Acta Chemica Scandinavica A 29 (1975) 76—88

The Molecular and Crystal Structures of $[Ni_2Cl_2(C_2H_6O_2)_4]Cl_2$ and $[Co_2Cl_2(C_2H_6O_2)_4]Cl_2$, Two Isostructural Compounds Containing {Di-μ-chlorobis[di(1,2-ethanediol)metal(II)]} Cations

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The crystal structures of the isostructural compounds $[Ni_2Cl_2(C_2H_6O_2)_4]Cl_2$ (I) and $[Co_2Cl_2(C_2H_6O_2)_4]Cl_2$ (II) have been determined and refined using three-dimensional X-ray diffraction data. The crystals are monoclinic, space group $C2/m$, with unit cell dimensions and corresponding standard deviations (the values in square brackets refer to the Co-compound), $a=12.445(1)$ Å [12.428(1) Å], $b=11.375(1)$ Å [11.456(1) Å], $c=9.258(1)$ Å [9.347(1) Å], and $\beta=133.086(4)°$ [133.017(7)°]. There are two formula units in the unit cell. The intensity materials were collected with the linear diffractometer PAILRED using Mo$K\alpha$-radiation. Both structures were solved by Patterson and heavy-atom Fourier methods and refined by full-matrix least-squares techniques.

With anisotropic temperature factors for all non-hydrogen atoms and isotropic temperature factors for the hydrogen atoms the refinements converged at R-values of 0.046 and 0.032 for structures I and II, respectively. The refinements were based on 1394 independent reflexions for structure I and 2041 for structure II.

The structures consist of dinuclear cations $[Me_2Cl_2(C_2H_6O_2)_4]^{2+}$ and chloride ions. In the cation, the metal ions are coupled together through two chlorine atoms forming a bridge. Oxygen atoms from the glycol* molecules complete an octahedral arrangement around each metal ion. These cations are linked through the chloride ions by means of hydrogen bonds of the type $Cl^-\cdots H-O$, to form layers. Between these layers there are only van der Waals contacts. The Me—Me distances are 3.458 and 3.470 Å, the Me—Cl distances 2.383 and 2.417 Å and the average Me—O distances 2.067 and 2.104 Å in the Ni- and Co-compounds, respectively.

* Throughout this paper 1,2-ethanediol will be referred to as glycol or ethylene glycol.

Crystal structure investigations of complexes between ethylene glycol and divalent transition metal ions are in progress at this department. Their aim is to elucidate the coordination changes within the series Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+} and Zn^{2+}, particularly when sulfate and chloride are used as anions. The first two papers in this series, the crystal structures of $[Cu(C_2H_6O_2)_3]SO_4$[1] and $[MnCl_2(C_2H_6O_2)_2]$[2] have recently been published. A compilation of compounds prepared hitherto together with some characteristics of crystals of them, is presented in Table 1. The structure determinations of the isostructural compounds $[Co_2Cl_2(C_2H_6O_2)_4]Cl_2$ and $[Ni_2Cl_2(C_2H_6O_2)_4]Cl_2$ are presented here. In a recent report by Knetsch and Groeneveld[3] the preparation and properties of two crystalline compounds, to which the formulas $Ni(C_2H_6O_2)_2Cl_2$ and $Co(C_2H_6O_2)_2Cl_2$ were assigned, were carefully described. From visible, UV and IR spectra and magnetic susceptibility measurements it was concluded that glycol in these compounds acts as a bidentate ligand and has *gauche* conformation while the coordination around the metal ion is octahedral or pseudo-octahedral. From X-ray powder data, the two compounds were seen to be isostructural. A comparison of IR spectra of our compounds with the spectra published by Knetsch and Groeneveld shows that the compounds are identical.

EXPERIMENTAL

Crystal preparation and analyses. The Ni- and Co-compounds were prepared similarly. The

Table 1. A compilation of compounds prepared hitherto and some characteristics of crystals of them.

Compound	a (Å)	b (Å)	c (Å)	β (°)	Space group	Z	D_m(g/cm³)
$[Co(C_2H_6O_2)_3]SO_4$[a]	8.818(1)	7.585(1)	19.238(1)	99.357(5)	$P2_1/c$	4	1.77
$[Ni(C_2H_6O_2)_3]SO_4$[b]	10.32	9.03	15.04	116.4	$P2_1/c$	4	1.81
$[Cu(C_2H_6O_2)_3]SO_4$	10.166(1)	9.013(1)	15.365(1)	115.666(6)	$P2_1/c$	4	1.82
$[Zn(C_2H_6O_2)_3]SO_4$[c]	9.544(1)	14.198(1)	9.180(1)		$Ac2a$	4	1.84
$[MnCl_2(C_2H_6O_2)_2]$	9.491(1)	7.223(1)	14.213(1)	92.229(7)	$P2_1/c$	4	1.68
$[Co_2Cl_2(C_2H_6O_2)_4]Cl_2$	12.428(1)	11.456(1)	9.347(1)	133.017(7)	$C2/m$	2	1.71
$[Ni_2Cl_2(C_2H_6O_2)_4]Cl_2$	12.445(1)	11.375(1)	9.258(1)	133.086(4)	$C2/m$	2	1.75
$CuCl_2(C_2H_6O_2)$[d]	7.424	10.939	7.518	95.67	$P2_1/c$	4	2.14
$[CuCl_2(C_2H_6O_2)]\frac{1}{2}H_2O$[e]	10.198(1)	18.769(1)	7.043(1)		$Pcnb$	8	2.04

[a] Structure determined and refined (present R-value 0.038). To be published. [b] Isostructural with $[Cu(C_2H_6O_2)_3]SO_4$; X-ray data not yet collected. [c] Structure determined and refined (present R-value 0.047). To be published. [d] Structure determined and refined (present R-value 0.059). To be published. [e] X-Ray data just collected.

hexahydrates of the Ni(II)- and Co(II)-dichlorides were dissolved in glycol (molar ratio 1:2) by heating on a waterbath. The decanted solutions were then placed in a desiccator over sulfuric acid; crystals in the form of distorted tabular hexagons formed after some time. The Ni-containing crystals were pale green while the Co-containing crystals were deep violet. The crystals were analysed for metal and chlorine and the following results (in weight-%) were obtained: Found in crystal I Ni 23.0; Cl 27.1 and in crystal II Co 23.1; Cl 27.2. Calc. for $[Ni_2Cl_2(C_2H_6O_2)_4]Cl_2$: Ni 23.1; Cl 27.9 and for $[Co_2Cl_2(C_2H_6O_2)_4]Cl_2$: Co 23.2; Cl 27.9. The IR-spectra showed that no water was present. The densities of the crystals as determined by the flotation method using bromoform and xylene are 1.75 ± 0.01 and 1.71 ± 0.02 g/cm³ for the Ni- and Co-compounds, respectively. Calculated for $[Me_2Cl_2(C_2H_6O_2)_4]Cl_2$ with $Z=2$ gave the corresponding values of 1.76 and 1.73 g/cm³.

Crystal data and space group. From rotation photographs and corresponding Weissenberg photographs (zero and first layers) taken from crystals mounted around their b- and c-axis, it was concluded that the crystals are monoclinic. The unit cell parameters determined using these photographs were refined from powder photographs taken with a camera of Guinier-Hägg type, with Cu$K\alpha$-radiation, and with Si ($a=5.43054$ Å) as internal standard. (For the Co-compound Cu-foil was used to avoid fluorescence). The accurate cell parameters and their estimated standard deviations are listed in Table 1. Systematic extinctions of intensities were found for hkl when $h+k=2n+1$, which is characteristic for the three space groups $C2$ (No. 5), Cm (No. 8), and $C2/m$ (No. 12).[4] Of these only $C2/m$ is centrosymmetric.

Intensity data. The diffracted intensities from single crystals of I and II were collected and measured with the automatic linear diffractometer PAILRED using graphite-monochromated Mo$K\alpha$-radiation. As the crystals were hygroscopic they were enclosed in capillaries of Lindeman glass during the data collection. Both were rotated around their b-axis and intensities for $h0l-h15l$ were measured ($\sin\theta\leq 0.63$ for I and ≤ 0.67 for II). Reflexions for which the total number of counts during one scan interval was less than 4 000 were measured again. For the crystal of I the half scan interval for $h0l$ reflexions was 1.2 for $\theta\geq 20°$ (Ω_1) and 1.9 for $\theta\leq 20°$ (Ω_2). These half scan intervals were gradually increased for each layer up to 1.3 and 2.2, respectively, for $h15l$. The corresponding values for the crystal of II were 1.4 and 2.1 for $h0l$ and 1.6 and 2.5 for $h15l$. The scan speed was 1°/min. Background intensities were measured for 40 s (t_B) before and after each scan. The net intensity I for a reflexion was calculated from the measured total intensity TI (peak+background) by subtracting the two background counts B_1 and B_2 according to the relation.

$$I=TI/N-[t_T/(t_B/60)]\,(B_1+B_2)$$

where t_T is total scanning time [$\Omega_{1\text{ or }2}$/(scan speed/min)] and N is the number of times the reflexion was measured. 2238 independent intensities were measured from the crystal of I and 2442 from the crystal of II. From these 1394 and 2041, respectively, were significantly above background at the 95 % level, *i.e.* they had $\Delta I/I\leq 0.5$.[3] These were used in the refinements. Because of difficulties in obtaining large crystals of the Ni-compound the crystal of II was much larger than that of I ($V_I=0.449\times10^{-3}$ mm³, $V_{II}=0.859\times10^{-3}$ mm³). Thus there are more significant reflexions for II. Besides the normal correction for Lorentz

and polarization factors, absorption correction was also made. For the crystal of I the linear absorption coefficient was 25.3 cm^{-1} and the transmission factors varied from 0.84 to 0.92. Corresponding values for the crystal of II were 23.1 cm^{-1} and 0.63 to 0.76. When the refinements were terminated, structure factors for all the unobserved reflexions were calculated. These all had amplitudes equal to or lower than the corresponding threshold values.

