference maps, representing the only other significant features in these maps. They were of height 1.0 - 1.1 $e\AA^{-3}$ and were aligned roughly along the a-xis. Inspection of ball and rod as well as space filling models clearly showed the presence of an infinite tunnel centred at $y = z = 0$ (see Figure 1) with intermolecular distances across the tunnel reaching 6Å. Such a tunnel would readily accommodate water and even larger solvent molecules. The assignment of a water oxygen atom to one of the peaks led to occupancy and temperature factor values of 0.38 and 12.9 Å^2 after one cycle of least squares refinement with no significant decrease in the R-factor. No further analysis of these electron density residuals was made.

A listing of observed and calculated structure factors is given in Table II.

The average values of the standard deviations of positional parameters may be summarised as $\sigma_{xa} \approx \sigma_{yb} \approx \sigma_{zc}$ = 0.004, 0.008, 0.02 and 0.03$\AA$ for Co, Cl and S, N and C respectively. The β_{ij} terms refer to the coefficients of the expression exp-$(h^2\beta_{11} + k^2\beta_{22} + l^2\beta_{33} + 2hk\beta_{12} + 2hl\beta_{13} + 2kl\beta_{23})$ and the U_{ij} terms are given by $U_{ij} = \beta_{ij}/2\pi^2a_i^*a_j^*$.

The atomic scattering factor curves were determined by linear interpolation of $f^{-1/2}$[8] from tabulated values for C, N and O,[9] S and Cl[10] and Co.[11] The curve for Co was corrected for anomalous scattering using the data of Dauben and Templeton.[12] The weighting scheme of Hughes[13] and the facility to refine together both isotropic and anisotropic thermal parameters were incorporated into the full matrix least squares program of Busing, Martin, and Levy.[4] Unobserved reflexions were given the value $|F^2| = \frac{1}{2}(L_p)^{-1}$ and were used to calculate R-factors on the basis that $\Delta F \neq 0$ only if $|F_o| < |F_c|$ but they were not used in setting up normal equations.

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Table V. Bond Angles.

S(1)-C(1)-N(1)	114.2±1.8°	S(2)-C(11)-N(4)	113.9±1.7°
N(1)-C(2)-C(3)	111.8±2.0	N(4)-C(12)-C(13)	112.5±1.8
N(1)-C(2)-C(10)	115.1±2.0	N(4)-C(12)-C(20)	118.0±1.8
C(3)-C(2)-C(10)	132.7±2.1	C(13)-C(12)-C(20)	129.0±1.9
C(2)-C(3)-N(2)	121.4±2.0	C(12)-C(13)-N(5)	124.1±1.9
C(2)-C(3)-N(3)	124.4±2.1	C(12)-C(13)-N(6)	123.1±1.9
N(2)-C(3)-N(3)	114.2±2.0	N(5)-C(13)-N(6)	112.6±1.9
C(5)-C(4)-C(9)	119.6±2.1	C(15)-C(14)-C(19)	120.2±2.0
C(5)-C(4)-N(2)	128.2±2.2	C(15)-C(14)-N(5)	133.9±2.1
C(9)-C(4)-N(2)	112.2±2.1	C(19)-C(14)-N(5)	105.6±2.0
C(4)-C(5)-C(6)	112.6±2.4	C(14)-C(15)-C(16)	116.7±2.2
C(5)-C(6)-C(7)	127.5±3.0	C(15)-C(16)-C(17)	123.1±2.5
C(6)-C(7)-C(8)	120.3±2.7	C(16)-C(17)-C(18)	119.3±2.6
C(7)-C(8)-C(9)	112.7±2.5	C(17)-C(18)-C(19)	116.5±2.5
C(4)-C(9)-C(8)	127.3±2.4	C(14)-C(19)-C(18)	124.0±2.4
C(8)-C(9)-N(3)	128.0±2.2	C(18)-C(19-N(6)	127.6±2.3
C(4)-C(9)-N(3)	104.7±1.9	C(14)-C(19)-N(6)	108.0±2.0
C(2)-C(10)-S(1)	111.0±1.7	C(12)-C(20)-S(2)	107.4±1.7
C(1)-N(1)-C(2)	108.5±2.1	C(11)-N(4)-C(12)	110.1±1.9
C(3)-N(2)-C(4)	103.2±1.8	C(13)-N(5)-C(14)	109.7±1.8
C(3)-N(3)-C(9)	105.6±1.8	C(13)-N(6)-C(19)	103.5±1.8
C(2)-N(1)-Co	116.1±0.7	C(12)-N(4)-Co	116.6±0.7
C(3)-N(2)-Co	111.4±0.7	C(13)-N(5)-Co	111.0±0.7
C(1)-S(1)-C(10)	91.0±1.1	C(11)-S(2)-C(20)	90.2±1.2
N(1)-Co-N(2)	78.4±0.7	N(4)-Co-N(5)	75.6±0.7
N(1)-Co-N(5)	94.0±0.7	N(4)-Co-Cl(1)	97.3±0.5
N(1)-Co-Cl(1)	91.3±0.5	N(4)-CoCl(2)	92.6±0.5
N(1)-Co-Cl(2)	97.7±0.5	N(5)-Co-Cl(1)	89.8±0.5
N(2)-Co-N(4)	92.9±0.7		
N(2)-Co-N(5)	91.1±0.7	Cl(1)-Co-Cl(2)	91.3±0.2
N(2)-Co-Cl(2)	89.9±0.5		