The diffractometer data correction program is a modified version of a program originally written by Ivarsson and Lundberg.[5] The other computer programs used were those described by Antti and Lundberg.[6]

STRUCTURE DETERMINATION AND REFINEMENT

Structure I. The space group was initially assumed to be $C2/m$. From a three-dimensional Patterson synthesis the positions of the nickel and chlorine atoms were located, Ni on the twofold axis (4*g*) and Cl(1) and Cl(2) in the mirror plane (4*i*). The positions of the oxygen and carbon atoms were found in general eightfold positions, using heavy-atom Fourier methods.

After two cycles of full matrix least-squares refinement of the atomic positional parameters the R-value was 0.22 (R is defined as $[\sum||F_o|-|F_c||]/\sum|F_o|$). When atomic isotropic temperature factors were added as parameters the R-value decreased to 0.11 after one cycle. At this point anisotropic temperature factors for all atoms were introduced and after further refinement the R-value decrease to 0.056. A difference Fourier synthesis was calculated and probable positions for the hydrogen atoms were found. When they were included and refined with isotropic temperature factors the refinement converged at an R-value of 0.046. During the refinement the observations were weighted according to the function suggested by Cruickshank;[7] $w=1/(a+|F_o|+c|F_o|^2+d|F_o|^3)$, using the constants $a=250$, $c=-0.015$, and $d=0.00005$. The atomic scattering factors for Ni^{2+}, Cl^-, O, and C were those given by Cromer and Waber [8] and account was taken of the real part of the dispersion correction for Ni^{2+} and Cl^-.[9] (The scattering curve for Ni^+ [8] was also tested but there was no improvement neither in the least-squares refinements nor in a final difference Fourier synthesis). The scattering factors for the hydrogen atoms were those proposed by Stewart, Davidson and Simpson.[10]

Attempts were made to refine the structure in both of the noncentrosymmetrical space groups $C2$ and Cm. The very strong correlation (± 1.0) found between the parameters that are symmetry-related in space group $C2/m$ indicated that the structure in fact has a centre of symmetry.

Structure II. The two structures were assumed to be isostructural so the atomic positional parameters from structure I were used for the first cycle of least squares refinement of structure II. The R-value after this cycle was 0.22 and when isotropic temperature factors for all atoms were included the R-value decreased to 0.11. The refinement then proceeded in the same way as for structure I to a final R-value of 0.032.

Cruickshank constants used were; $a=175$, $c=-0.015$, and $d=0.0006$. The atomic scattering factors for Co^{2+} were those proposed by Cromer and Waber [8] and account was taken of the real part of the dispersion correction. Atomic scattering factors for the other atoms were as for structure I. Final positional and thermal parameters for the two structures are listed in Tables 2 and 3. The corresponding observed and calculated structure amplitudes are listed in Tables 4 and 5. For some of the strongest reflexions (those with $\sin\theta<0.2$) F_o is considerably less than F_c. This was noticed at the beginning of the refinements and as the intensities were believed to be affected by secondary extinction, attempts were made to introduce an isotropic extinction coefficient to correct the whole data. These were unsuccessful so the strong reflexions were excluded from further refinements. When the refinement had converged they were introduced again and were seen to have no significant effect on the atomic positional and thermal parameters. As the reflexions were measured with an Ω-scan there is a possibility that the chosen scan interval was too small for strong broad reflexions with low $\sin\theta$-values and hence that the intensities measured are too low.

DESCRIPTION AND DISCUSSION OF THE STRUCTURES

The structures consist of discrete dinuclear $[Me_2Cl_2(C_2H_6O_2)_4]^{2+}$-cations and Cl^--ions. They

Table 2. Atomic positional and thermal parameters for $[Ni_2Cl_2(C_2H_6O_2)_4]Cl_2$. For the non-hydrogen atoms all parameters have been multiplied by 10^4. The anisotropic temperature factors have been calculated according to the formula $\exp[-(h^2\beta_{11}+k^2\beta_{22}+l^2\beta_{33}+2hk\beta_{12}+2hl\beta_{13}+2kl\beta_{23})]$. For the hydrogen atoms the positional parameters have been multiplied by 10^3. The labelling of atoms is shown in Fig. 3. (Standard deviations for the last significant figure are given in parentheses).

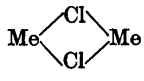
	x/a	y/b	z/c	$\beta_{11}(B)$	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Ni	0	1520(1)	0	55(1)	34(0.5)	90(1)	0	49(1)	0
Cl(1)	2563(2)	5000	1793(3)	127(2)	48(1)	317(5)	0	177(3)	0
Cl(2)	1649(2)	0	2232(2)	74(2)	44(1)	96(2)	0	33(2)	0
O(1)	3970(3)	3236(3)	988(4)	85(3)	63(3)	159(6)	18(2)	94(4)	18(3)
O(2)	1342(3)	2797(3)	2187(4)	88(3)	52(2)	153(6)	−13(2)	86(4)	−13(3)
C(1)	4905(5)	2684(5)	2906(6)	112(6)	82(4)	149(9)	15(4)	106(6)	17(5)
C(2)	680(5)	3295(4)	2842(7)	98(5)	59(4)	156(9)	−13(9)	86(6)	−30(4)
H(1)	357(6)	369(6)	105(9)	5(2)					
H(2)	168(5)	322(5)	200(7)	2(1)					
H(3)	60(5)	165(5)	398(7)	3(1)					
H(4)	428(5)	233(5)	310(7)	3(1)					
H(5)	500(6)	110(6)	200(8)	4(1)					
H(6)	147(5)	359(4)	415(6)	2(1)					

Table 3. Atomic positional and thermal parameters for $[Co_2Cl_2(C_2H_6O_2)_4]Cl_2$. Legend as for Table 2.

	x/a	y/b	z/c	$\beta_{11}(B)$	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Co	0	1515(0.3)	0	64(0.3)	38(0.2)	99(0.5)	0	57(0.3)	0
Cl(1)	2567(1)	5000	1798(1)	140(1)	51(0.5)	336(2)	0	191(1)	0
Cl(2)	1716(1)	0	2231(1)	81(1)	46(0.4)	101(1)	0	32(1)	0
O(1)	3984(2)	3225(1)	1036(2)	93(1)	67(1)	169(3)	21(1)	101(2)	22(1)
O(2)	1337(2)	2819(1)	2203(2)	101(2)	56(1)	170(3)	−19(1)	99(2)	−19(1)
C(1)	4903(3)	2668(2)	2914(3)	127(3)	86(2)	155(4)	17(2)	114(3)	21(2)
C(2)	667(2)	3311(2)	2848(3)	116(2)	62(2)	162(4)	−15(2)	97(3)	−32(2)
H(1)	355(3)	361(3)	101(4)	4.1(7)					
H(2)	167(3)	323(2)	204(3)	2.1(4)					
H(3)	55(3)	170(3)	389(4)	4.4(6)					
H(4)	432(3)	236(3)	318(3)	3.3(5)					
H(5)	493(3)	108(3)	189(4)	3.7(6)					
H(6)	139(3)	369(3)	409(4)	3.9(6)					

are shown in Fig. 1. The ions are linked together by hydrogen bonds of the type $Cl^-\cdots H-O$, forming layers parallel to the *ab*-plane. These layers are separated by *c*, the contacts between them being solely of van der Waals type. Part of the coupling of the layers is shown in Fig. 2.

The $[Me_2Cl_2(C_2H_6O_2)_4]^{2+}$*-cation.* In the $[Me_2Cl_2(C_2H_6O_2)_4]^{2+}$-cation the two metal ions are coupled through two chlorines forming a bridge and the four oxygens from two bidentate coordinated glycol ligands complete the octahedral arrangement around each metal ion. The bridging arrangement



is nearly square. The angles Cl—Me—Cl are 87.0 and 88.2°, the distances Me—Me 3.458(1) and 3.470(1) Å and the distances Me—Cl 2.383(1) and 2.417(1) Å for the Ni- and Co-compounds, respectively. These distances agree well with earlier reported values. Since the glycol molecules are coordinated to the metal ion as bidentate chelates, puckered five-membered rings are obtained. The dimensions

Table 4. Observed and calculated structure amplitudes (× 10) for $[Ni_2Cl_2(C_2H_6O_2)_4]Cl_2$.

L	H			L	H			L	H			L	H			L	H			L	H		
				-8	4	542	536	6	3	197	195	-2	2	882	844	4	5	541	-552	-2	6	912	-904
K=	0			-11	4	231	250	5	3	120	144	-1	2	515	-478	5	5	143	-149	-1	6	830	-832
				-12	4	201	212	4	3	259	269	0	2	1552	-1596	7	5	231	-221	0	6	167	-180
-2	16	129	123	-13	4	139	97	3	3	546	545	1	2	514	-495	8	5	171	-174	1	6	154	-158
-3	16	161	167	-11	2	247	243	2	3	608	608	2	2	117	123	9	3	192	-173	2	6	439	-450
-4	16	179	163	-10	2	377	364	1	3	187	193	3	2	191	-176	8	3	138	-154	3	6	317	-317
-5	16	198	186	-9	2	151	185	-1	3	516	490	4	2	296	-308	6	3	161	-156	4	6	185	-183
-6	16	288	299	-8	2	229	235	-2	3	1318	1300	5	2	246	-226	5	3	555	-550	7	6	160	-157
-7	16	275	277	-7	2	697	676	-3	3	672	662	6	2	146	-150	4	3	634	-641	8	4	188	-176
-10	16	163	177	-6	2	838	823	-4	3	296	-293	7	0	282	-272	3	3	310	-313	5	4	223	-208
-11	16	222	272	-5	2	417	423	-6	3	684	659	5	0	273	270	2	3	560	-552	4	4	482	-483
-12	16	220	237	-4	2	162	161	-7	3	653	652	4	0	206	-185	1	3	1412	-1428	3	4	552	-557
-13	16	184	220	-3	2	535	520	-8	3	214	220	3	0	800	-788	0	3	1343	-1358	2	4	313	-322
-15	14	133	134	-2	2	843	776	-11	3	167	149	2	0	338	-332	-1	3	298	273	0	4	419	-410
-14	14	248	262	-1	2	1601	1636	-10	1	190	213	1	0	180	-155	-2	3	627	607	-1	4	942	-938
-13	14	224	214	0	2	944	904	-9	1	271	255					-3	3	582	-575	-2	4	491	-488
-10	14	348	339	1	2	193	-196	-6	1	349	334	K=	3			-4	3	1243	-1255	-3	4	142	-170
-9	14	361	380	2	2	1096	1087	-5	1	632	642					-5	3	1095	-1108	-4	4	858	-837
-8	14	272	283	3	2	1828	1874	-4	1	443	440	-3	15	128	-143	-6	3	517	-514	-5	4	1006	-982
-7	14	279	301	4	2	844	856	-2	1	137	119	-4	15	283	-284	-7	3	217	-208	-6	4	332	-317
-6	14	286	265	5	2	157	-130	1	1	1051	1046	-5	15	381	-371	-8	3	358	-365	-8	4	286	-302
-5	14	247	255	7	2	408	412	2	1	775	776	-6	15	265	-260	-9	3	503	-502	-9	4	444	-427
-4	14	335	329	8	2	279	269	3	1	543	539	-9	15	204	-226	-10	3	277	-264	-10	4	208	-222
-3	14	287	287	10	0	250	241	4	1	335	343	-10	15	234	-240	-13	3	142	-143	-9	2	262	-245
-4	12	141	117	9	0	350	319	5	1	151	130	-11	15	159	-168	-12	1	137	-155	-8	2	484	-468
1	12	233	241	8	0	240	245	6	1	97	22	-12	15	140	-158	-11	1	133	-131	-7	2	259	-265
0	12	337	319	7	0	181	177	7	1	164	156	-13	15	138	-160	-9	1	168	-195	-6	2	153	-147
-1	12	162	152	6	0	212	217	8	1	246	260	-14	15	140	-133	-8	1	465	-463	-5	2	596	-598
-3	12	238	227	5	0	649	663	9	1	141	145	-16	13	129	-128	-7	1	605	-606	-4	2	845	-849
-4	12	257	242	4	0	1037	1041					-14	13	139	-107	-6	1	359	-363	-3	2	365	-354
-5	12	294	291	3	0	240	228	K=	2			-13	13	145	-165	-5	1	114	71	-2	2	185	147
-6	12	615	625	2	0	840	-854					-12	13	192	-213	-3	1	1027	-1031	-1	2	427	-416
-7	12	658	661	1	0	1650	1765	-3	16	118	-43	-11	13	143	-124	-2	1	1491	-1485	0	2	1228	-1233
-8	12	311	316					-9	16	179	-190	-9	13	220	-226	1	1	1526	-1569	1	2	1346	-1352
-9	12	272	279	K=	1			-10	16	209	-205	-8	13	521	-525	2	1	1406	-1423	2	2	556	-550
-10	12	350	339					-13	16	127	-89	-7	13	580	-582	3	1	542	-530	3	2	168	142
-11	12	208	210	-2	15	185	180	-14	16	172	-171	-6	13	349	-368	4	1	244	-251	4	2	204	-210
-12	12	141	161	-3	15	157	142	-15	14	113	39	-5	13	171	-156	5	1	485	-488	5	2	613	-620
-13	12	239	234	-6	15	189	198	-13	14	129	-134	-4	13	128	-143	6	1	452	-451	6	2	377	-397
-13	10	189	184	-7	15	312	308	-12	14	132	-98	-3	13	236	-247	7	1	186	-186	9	2	187	-155
-12	10	187	189	-8	15	206	214	-7	14	206	-215	-2	13	236	-255	10	1	196	-198	11	0	114	-155
-11	10	298	293	-12	15	150	160	-6	14	191	-173	-1	13	167	-130	11	1	172	-151	8	0	191	-212
-10	10	493	506	-13	15	135	147	-5	14	116	-100	2	13	127	-144					7	0	408	-422
-9	10	507	506	-11	13	161	154	-4	14	124	-152	3	11	171	-188	K=	4			6	0	321	-323
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3	8	248	250	-7	11	436	455	-4	10	240	245	-12	11	131	-101	-4	14	144	-144	-8	13	157	-174
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-5	8	966	955	-7	9	222	227	0	8	255	-242	-8	9	612	-611	-5	12	178	-201	-6	11	141	-159
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-7	8	257	224	-5	9	276	263	-3	8	619	-613	0	10	104	-94	-7	12	210	-213	-8	11	330	329
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2	6	236	213	-11	7	167	126	6	6	146	-148	-6	7	426	-412	5	8	137	-175	-5	7	166	-148
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6	4	492	485	-7	5	128	154	-2	4	338	-333	-13	7	173	-151	-5	8	161	-189	-5	5	338	338
5	4	335	329	-6	5	262	192	-3	4	720	-688	-11	5	187	-207	-7	8	254	-254	-4	5	651	657
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3	4	508	507	-4	5	1257	1242	-6	4	234	-238	-7	5	731	-738	-9	8	428	-419	-2	5	536	-618
2	4	881	881	-3	5	968	951	-7	4	274	-274	-6	5	1237	-1229	-12	8	225	-249	-1	5	475	-457
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Table 4. Continued.

L	H			L	H			L	H			L	H			L	H			L	H		
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K=	5			-8	4	411	416	-5	5	462	469	4	2	123	121	-8	12	195	-208	-8	9	189	-199
				-9	4	159	128	-4	5	964	936	5	2	124	-133	-7	12	219	-201	-9	9	106	-125
-1	3	103	-94	-11	4	144	142	-3	5	840	831	7	2	176	162	-6	12	137	-142	-13	9	94	-102
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-5	3	253	-254	-9	2	170	186	2	5	486	485	3	0	157	-168	-2	12	244	-224	-4	7	131	-144
-6	3	272	265	-8	2	341	285	4	5	133	108	2	0	303	-318	-1	12	131	-105	-3	7	197	-211
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10	1	117	101	-6	2	341	350	6	5	240	215					0	10	229	-237	1	7	232	-239
-7	1	137	-129	-5	2	323	322	10	3	126	50	K=	9			-1	10	271	-286	2	7	217	-230
-5	1	153	144	-4	2	283	284	8	3	109	125					-2	10	160	-178	4	7	90	17
-3	1	160	-122	-3	2	468	430	7	3	235	224	-2	13	145	-127	-4	10	151	-186	4	5	135	-125
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4	1	97	-28	2	2	962	954	2	3	670	679	-10	13	122	104	-9	10	168	-168	-2	5	378	-368
5	1	133	-135	3	2	930	924	1	3	162	165	-11	13	99	-38	-10	10	226	-233	-4	5	173	162
6	1	143	-130	4	2	351	360	-1	3	824	797	-12	13	168	-176	-11	10	150	-158	-6	5	230	-241
				7	2	198	224	-2	3	1381	1369	-11	11	238	-246	-12	10	103	-96	-7	5	149	-166
K=	6			8	2	129	149	-3	3	584	582	-10	11	220	-216	-10	8	109	-137	-10	5	137	-148
				10	0	150	139	-4	3	175	-156	-9	11	147	-139	-9	8	276	-294	-11	5	95	-107
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-7	8	232	214	-8	9	131	132	-8	8	112	-108	0	3	322	-320	-3	2	384	-372	-6	4	131	131
-9	8	139	150	-7	9	190	205	-10	8	137	141	1	3	508	-505	-4	2	548	-535	-5	4	162	168
-10	8	224	244	-6	9	451	433	-10	6	112	119	2	3	321	-323	-5	2	353	-357	-4	4	159	164
-11	8	288	294	-5	9	549	545	-9	6	217	236	3	3	149	-154	-6	2	168	-175	-1	4	70	82
-12	8	226	226	-4	9	373	367	-8	6	179	178	4	3	225	-257	-7	2	224	-223	0	4	169	173
-13	8	129	92	-3	9	243	245	-6	6	191	-175	5	3	234	-233	-8	2	283	-270	1	4	187	194
-15	8	136	97	-2	9	349	347	-5	6	97	-85	6	3	135	-105	-9	2	145	-159	2	4	128	134
13	6	132	141	-1	9	307	298	-4	6	249	243	6	1	167	-162	1	0	254	-272	4	2	124	104
-9	6	428	447	0	9	152	153	-3	6	208	216	5	1	292	-305	2	0	668	-666	3	2	332	338
-8	6	394	384	1	9	153	167	-2	6	118	-113	4	1	164	-187	3	0	628	-619	2	2	235	249
-6	6	171	159	2	9	218	239	0	6	255	263	3	1	144	-156	4	0	232	-234	-1	2	139	147
-5	6	792	774	3	9	140	181	1	6	157	175	2	1	392	-393	5	0	82	-72	-2	2	198	207
-4	6	865	859	5	7	143	159	3	6	88	55	1	1	394	-398	6	0	237	-229	-3	2	141	161
-3	6	591	576	4	7	280	294	4	6	153	153	-2	1	594	-582	7	0	316	-325	-4	2	74	82
-2	6	573	570	3	7	183	216	6	4	120	115	-3	1	203	-195	8	0	160	-174	-7	2	141	129
-1	6	466	447	1	7	118	125	3	4	140	-152	-5	1	85	-117					1	0	222	244
0	6	188	181	0	7	437	438	2	4	80	55	-6	1	176	-203	K=	11			2	0	94	-82
1	6	140	162	-1	7	651	649	1	4	391	406	-7	1	209	-209					4	0	156	169
2	6	235	232	-2	7	416	421	0	4	303	331	-8	1	189	-212	-2	13	108	-122	5	0	111	130
3	6	181	202	-3	7	187	193	-2	4	149	148	-9	1	116	-122	-3	13	132	-139				
4	6	261	237	-4	7	384	387	-3	4	231	236					-7	13	178	-173	K=	13		
5	6	243	242	-5	7	548	534	-5	4	130	-134	K=	10			-12	13	97	-80				
6	4	342	337	-6	7	375	369	-6	4	116	115					-13	13	106	-92	-1	11	105	103
5	4	319	323	-7	7	253	251	-7	4	179	176	-3	14	128	-106	-10	11	204	-190	-3	11	188	189
3	4	228	228	-8	7	347	360	-9	4	107	-45	-4	14	131	-114	-8	11	127	112	-4	11	180	167
2	4	544	537	-9	7	356	347	-11	4	108	78	-5	14	136	-144	-6	11	162	-177	-6	11	102	100
1	4	518	508	-10	7	234	207	-12	4	96	78	-6	14	206	-207	-5	11	216	-236	-7	11	202	192
0	4	412	406	-13	7	120	121	-6	2	163	168	-7	14	202	-218	-4	11	144	-152	-8	11	218	218
-1	4	478	464	-14	7	132	130	-7	2	344	374	-8	14	151	-140	1	9	106	-85	-9	11	142	149
-2	4	208	208	-12	5	161	178	-2	2	554	572	-10	14	136	-121	0	9	122	-112	-10	9	129	146
-3	4	204	203	-11	5	121	116	-1	2	193	183	-11	14	145	-173	-3	9	145	-158	-9	9	110	104
-4	4	652	639	-9	5	288	282	0	2	259	-274	-12	14	178	-170	-4	9	101	-128	-8	9	89	114
-5	4	745	729	-8	5	452	453	1	2	232	-232	-11	12	162	-147	-5	9	72	-69	-7	9	198	184
-6	4	507	488	-7	5	239	241	2	2	108	110	-10	12	222	-213	-6	9	120	-118	-6	9	179	200