Discussion

Molecular Structure. Both thiabendazole ligand molecules are coordinated to the cobalt atom through their two trigonal nitrogen atoms to form two 5-membered bidentate chelate rings in *cis*-configuration. The preferential formation of *cis* isomers of complexes between dipyridyl and *o*-phenanthroline with Co,^{II} Co,^{III} Pd^{II} and Pt^{II} has already been pointed out[14] and rationalized in terms of steric hindrance between the hydrogen atoms at C_2 and C_9 which would occur in the *trans* isomers of the above complexes. A *trans* square or octahedral complex of thiabendazole would also result in severe steric interactions between the hydrogen atoms at C(5) and C(15) with those ot C-(11) and C(1) respectively.

The two chlorine atoms complete the octahedral coordination which is distorted by displacements of the nitrogen atoms, especially N(1) and N(4) of the thiazole rings, from their expected positions. The extent of these displacements is shown by the bond angles in Table V though it should be noted from Table IV that the lengths of the coordinate bonds remain normal.[15,16,17,18] These displacements are a consequence of the angle adjustments required to form the 5-membered chelate rings, resulting in reductions of the normal chelate ring angles at C(2) and C(12) and at the Co atom on the one hand and in increases of the bond angles at N(1) and N(4) on the other. The thiazole rings are *trans* to each other, resulting in a complex possessing aproximate 2-fold symmetry with the axis running between the two chlorine atoms and between the imidazole nitrogen atoms N(2) and N(5).

Both ligand molecules are virtually planar as would be expected from the many limiting resonance forms resulting from the transfer into the molecule of lone pair electrons from the sulphur or secondary nitrogen atoms. The equations of the least squares planes for the thiabendazole molecules containing S(1) and S(2) are, respectively,

$$9.984x+1.471y-6.692z+0.325 = 0$$

and

$$5.500x+5.585y-8.142z-5.764 = 0,$$

where the constants are referred to the monoclinic axes and expressed in Ångstrom units. The maximum deviations of atoms from each plane is 0.083 and 0.090 Å respectively and the standard deviations as defined by $(\Sigma_i^n(d-d_i)^2/(n-3))^{1/2}$ are 0.049 and 0.051 Å respectively. The dihedral angle formed by the least squares planes of the ligands is 89°19′. Similarly, the ligand bond lengths and angles listed in Tables IV and V are consistent with a highly conjugated system and resemble closely those found in comparable structures such as those of « hydrolyzed cocarboxylase »,[19] 5-anilino-3-oxo-2-phenyl-2,3-dihydro-1-H-pyrazolo[3,4-d]thiazole,[20] imidazole,[21] thiamine hydrochloride,[22] N-benzyl-4-methylthiazolium bromide[23] and pu-

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Table VI. Intermolecular distances less than 3.5 Å.

C(1)...C(14)*	3.42 Å	(thiazole and aromatic rings at right angles to each other)
S(1)...C(19)	3.47	
C(1)...N(3)	3.36	(thiazole and imidazole rings parallel to each other)
C(1)...C(3)	3.37	
N(1)...N(3)		

* Each atom in this column is related to that listed in Table III by the symmetry relation ($x, \frac{1}{2}-y, -\frac{1}{2}+z$).

rine.[24] Only C(3) - N(3) appears to be abnormally different from expected values but the shortening is only by aproximately 2σ.

Crystal Structure. The shortest intermolecular contacts are those between the two secondary nitrogen atoms N(6) and N(3) and the chlorine atoms Cl(1) and Cl(2) respectively, the corresponding distances being 3.33 and 3.28 Å. No attempt was made to locate hydrogen atoms, but stereochemical considerations make it clear that both of these close contacts represent hydrogen bonds.

Other close van der Waals contacts are listed in Table VI.

Finally, we interpret the diffuse, low electron density peaks near the origin as indicating that solvent loss had occurred either prior to or during data collection. In turn, this implied that the solvent molecules were able to move in and out of the tunnels without disturbing the structure. This problem had not been anticipated and no precautions such as coating the crystal or sealing it in a capillary with mother liquor had been taken. Indeed, the initial elemental analysis had clearly indicated a dihydrate, 4.9% loss in weight (equivalent to 1.54 H_2O) on drying at 100°C under vacuum. An atomic absorption analysis for cobalt, determined at a later time, confirmed a dihydrate stoichiometry but gas chromatographic assays for water gave values ranging from 0.65 to 2.0 H_2O. Some of the G.C. assays also showed the presence of methanol and ethanol in addition to water to the extent of 0.42 and 0.14 moles respectively depending upon which solvent had been used during the preparation of the complex. Neither ether nor benzene which were also used as recrystallizing solvents could be detected.

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