Table 4. Continued.

L	H			L	H			L	H			L	H			L	H		
				-7	5	126	124	-7	1	125	99	-9	8	75	49	1	4	240	244	-4	7	89	-116
K= 13				-6	5	119	107	-6	1	199	207	-7	8	152	149	2	4	154	154	-7	5	87	-90
				-5	5	254	246	-5	1	284	284	-6	8	270	269	4	2	150	144	-6	5	126	-139
-5	9	178	185	-4	5	421	408	-4	1	307	295	-5	8	222	216	3	2	247	248	-4	5	84	94
-4	9	235	233	-3	5	294	289	-3	1	233	216	-1	8	185	188	2	2	135	157	-2	5	109	-136
-3	9	263	246	0	5	315	322	-2	1	137	147	0	8	124	134	-1	2	232	239	-1	5	97	-115
-2	9	163	149	1	5	363	347	1	1	275	275	3	6	82	70	-2	2	378	375	1	5	100	90
0	9	106	95	2	5	155	172	2	1	236	228	2	6	88	70	-3	2	192	197	1	3	113	-147
1	9	118	136	4	5	114	118	3	1	247	244	1	6	170	168	-4	2	59	46	0	3	134	-147
3	7	169	164	5	3	111	100	4	1	214	197	0	6	195	188	-5	2	127	137	-1	3	79	70
0	7	185	190	4	3	123	137	5	1	124	121	-3	6	199	205	-6	2	204	186	-2	3	144	151
-1	7	291	293	3	3	224	224	6	1	115	116	-4	6	235	240	-7	2	86	68	-4	3	135	-153
-2	7	260	260	2	3	234	232	7	1	151	141	-7	6	76	64	-6	0	99	100	-5	3	102	-107
-3	7	148	154	1	3	149	154					-8	6	166	174	-5	0	274	277	-5	1	85	88
-5	7	149	164	0	3	192	187	K= 14				-9	6	179	189	-4	0	220	220	-3	1	98	-111
-6	7	286	275	-1	3	343	322					-7	4	171	170	-2	0	57	-33	-2	1	108	-128
-7	7	256	247	-2	3	442	426	-2	10	133	120	-6	4	143	141	-1	0	170	201	1	1	67	-76
-8	7	153	145	-3	3	350	337	-3	10	178	194	-4	4	62	67					2	1	71	-79
-9	7	110	131	-4	3	98	107	-4	10	156	156	-3	4	238	214	K= 15							
-10	7	138	153	-6	3	243	239	-7	10	155	140	-2	4	214	203								
-9	5	158	160	-7	3	285	294	-8	10	130	136	-1	4	83	112	-1	7	70	89				
-8	5	153	163	-8	3	127	125	-10	8	130	126	0	4	161	169	-3	7	139	-147				

of these rings are given in Tables 6 and 7. All the Me—O distances are approximately the same so the five-membered rings are very symmetrical. The average Me—O distance is 2.067(3) Å in the Ni-compound and 2.104(2) Å in the Co-compound.

The glycol oxygens taking part in the Me—O bonds have three neighbours each, one hydrogen atom, one carbon atom, and one Me^{2+}-ion (Fig. 3). The arrangement around each of these oxygens can be considered as being tetrahedral, although distorted, if a lone pair of electrons is assumed to complete each tetrahedron.

The glycol ligands. As mentioned above the glycol molecule acts as a bidentate ligand in its coordination to the metal ion. It has a *gauche* conformation with dihedral angles of 52.39 and 52.12° for the Ni- and Co-compounds, respectively. [The dihedral angle is defined as the angle between the planes O(1)—C(1)—C(2) and O(2)—C(2)—C(1)]. These dihedral angles are in good agreement with the mean value of 52.2° found in $[MnCl_2(C_2H_6O_2)_2]$.[2] In $[Cu(C_2H_6O_2)_3]SO_4$[1] this angle varies between 45.9 and 55.3°. *Gauche* conformation of glycol molecules (dihedral angle 65°) has also been reported in (1-phenylbutane-1,3-dionato)-(ethyleneglycol) sodium,[11] where the glycol molecules act as bridging ligands.

Bastiansen [12] found by the method of electron diffraction on the free glycol molecule a single O···O distance of 2.96(2) Å which reflects a dihedral angle of $\approx 75°$ if normal values are assumed for the other parameters. There was no indication of a *trans* isomer. Infrared spectra of liquid, gaseous, and crystalline ethylene glycol, measured and discussed by Buckley and Giguère, also seem to indicate that the molecule exists only as *gauche* isomer.[13] These authors claim that the *gauche*-form should be more stable than the *trans*-form because of intramolecular hydrogen bonding and that the structure of the molecule should be fairly rigid because of energy barriers to rotation around C—C and C—O, respectively.

From the above discussion it may be concluded that the dihedral angle of the glycol molecule decreases as it changes from being free to acting as bridging ligand and bidentate ligand, respectively.

There are no significant differences between the values obtained for the C—C and C—O distances in the Ni- and Co-compounds, respectively. They also agree well with previously reported distances.[1,2] The intramolecular angles, *i.e.* the O—C—C angles, are significantly smaller than the tetrahedral angle; for $[Ni_2Cl_2(C_2H_6O_2)_4]Cl_2$ there is a mean value of 106.5(4)° and for $[Co_2Cl_2(C_2H_6O_2)_4]Cl_2$ 106.6(2)°. These values are similar to those reported for $[MnCl_2(C_2H_6O_2)_2]$.[2]

The C—H and O—H distances in these structures are not significantly different from other reported values obtained using X-ray data.

The hydrogen bonds. As mentioned above the hydrogen bonds are in layers parallel to the *ab*-plane. A drawing showing a layer and with hydrogen bonds marked (dashed lines) is given in Fig. 1. All hydrogen bonds are of the $Cl^-\cdots H-O$ type. Around each Cl^- there are four such hydrogen bonds. The four oxygen atoms taking part in this arrangement form a nearly square plane; in the middle of this

Table 5. Observed and calculated structure amplitudes ($\times 10$) for $[Co_2Cl_3(C_2H_6O_2)_4]Cl_2$.

L	H			L	H			L	H			L	H			L	H			L	H		
K=	0			-13	6	228	222	-2	13	47	47	4	1	313	313	2	4	265	-264	-10	9	270	-269
				-12	6	146	143	-4	13	169	169	3	1	524	514	1	4	271	257	-9	9	367	-372
				-11	6	62	59	-5	13	386	389	2	1	781	752	0	4	302	295	-8	9	539	-546
0	16	74	70	-10	6	214	216	-6	13	278	280	1	1	1033	1008	-1	4	69	4	-7	9	512	-507
-1	16	64	61	-9	6	515	509	-8	13	198	207	-2	1	163	125	-2	4	400	-393	-6	9	141	-136
-2	16	88	77	-8	6	522	513	-10	13	296	302	-4	1	403	403	-3	4	697	-688	-5	9	104	-72
-3	16	138	134	-7	6	132	136	-11	13	182	170	-5	1	625	619	-4	4	324	-317	-4	9	400	-411
-4	16	158	159	-5	6	871	858	-14	13	82	85	-6	1	337	334	-5	4	70	-73	-3	9	438	-447
-5	16	173	170	-4	6	1710	1777	-15	13	105	108	-8	1	68	53	-6	4	278	-275	-2	9	408	-412
-6	16	236	231	-3	6	1353	1372	-16	13	61	67	-9	1	233	233	-7	4	282	-282	-1	9	548	-555
-7	16	208	207	-2	6	475	465	-14	11	83	79	-10	1	193	194	-8	4	78	-74	0	9	486	-494
-8	16	46	46	-1	6	306	310	-13	11	153	150					-9	4	57	-66	1	9	176	-179
-10	16	158	158	0	6	556	553	-12	11	140	143	K=	2			-10	4	144	-146	3	9	120	-127
-11	16	223	223	1	6	422	417	-9	11	264	262					-11	4	57	-48	4	9	157	-168
-12	16	213	216	2	6	167	161	-8	11	517	517	-3	16	53	-38	-14	4	59	-62	5	9	102	-99
-13	16	228	223	3	6	206	207	-7	11	382	384	-4	16	68	-70	-13	2	53	-47	7	9	49	-29
-14	16	162	157	4	6	360	355	-6	11	52	55	-5	16	79	-82	-10	2	44	-53	7	7	110	-107
-15	16	62	72	5	6	303	299	-4	11	193	187	-7	16	56	52	-9	2	71	-76	6	7	186	-191
-16	16	71	76	6	6	117	118	-3	11	188	187	-8	16	52	22	-8	2	153	-151	5	7	138	-142
-17	16	80	83	7	6	49	46	-2	11	120	116	-9	16	145	-154	-7	2	254	-248	4	7	77	-62
-17	14	95	103	8	6	95	92	-1	11	156	150	-10	16	184	-186	-6	2	216	-224	3	7	110	-109
-16	14	86	105	9	6	97	102	0	11	202	201	-11	16	47	20	-5	2	227	-225	2	7	310	-310
-15	14	116	114	10	4	121	113	1	11	139	140	-12	16	86	90	-4	2	250	-251	1	7	509	-506
-14	14	234	227	7	4	193	194	5	11	78	71	-13	16	76	-75	-3	2	284	276	0	7	383	-385
-13	14	216	216	6	4	445	434	7	9	67	68	-14	16	138	-146	-2	2	916	911	-1	7	146	-142
-10	14	265	264	5	4	319	318	6	9	71	85	-15	16	71	-61	-1	2	508	-463	-2	7	451	-441
-9	14	311	315	4	4	167	169	3	9	102	99	-17	14	74	-72	0	2	1476	-1522	-3	7	1212	-1239
-8	14	264	267	3	4	443	438	2	9	246	242	-15	14	48	36	1	2	487	-474	-4	7	1063	-1078
-7	14	288	290	2	4	820	814	1	9	223	229	-14	14	63	-57	2	2	181	160	-5	7	328	-328
-6	14	224	221	1	4	820	819	0	9	119	116	-13	14	162	-162	3	2	182	-162	-6	7	321	-318
-5	14	176	180	0	4	447	451	-1	9	82	83	-12	14	74	-76	4	2	286	-290	-7	7	409	-407
-4	14	276	272	-1	4	146	132	-2	9	228	231	-7	14	155	-154	5	2	214	-205	-8	7	209	-209
-3	14	280	272	-2	4	324	305	-3	9	427	430	-6	14	163	-164	6	2	122	-124	-9	7	144	-148
-2	14	146	137	-3	4	1094	1111	-4	9	430	427	-5	14	134	-125	8	2	51	47	-10	7	281	-284
-1	14	77	61	-4	4	985	981	-5	9	201	196	-4	14	129	-133	9	2	64	-68	-11	7	300	-304
0	14	51	61	-5	4	528	529	-6	9	165	161	-3	14	47	-46	10	2	93	-98	-12	7	215	-216
1	14	67	63	-6	4	849	852	-7	9	230	227	-2	14	60	63	12	0	47	-24	-13	7	150	-150
2	14	69	75	-7	4	970	988	-8	9	146	148	0	14	93	-92	11	0	92	-91	-14	7	95	-87
3	14	76	74	-8	4	486	486	-9	9	141	140	1	14	59	-59	10	0	79	-80	-15	5	78	-83
5	12	57	58	-10	4	61	55	-10	9	262	261	2	12	110	-112	8	0	68	-62	-14	5	114	-111
4	12	100	103	-11	4	213	218	-11	9	291	285	1	12	96	-91	7	0	276	-270	-13	5	83	-91
3	12	80	76	-12	4	186	195	-12	9	139	143	-1	12	110	108	6	0	58	-51	-12	5	75	-75
2	12	53	54	-13	4	86	99	-15	9	58	59	-2	12	136	-137	5	0	303	292	-11	5	202	-202
1	12	175	168	-11	2	209	216	-15	7	66	58	-3	12	343	-342	4	0	157	-148	-10	5	301	-300
0	12	270	266	-10	2	325	321	-14	7	104	106	-4	12	75	-68	3	0	786	-767	-9	5	94	-89
-1	12	179	178	-9	2	145	148	-13	7	85	86	-5	12	230	227	2	0	327	-307	-8	5	63	-61
-2	12	103	104	-8	2	209	209	-12	7	56	55	-7	12	330	-330	1	0	165	-134	-7	5	695	-699
-3	12	150	143	-7	2	672	669	-11	7	147	149	-8	12	250	-244	K=	3			-6	5	1159	-1169
-4	12	155	153	-6	2	827	824	-10	7	229	225	-9	12	147	-147					-5	5	597	-596
-5	12	301	294	-5	2	401	397	-9	7	126	124	-10	12	109	-107					-4	5	183	-178
-6	12	649	643	-4	2	135	136	-8	7	119	115	-13	12	58	-57	0	15	79	-80	-3	5	831	-834
-7	12	599	599	-3	2	540	507	-7	7	393	390	-16	12	69	-69	-1	15	91	-90	-2	5	1130	-1172
-8	12	225	224	-2	2	755	741	-6	7	516	515	-17	12	53	-55	-2	15	71	-71	-1	5	906	-926
-9	12	214	222	-1	2	1359	1541	-5	7	179	175	-11	10	187	-181	-3	15	95	-90	0	5	270	-267
-10	12	328	328	0	2	875	845	-4	7	58	54	-10	10	355	-355	-4	15	223	-215	1	5	114	115
-11	12	191	197	1	2	202	-203	-3	7	335	336	-8	10	271	272	-5	15	333	-336	2	5	210	-213
-12	12	145	145	2	2	1106	1082	-2	7	695	707	-9	10	227	-220	-6	15	254	-253	3	5	600	-608
-13	12	201	201	3	2	1759	1806	-1	7	751	761	-6	10	642	-642	-7	15	50	-52	4	5	458	-469
-14	12	113	114	4	2	756	745	0	7	283	279	-5	10	204	-200	-9	15	165	-177	5	5	109	-111
-16	12	103	108	5	2	178	-177	1	7	133	-130	-4	10	313	310	-10	15	230	-240	6	5	73	-87
-17	12	115	118	6	2	69	64	2	7	39	-25	-3	10	218	210	-11	15	172	-182	7	5	203	-202
-16	10	103	97	7	2	394	390	3	7	270	271	-2	10	179	-177	-12	15	135	-140	8	5	140	-140
-15	10	62	51	8	2	237	240	4	7	251	250	-1	10	338	-346	-13	15	184	-187	10	3	79	-73
-14	10	85	94	9	2	47	56	5	7	46	37	0	10	189	-193	-14	15	119	-123	9	3	159	-159
-13	10	183	183	10	2	52	53	7	7	73	66	3	10	104	-102	-15	15	122	-137	8	3	151	-146
-12	10	156	148	11	2	97	93	8	7	98	88	4	10	90	-89	-16	15	103	-122	6	3	100	-105
-11	10	213	210	10	0	220	216	9	5	65	71	5	10	46	14	-17	13	74	-77	5	3	482	-487
-10	10	465	472	9	0	313	300	6	5	146	138	5	8	116	-114	-16	13	104	-108	4	3	601	-609
-9	10	543	546	8	0	250	237	5	5	283	280	4	8	71	-80	-15	13	113	-114	3	3	299	-300
-8	10	469	454	7	0	172	167	4	5	181	185	3	8	76	66	-14	13	123	-120	2	3	508	-494
-7	10	491	483	6	0	202	202	2	5	192	190	2	8	44	36	-13	13	171	-174	1	3	1316	-1353
-6	10	281	285	5	0	627	613	1	5	697	687	1	8	223	-228	-12	13	190	-188	0	3	1274	-1307
-5	10	49	-47	4	0	992	978	0	5	592	591	0	8	268	-269	-11	13	71	-74	-1	3	272	259
-4	10	287	273	3	0	187	183	-1	5	264	-253	-1	8	54	-25	-9	13	220	-222	-2	3	640	628
-3	10	708	705	2	0	945	-929	-2	5	349	-338	-2	8	75	-57	-8	13	486	-491	-3	3	504	-507
-2	10	494	490	1	0	1531	1709	-3	5	850	839	-3	8	510	-506	-7	13	482	-489	-4	3	1204	-1225
-1	10	135	140					-4	5	1207	1235	-4	8	609	-598	-6	13	277	-286	-5	3	1109	-1120
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2	10	241	239	-3	17	69	55	-7	5	68	74	-7	8	199	197	-3	13	204	-202	-8	3	308	-309
3	10	82	80	-6	17	112	111	-8	5	229	225	-8	8	217	-207	-2	13	169	-168	-9	3	457	-461
4	10	55	49	-5	17	129	120	-9	5	255	260	-9	8	397	-396	-1	13	89	-95	-10	3	230	-240
5	10	75	80	-6	17	50	56	-10	5	128	127	-10	8	167	-169	0	13	82	-85	-12	3	58	-42
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8	8	84	82	-10	17	163	167	-13	5	112	120	-13	8	143	-148	2	13	101	-102	-14	3	86	-88
7	8	117	114	-11	17	125	132	-14	5	59	59	-14	8	78	-71	3	11	149	-153	-13	1	56	-68
6	8	71	68	-12	17	94	88	-12	3	86	90	-13	6	53	-48	2	11	169	-172	-12	1	130	-136
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4	8	161	158	-14	17	48	45	-10	3	78	75	-11	6	134	-139	0	11	199	-199	-9	1	174	-178
3	8	236	224	-16	17	58	64	-8	3	213	218	-9	6	152	149	-1	11	269	-266	-8	1	446	-443
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-11	8	345	341	-2	15	132	133	7	3	178	177	7	6	99	-101	-16	11	70	-83	8	1	51	-50
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-14	8	125	126	3	13	65	70	9	1	134	134	6	4	53	43	-14	9	135	-138	11	1	123	-132
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Table 5. Continued.

L	H			L	H			L	H			L	H			L	H			L	H		
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K=	4			-2	6	800	-819	-6	9	167	-165	-6	14	154	161	-6	4	420	406	-5	9	486	483
				-1	6	700	-719	-5	9	206	-201	-5	14	122	130	-7	4	400	392	-4	9	386	380
-1	16	71	-65	0	6	150	-154	-4	9	134	140	-4	14	145	143	-8	4	399	395	-3	9	262	260
-2	16	78	-72	1	6	199	-197	-3	9	244	249	-3	14	165	158	-9	4	115	111	-2	9	270	277
-3	16	93	-87	2	6	433	-442	-1	9	126	-127	-2	14	138	133	-11	4	128	119	-1	9	205	215
-4	16	130	-127	3	6	253	-258	1	9	116	119	-1	14	76	66	-12	4	160	166	0	9	123	131
-5	16	111	-111	5	6	79	-86	2	9	125	131	1	14	57	29	-13	4	67	70	1	9	167	175
-6	16	58	-47	6	6	177	-182	4	9	107	-100	2	14	59	67	-12	2	93	50	2	9	214	214
-7	16	80	-80	7	6	136	-131	5	9	48	-45	3	14	63	63	-11	2	141	138	3	9	138	131
-8	16	180	-187	8	6	50	-35	6	9	49	45	4	12	71	80	-10	2	150	146	5	9	44	42
-9	16	185	-190	9	4	108	-100	8	7	46	49	3	12	63	56	-9	2	140	136	6	9	74	79
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-14	16	116	-128	3	4	544	-554	3	7	140	144	-3	12	54	-45	-4	2	238	245	3	7	222	222
-15	16	118	-132	2	4	325	-335	2	7	180	-171	-4	12	104	101	-3	2	405	392	2	7	52	63
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-17	14	44	-49	0	4	330	-329	-1	7	415	411	-6	12	423	416	-1	2	641	626	0	7	361	362
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-14	14	82	-76	-3	4	161	-165	-4	7	300	-298	-9	12	197	204	2	2	919	913	-3	7	182	185
-13	14	83	-85	-4	4	768	-773	-5	7	181	-182	-10	12	201	203	3	2	873	878	-4	7	297	301
-12	14	205	-206	-5	4	916	-921	-6	7	254	252	-11	12	147	142	4	2	306	299	-5	7	455	454
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0	14	98	-105	-11	2	42	-45	-6	5	36	24	-10	10	164	153	4	0	397	390	-12	5	155	151
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-9	10	236	-237	1	0	474	-458	-6	3	238	236	-8	8	66	68	-12	13	144	140	-1	3	742	729
-8	10	166	-175					-7	3	314	312	-9	8	128	124	-11	13	199	197	-2	3	1294	1321
-7	10	191	-191	K=	5			-8	3	57	60	-10	8	215	208	-10	13	226	223	-3	3	567	578
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2	10	62	-59	-8	15	60	62	-2	1	288	-291	-11	6	63	61	-1	13	139	138	-12	1	114	119
3	10	109	-108	-9	15	105	-114	1	1	494	505	-10	6	113	121	0	13	101	103	-13	1	45	44
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6	8	97	-97	-12	15	87	78	4	1	81	-58	-7	6	67	-51	3	13	57	63	-9	1	245	244
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-4	8	633	-647	-7	13	118	-115	-3	16	105	103	2	6	188	192	-3	11	259	253	4	1	478	477
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-9	8	432	-432	3	11	48	-39	-8	16	114	111	8	6	67	75	-8	11	436	430				
-10	8	75	-74	2	11	45	-31	-9	16	48	-39	9	6	76	80	-9	11	179	174	K=	8		
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-11	6	268	-271	-8	11	292	298	-15	14	144	147	3	4	179	184	-15	9	114	107	-14	14	39	25
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-5	6	686	-696	-10	9	100	99	-9	14	155	160	-3	4	195	195	-8	9	158	156	-8	12	78	-83
-4	6	87	-64	-9	9	59	-51	-8	14	204	201	-4	4	648	658	-7	9	190	190	-6	12	112	113

Table 5. Continued.

L	H		
K=	8		
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1	10	70	74
0	10	58	-51
-1	10	126	-132
-2	10	54	47
-3	10	320	334
-4	10	258	277
-5	10	57	-56
-6	10	107	-115
-7	10	104	108
-8	10	160	170
-9	10	36	40
-13	10	64	58
-14	10	39	49
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-10	8	108	108
-9	8	104	-110
-8	8	88	-93
-7	8	279	297
-6	8	435	453
-5	8	161	164
-4	8	140	-143
-3	8	142	-145
-2	8	42	34
-1	8	146	152
0	8	48	55
1	8	53	-50
2	8	50	55
3	8	135	143
4	8	42	47
6	6	51	-57
4	6	150	158
3	6	75	76
2	6	42	-43
1	6	121	128
0	6	252	260
-2	6	84	-79
-3	6	148	156
-4	6	191	189
-5	6	42	-45
-6	6	96	-102
-8	6	133	141
-9	6	211	221
-10	6	126	134
-13	6	41	45
-12	4	66	67
-11	4	63	62
-8	4	35	33
-7	4	151	150
-6	4	83	90
-5	4	103	-104
-4	4	26	13
-3	4	214	210
-2	4	NA	92
-1	4	46	55
0	4	350	375
1	4	389	414
2	4	53	20
3	4	159	-174
4	4	75	-71
5	4	69	74
6	4	105	115
7	4	44	41
8	2	112	119
7	2	164	168
5	2	116	-124
4	2	103	104
3	2	287	296
2	2	126	129
1	2	202	-208
0	2	263	-277
-1	2	162	155
-2	2	543	570
-3	2	379	409
-4	2	29	22
-5	2	35	27
-6	2	138	142
-7	2	33	27
-8	2	71	-75
-10	2	79	84
-11	2	43	55
1	0	150	141
2	0	288	-295
3	0	128	-129
4	0	291	307
5	0	326	342
6	0	56	60
7	0	45	-48
8	0	54	47
9	0	72	78
K=	9		
1	13	77	-81
0	13	41	-31
-2	13	78	-75
-3	13	126	-121
-4	13	107	-98
-7	13	247	-248
-8	13	355	-350
-9	13	110	-101
-10	13	127	112
-12	13	153	-155
-13	13	94	-92
-13	11	49	46
-12	11	87	-82
-11	11	236	-228
-10	11	174	-176
-9	11	90	-90
-8	11	103	-96
-7	11	132	-130
-6	11	185	-186
-5	11	195	-190
-4	11	81	-73
-2	11	145	-146
-1	11	139	-145
2	11	124	-114
3	11	84	-89
4	9	103	-105
3	9	78	-68
0	9	240	-234
-1	9	382	-365
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-4	9	102	-111
-5	9	175	-175
-6	9	98	-105
-7	9	129	-127
-8	9	209	-207
-9	9	182	-181
-10	9	143	-134
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-13	9	61	-57
-14	9	73	-82
-13	7	79	-77
-12	7	122	-117
-11	7	115	-113
-10	7	78	-83
-9	7	133	-137
-8	7	182	-180
-7	7	33	-36
-6	7	52	38
-5	7	285	-280
-4	7	631	-609
-3	7	426	-422
-1	7	54	45
0	7	210	-211
1	7	306	-308
2	7	126	-130
5	7	105	-109
6	7	111	-105
7	5	99	-101
6	5	59	-54
5	5	49	-50
4	5	155	-158
3	5	247	-249
2	5	197	-197
1	5	31	-12
0	5	67	56
-1	5	272	-267
-2	5	605	-595
-3	5	371	-368
-4	5	32	22
-5	5	88	-95
-6	5	421	-412
-7	5	370	-362
-8	5	103	-100
-10	5	70	-71
-11	5	104	-113
-12	5	78	-71
-13	3	102	-107
-9	3	204	-203
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-6	3	275	-279
-5	3	511	-505
-4	3	328	-316
-3	3	86	-93
-2	3	25	-32
-1	3	78	-78
0	3	301	-293
1	3	461	-452
2	3	274	-274
3	3	131	-135
4	3	237	-235
5	3	198	-194
8	3	92	-96
9	3	78	-83
8	1	58	-46
6	1	140	-145
5	1	275	-270
4	1	146	-147
3	1	103	-110
2	1	354	-353
1	1	369	-364
-2	1	531	-519
-3	1	165	-165
-4	1	53	37
-5	1	93	-106
-6	1	177	-175
-7	1	188	-188
-8	1	201	-202
-9	1	111	-107
K=	10		
0	14	103	-94
-1	14	79	-75
-2	14	50	-55
-3	14	72	-64
-4	14	92	-91
-5	14	140	-139
-6	14	192	-188
-7	14	169	-168
-8	14	98	-99
-9	14	83	-83
-10	14	128	-128
-11	14	149	-151
-12	14	139	-134
-13	14	111	-105
-14	14	81	-73
-14	12	104	-103
-13	12	99	-101
-12	12	83	-79
-11	12	116	-112
-10	12	184	-180
-9	12	222	-209
-8	12	211	-202
-7	12	170	-166
-6	12	90	-90
-5	12	67	-71
-4	12	179	-174
-3	12	261	-250
-2	12	184	-176
-1	12	59	-64
0	12	52	-55
1	12	96	-99
2	12	98	-91
3	10	77	-87
2	10	53	-54
1	10	75	-72
0	10	173	-172
-1	10	253	-246
-2	10	188	-187
-3	10	84	-82
-4	10	122	-129
-5	10	330	-322
-6	10	406	-391
-7	10	222	-214
-8	10	57	-59
-9	10	124	-125
-10	10	221	-209
-11	10	150	-149
-12	10	93	-88
-13	10	108	-106
-14	10	103	-101
-13	8	132	-126
-12	8	104	-103
-11	8	62	-60
-10	8	134	-132
-9	8	292	-285
-8	8	347	-339
-7	8	213	-212
-6	8	73	-70
-5	8	171	-166
-4	8	421	-417
-3	8	458	-449
-2	8	216	-212
-1	8	66	-69
0	8	151	-154
1	8	227	-220
2	8	143	-143
3	8	78	-72
4	8	94	-95
5	8	123	-115
6	6	108	-116
5	6	71	-67
4	6	75	-80
3	6	193	-195
2	6	262	-258
1	6	218	-217
0	6	235	-230
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-2	6	369	-371
-3	6	194	-201
-4	6	97	-103
-5	6	293	-279
-6	6	487	-471
-7	6	379	-368
-8	6	120	-129
-9	6	62	-66
-10	6	159	-154
-11	6	195	-190
-12	6	127	-127
-13	6	51	-55
-12	4	46	-43
-11	4	94	-93
-10	4	197	-192
-9	4	229	-225
-8	4	152	-151
-7	4	109	-109
-6	4	219	-221
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-4	4	394	-384
-3	4	338	-329
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-1	4	454	-449
0	4	336	-331
1	4	141	-143
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3	4	359	-354
4	4	297	-291
5	4	84	-83
7	4	84	-91
8	4	113	-115
9	2	95	-93
8	2	47	-47
7	2	88	-89
6	2	227	-228
5	2	322	-315
4	2	203	-202
3	2	30	-19
2	2	149	-157
1	2	616	-598
0	2	717	-710
-1	2	296	-291
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-3	2	351	-343
-4	2	542	-530
-5	2	330	-329
-6	2	128	-135
-7	2	195	-192
-8	2	254	-246
-9	2	144	-143
-10	2	54	-48
-11	2	55	-55
-1	0	231	-232
-2	0	646	-623
3	0	613	-594
4	0	207	-208
6	0	215	-212
7	0	319	-310
8	0	151	-152
9	0	49	-25
10	0	56	-66
K=	11		
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-2	13	85	-88
-3	13	122	-119
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-6	13	42	-45
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-9	11	69	-71
-8	11	94	88
-7	11	31	24
-6	11	153	-152
-5	11	181	-189
-4	11	131	-134
-3	11	90	-94
-2	11	63	-64
-1	11	54	-52
0	11	42	-40
4	9	74	-87
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0	9	102	-103
-1	9	57	-64
-2	9	66	-67
-3	9	114	-113
-4	9	97	-98
-5	9	82	-87
-6	9	134	-140
-7	9	164	-173
-8	9	146	-157
-9	9	101	-102
-11	9	39	30
-12	9	43	-46
-13	9	90	-87
-12	7	52	-59
-11	7	72	-72
-10	7	53	-62
-9	7	79	-75
-8	7	129	-132
-7	7	156	-156
-6	7	106	-111
-5	7	80	-90
-4	7	167	-176
-3	7	190	-191
-1	7	102	95
0	7	38	-56
1	7	234	-242
2	7	190	-194
3	7	38	-30
5	7	41	-48
6	7	68	-67
7	5	60	-68
5	5	53	37
4	5	89	-87
3	5	209	-222
2	5	82	-92
1	5	91	88
0	5	110	-118
-1	5	433	-458
-2	5	368	-372
-3	5	27	9
-4	5	172	163
-5	5	31	-28
-6	5	226	-227
-7	5	176	-185
-8	5	40	-42
-9	5	45	-46
-10	5	127	-129
-11	5	93	-99
-10	3	77	-88
-9	3	127	-131
-8	3	75	-70
-7	3	70	66
-6	3	79	74
-5	3	247	-254
-4	3	483	-501
-3	3	154	-165
-2	3	170	169
-1	3	119	-126
0	3	449	-461
1	3	246	-247
3	3	44	41
3	3	32	11
4	3	110	-113
5	3	114	-121
6	3	42	-45
8	1	49	41
7	1	100	-103
6	1	233	-235
5	1	134	-141
4	1	43	-51
3	1	90	-99
2	1	115	-118
1	1	92	-95
-2	1	279	-290
-3	1	438	-445
-4	1	151	-160
-5	1	120	115
-6	1	63	-68
-7	1	240	-245
-8	1	100	-106
-9	1	36	34
K=	12		
1	12	42	36
0	12	95	95
-1	12	57	66
-3	12	47	-45
-5	12	121	123
-6	12	147	147
-7	12	59	51
-9	12	54	59
-10	12	91	92
-13	12	43	43
-14	12	49	44
-13	10	59	58
-12	10	38	41
-10	10	49	40
-9	10	155	153
-8	10	168	171
-7	10	43	52
-6	10	86	-86
-5	10	73	-67
-4	10	109	121
-3	10	214	222
-2	10	75	81
-1	10	62	-56
1	10	114	118
2	10	48	63
4	8	37	13
3	8	62	62
2	8	66	65
-1	8	157	166
-2	8	209	218
-4	8	104	-92
-5	8	103	104
-6	8	240	246
-7	8	98	106
-8	8	51	-46
-10	8	69	73
-11	8	101	103
-12	8	64	64
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-9	6	121	125
-8	6	68	78
-7	6	60	-51
-5	6	176	184
-4	6	202	210
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-2	6	84	91
-1	6	104	112
0	6	48	52
1	6	64	69
3	6	99	110
5	6	60	68
8	4	39	-28
6	4	106	107
5	4	97	100
2	4	84	98
1	4	174	187
0	4	167	182
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-2	4	62	-55
-3	4	29	32
-4	4	164	174
-5	4	145	153
-6	4	82	85
-7	4	117	123
-8	4	104	107
-11	4	48	43
-12	4	39	52
-11	2	41	51
-10	2	56	50
-8	2	56	64
-7	2	120	127
-6	2	66	71
-4	2	61	73
-3	2	150	161
-2	2	171	183
-1	2	100	105
0	2	43	-30
1	2	29	-10
2	2	213	226
3	2	291	299
4	2	64	67
5	2	89	-85
7	2	95	100
10	0	40	38
9	0	53	59
8	0	56	60
7	0	37	38
5	0	95	106
4	0	139	147
3	0	29	-17
2	0	113	-103
1	0	193	208
K=	13		
1	11	71	73
0	11	130	119
-1	11	104	98
-2	11	93	90
-3	11	143	140
-4	11	151	146
-5	11	91	86
-6	11	90	84
-7	11	155	150
-8	11	188	182
-9	11	140	133
-11	11	64	55
-11	11	45	42
-12	11	94	95
-12	9	86	87
-11	9	131	125
-10	9	126	116
-9	9	89	85
-8	9	111	110
-7	9	168	163
-6	9	165	156
-5	9	157	153
-4	9	234	222
-3	9	242	227
-2	9	110	107
-1	9	34	35
0	9	83	78
1	9	134	125
2	9	116	111
3	9	55	64
4	7	130	133
3	7	156	151
2	7	67	65
1	7	38	38
0	7	146	148
-1	7	257	255
-2	7	247	240
-3	7	134	130
-4	7	48	53
-5	7	128	130
-6	7	273	261
-7	7	251	234
-8	7	120	116
-9	7	104	104
-10	7	145	142
-11	7	107	100
-11	5	70	64
-10	5	125	118
-9	5	161	155
-8	5	143	141
-7	5	94	93
-6	5	86	84
-5	5	230	223
-4	5	384	373
-3	5	253	245
-1	5	59	69
0	5	306	302
1	5	325	311
2	5	134	134
3	5	50	57
4	5	111	105
5	5	122	121
6	5	54	69
7	3	104	103
6	3	118	113
5	3	88	81
4	3	109	105
3	3	184	187
2	3	195	199
1	3	138	138
0	3	146	144
-1	3	288	277
-2	3	414	400
-3	3	333	320
-4	3	69	78
-6	3	217	211
-7	3	271	259
-8	3	108	107
-10	3	87	77
-9	1	99	96
-8	1	39	37
-7	1	78	77
-6	1	203	196
-5	1	273	264
-4	1	260	251
-3	1	185	179
-2	1	129	132
1	1	235	231
2	1	194	191
3	1	216	211
4	1	182	178
5	1	105	109

Table 5. Continued.

L	H			L	H			L	H			L	H			L	H		
				-11	10	55	56	-3	6	163	169	6	4	100	99	-2	0	54	-39
K=	13			-11	8	75	75	-4	6	208	207	7	2	109	108	-1	0	175	188
				-10	8	109	102	-5	6	74	79	5	2	29	3				
6	1	93	95	-9	8	30	36	-7	6	59	54	4	2	126	126	K=	15		
7	1	120	116	-7	8	148	144	-8	6	161	152	3	2	234	235				
8	1	116	118	-6	8	250	245	-9	6	174	173	2	2	148	151	0	7	24	-16
				-5	8	190	183	-10	6	85	84	1	2	59	-39	-1	7	98	101
K=	14			-4	8	37	36	-10	4	37	36	0	2	44	-37	-2	7	41	45
				-2	8	59	66	-9	4	47	43	-1	2	213	223	-3	7	112	-125
1	10	47	50	-1	8	154	156	-8	4	89	91	-2	2	356	359	-4	7	100	-119
-1	10	34	21	0	8	100	101	-7	4	156	148	-3	2	177	178	-6	7	27	27
-2	10	88	87	2	8	55	59	-6	4	122	120	-4	2	29	33	-7	5	73	-85
-3	10	174	166	3	8	98	98	-4	4	58	66	-5	2	118	121	-6	5	101	-116
-4	10	154	154	4	6	93	[illegible]	-3	4	195	192	-6	2	169	168	-5	5	31	41
-5	10	54	56	3	6	66	66	-2	4	173	176	-7	2	58	60	-4	5	94	105
-6	10	34	32	2	6	51	55	-1	4	92	98	-9	2	50	48	-3	5	21	-28
-7	10	102	107	1	6	135	135	0	4	152	158	-8	0	53	60	-2	5	110	-132
-8	10	122	123	0	6	170	170	1	4	231	226	-6	0	79	81	-1	5	67	-82
-9	10	60	64	-1	6	55	64	2	4	138	134	-5	0	266	257	0	5	32	35
-10	10	49	42	-2	6	31	38	5	4	63	65	-4	0	215	212	1	5	78	80

L	H			L	H		
2	5	26	-1				
3	3	30	25				
2	3	28	29				
1	3	93	-113				
0	3	106	-126				
-1	3	60	58				
-2	3	123	136				
-4	3	99	-121				
-5	3	77	-96				
-5	1	76	79				
-4	1	54	51				
-3	1	74	-88				
-2	1	89	-106				
1	1	50	-60				
2	1	45	-53				
3	1	28	30				
4	1	28	24				

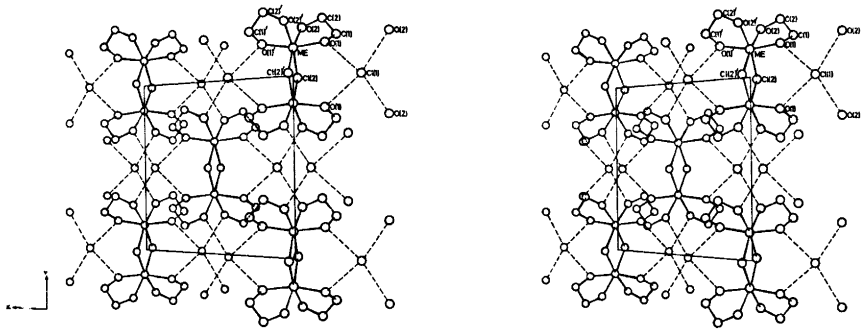

Fig. 1. A stereoscopic illustration of the *ab*-plane of the unit cell, showing the dinuclear $[Me_2Cl_2(C_2H_6O_2)_4]^{2+}$-ions, the Cl^--ions and the hydrogen bonds between these.

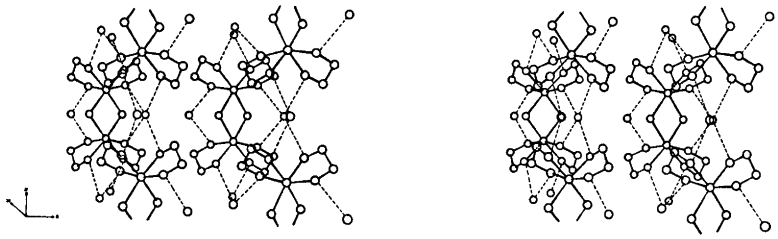

Fig. 2. A stereoscopic view of the layers which repeat themselves with displacement *c*. For the sake of clarity only half the unit cell in the *a*-direction is illustrated.

plane and a little below it (0.088 and 0.075 Å for the Ni- and Co-compounds, respectively) the chloride ion is situated. The mean Cl···O distance is 3.075 and 3.080 Å for the Ni- and Co-compounds, respectively.

In Fig. 3 the positions of the hydrogen atoms between the oxygen and chlorine atoms are shown. The O—H and Cl—H distances are quite reasonable and are given in Table 8. The angles Cl—H—O vary between 162

Table 6. Interatomic distances and angles in the two compounds. The roman figures I and II refer to the Ni- and Co-compounds respectively. (Standard deviations for the last significant figure are given in parentheses).

Atoms	I d/Å	II d/Å	Atoms	I angle/°	II angle/°
Me—Me	3.458(1)	3.470(1)	Cl(2)—Me—Cl(2)′	86.97(5)	88.22(2)
Me—O(1)	2.040(3)	2.071(1)	Cl(2)—Me—O(1)	98.24(9)	99.24(4)
Me—O(2)	2.093(3)	2.137(2)	Cl(2)—Me—O(1)′	93.14(9)	92.66(4)
Me—Cl(2)	2.383(1)	2.417(1)	Cl(2)—Me—O(2)	91.10(9)	91.27(4)
O(1)—O(2)	2.617(4)	2.612(2)	Cl(2)—Me—O(2)′	171.16(9)	169.14(4)
O(1)—C(1)	1.442(6)	1.434(3)	O(1)—Me—O(1)′	164.3 (2)	163.4 (1)
O(2)—C(2)	1.432(6)	1.436(3)	O(1)—Me—O(2)	78.6 (1)	76.7 (1)
C(1)—C(2)	1.501(7)	1.497(3)	O(1)—Me—O(2)′	90.5 (1)	91.6 (1)
Cl(1)—O(1)	3.071(3)	3.075(2)	O(2)—Me—O(2)′	92.1 (2)	91.2 (1)
Cl(1)—O(2)	3.079(3)	3.084(2)	Me—Cl(2)—Me	93.03(5)	91.78(2)
			Me—O(1)—C(1)	112.7 (3)	113.9 (1)
			Me—O(2)—C(2)	112.0 (3)	112.7 (1)
			O(1)—C(1)—C(2)	105.9 (4)	106.3 (2)
			O(2)—C(2)—C(1)	107.1 (4)	106.8 (2)
			Me—O(1)—Cl(1)	131.1 (1)	129.9 (1)
			Me—O(2)—Cl(1)	125.6 (1)	125.0 (1)

Table 7. Interatomic distances and angles involving hydrogen atoms. The roman figures I and II refer to the Ni- and Co-compounds respectively. (Standard deviations for the last significant figure are given in parentheses).

Atoms	I d/Å	II d/Å	Atoms	I angle/°	II angle/°
O(1)—H(1)	0.75(6)	0.68(3)	Me—O(1)—H(1)	127(5)	127(3)
O(2)—H(2)	0.73(5)	0.70(2)	Me—O(2)—H(2)	116(4)	116(2)
C(1)—H(3)	1.06(5)	1.00(3)	C(1)—O(1)—H(1)	103(5)	106(2)
C(1)—H(4)	1.00(5)	0.98(2)	C(2)—O(2)—H(2)	116(4)	115(2)
C(2)—H(5)	0.94(6)	1.00(3)	O(1)—C(1)—H(3)	107(3)	105(2)
C(2)—H(6)	0.96(4)	0.96(3)	O(1)—C(1)—H(4)	109(3)	111(1)
			C(2)—C(1)—H(3)	115(3)	116(2)
			C(2)—C(1)—H(4)	108(3)	110(2)
			H(3)—C(1)—H(4)	111(4)	108(2)
			O(2)—C(2)—H(5)	113(3)	109(2)
			O(2)—C(2)—H(6)	106(3)	111(2)
			C(1)—C(2)—H(5)	110(3)	110(2)
			C(1)—C(2)—H(6)	110(3)	113(2)
			H(5)—C(2)—H(6)	111(5)	107(2)

Table 8. Hydrogen bond distances (Å) and angles (°). The roman figures I and II refer to the Ni- and Co-compounds respectively. (Standard deviations for the last significant figure are given in parentheses.)

	Cl(1)···H(1)—O(1)		Cl(1)···H(2)—O(2)	
	I	II	I	II
Cl—H	2.32 (6)	2.41 (3)	2.37 (5)	2.40 (3)
O—H	0.75 (6)	0.68 (3)	0.73 (5)	0.70 (2)
Cl—O	3.071(3)	3.075(2)	3.079(3)	3.084(2)
∠Cl—H—O	171 (6)	166 (3)	162 (5)	164 (3)

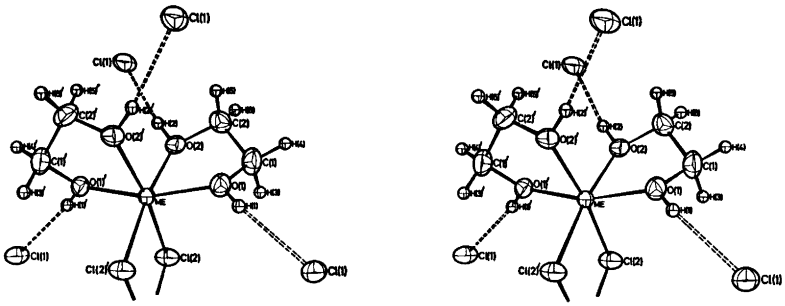

Fig. 3. A stereoscopic illustration, showing the coordination around the metal ion and four adjacent chloride ions. Thermal ellipsoids for the nonhydrogen atoms are scaled to enclose 50 % probability.

and 171° for the two compounds but there is no significant difference between these values.

Acknowledgements. I wish to express my sincere thanks to Professor Nils Ingri for much valuable advice and for all the facilities placed at my disposal. I also thank Dr. Britt Hedman for much valuable help with computational problems. The English of this paper has been corrected by Dr. Michael Sharp. This work forms part of a program supported by the Swedish Natural Science Research Council.

REFERENCES

1. Antti, B.-M., Lundberg, B. K. S. and Ingri, N. *Acta Chem. Scand. 26* (1972) 3984.
2. Antti, B.-M. *Acta Chem. Scand. 27* (1973) 3513.
3. Knetsch, D. and Groeneveld, W. L. *Inorg. Chim. Acta 7* (1973) 81.
4. *International Tables for X-Ray Crystallography*, Kynoch Press, Birmingham 1965, Vol. I.
5. Ivarsson, G., Lundberg, B. K. S. and Ingri, N. *Acta Chem. Scand. 26* (1972) 3005.
6. Antti, C.-J. and Lundberg, B. K. S. *Acta Chem. Scand. 25* (1971) 1758.
7. Cruickshank, D. W. J. *Computing Methods in Crystallography*, Pergamon, London 1965, p. 114.
8. Cromer, D. T. and Waber, J. T. *Acta Crystallogr. 18* (1965) 104.
9. *International Tables for X-Ray Crystallography*, Kynoch Press, Birmingham 1962, Vol. III.
10. Stewart, R. F., Davidson, E. R. and Simpson, W. T. *J. Chem. Phys. 42* (1965) 3175.
11. Bright, D., Milburn, G. H. W. and Truter, M. R. *J. Chem. Soc. A* (1971) 1582.
12. Bastiansen, O. *Acta Chem. Scand. 3* (1949) 415.
13. Buckley, P. and Giguère, P. A. *Can. J. Chem. 45* (1967) 397.

Received May 21, 1974.