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The Crystal Structure of Bis(isopropylammonium)tetrachlorocuprate(II)

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The structure of the low temperature (green) phase of the thermochromic compound bis(isopropylammonium)tetrachlorocuprate(II), $[(CH_3)_2CHNH_3]_2CuCl_4$*, has been determined by X-ray diffraction. The compound crystallizes in the triclinic space group P1 with lattice constants of* $a = 7.245(1)$ Å, $b = 14.588(1)$ Å, $c = 21.738(1)$ Å, $\alpha = 87.08(1)°$, $\beta = 103.59(1)°$ *and* $\gamma = 104.73(1)°$ *at 20° C. There are six formula units per unit cell. Least squares refinement of 3240 reflections with* $I > 2\sigma_I$ *led to a final value of* $R = 7.3\%$*. The structure contains discrete* $CuCl_4^{2-}$ *ions which pack together to form infinite ribbons parallel to the a-axis. The ribbons are held together by hydrogen bonds between the* $CuCl_4^{2-}$ *ions and the isopropylammonium ions. One-third of the* $CuCl_4^{2-}$ *ions have a square-planar geometry; the other two-thirds have a small tetrahedral distortion superimposed on the square-planar configuration.*

Introduction

A number of yellow (high temperature) thermochromic salts of the series $(R\text{–}NH_3)_2CuCl_4$[1–3] have now been studied and their structures determined. They all contain square planar $CuCl_4^{2-}$ ions arranged to form infinite sheets as shown in Fig. 1. Of these compounds, only the isopropylammonium salt shows a first order phase transition, which occurs at 56° C.[4] The room temperature structure of this compound has been determined.

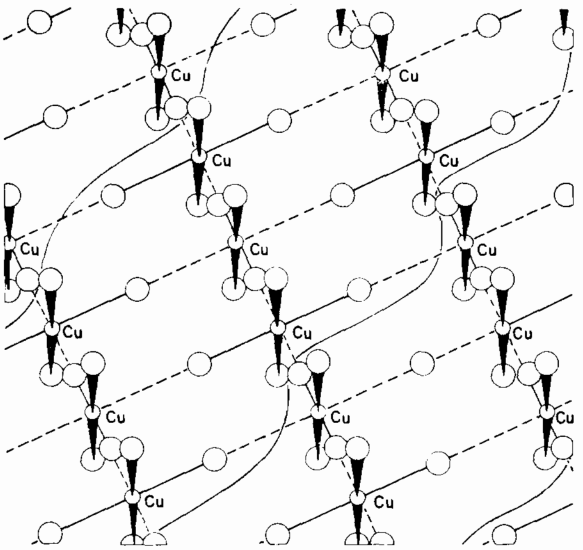

Figure 1. The infinite two-dimensional sheets found in the high temperature (yellow) phase of the $(R\text{–}NH_3)_2CuCl_4$ salts. The dashed lines indicate Cu–Cl distance in excess of 2.79 Å. The curved lines represent possible fracture points for change to the ribbon structure of $[(CH_3)_2CHNH_3]_2CuCl_4$.

Preparation and Data Collection

The compound $[(CH_3)_2CHNH_3]_2CuCl_4$ was prepared by the evaporation of a methanol solution containing a 2 : 1 molar ratio of $(CH_3)_2CHNH_2 \cdot HCl$ and $CuCl_2$. It crystallizes as needles along the <100> direction which, in the sample used for data collection, was .05 cm long by .03 cm by .03 cm. The lattice constants for the triclinic cell, determined from 24 measurements of 2Θ on a Picker 4-circle diffractometer, are a = 7.245(1)A, b = 14.588(1)Å, c = 21.738(1)Å, $\alpha = 87.08(1)°$, $\beta = 103.59(1)°$, and $\gamma = 104.73(1)°$. (The reduced cell has constants a = 14.545A, b = 21.237Å, c = 7.245Å, $\alpha = 95.79°$, $\beta = 104.07°$ and $\gamma = 89.12°$). The crystals sink very slowly in chloroform (1.47 g/cc), and the calculated density for z = 6 (six molecules per unit cell) is 1.50 g/cc.

Intensity data were collected on a manual Picker 4-circle diffractometer using Ni filtered Cu K_α radiation. A Θ–2Θ scan technique was used with 60 second scans and 20 second backgrounds before and after each scan. The linear absorption coefficient was 86.8 cm^{-1}. No absorption corrections were applied. Of the 4454 reflections collected, 3240 were considered observed.[5]

TABLE I. Parameters for $[(CH_3)_2CHNH_3]_2CuCl_4$.[a, b]

ATOM	X	Y	Z	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
CU-1	0.5000	0.5000	0.0	0.0515(26)	0.0452(24)	0.0399(23)	0.0040(10)	0.0036(10)	-0.0001(9)
CU-2	0.0	0.0	0.5000	0.0530(26)	0.0492(25)	0.0416(24)	0.0072(10)	0.0005(10)	-0.0008(10)
CU-3	0.1901(4)	0.7060(2)	0.1285(1)	0.0548(19)	0.0503(18)	0.0498(18)	0.0091(8)	0.0043(7)	-0.0004(7)
CU-4	0.4749(4)	0.1878(2)	0.3559(1)	0.0593(20)	0.0660(20)	0.0492(18)	0.0073(8)	0.0060(8)	-0.0007(8)
CL-1	0.5337(7)	0.3937(3)	0.0810(2)	0.0485(34)	0.0321(30)	0.0294(30)	0.0032(13)	0.0039(13)	0.0037(12)
CL-2	0.4237(8)	0.6930(4)	0.5708(3)	0.0805(46)	0.0535(37)	0.0680(42)	-0.0032(17)	0.0150(18)	-0.0146(16)
CL-3	0.3241(7)	0.6189(3)	0.0745(2)	0.0439(34)	0.0379(32)	0.0527(35)	0.0061(13)	0.0093(14)	-0.0046(13)
CL-4	0.2522(7)	0.7673(3)	0.6833(2)	0.0483(36)	0.0554(36)	0.0415(33)	0.0080(15)	0.0104(14)	0.0050(14)
CL-5	0.2493(6)	0.9472(3)	0.5616(2)	0.0339(31)	0.0442(32)	0.0301(30)	0.0073(13)	-0.0001(12)	0.0023(12)
CL-6	0.2799(8)	0.8360(3)	0.0731(3)	0.0627(40)	0.0441(36)	0.0786(43)	0.0137(16)	0.0160(17)	0.0108(15)
CL-7	0.2715(7)	0.0965(3)	0.4137(2)	0.0364(32)	0.0503(34)	0.0315(31)	0.0032(13)	0.0046(13)	0.0016(13)
CL-8	0.1928(6)	0.4116(3)	0.9598(2)	0.0329(30)	0.0300(29)	0.0339(30)	0.0006(12)	-0.0000(12)	-0.0033(12)
CL-9	0.0888(7)	0.1357(3)	0.5624(2)	0.0478(35)	0.0372(32)	0.0352(31)	0.0039(14)	0.0003(13)	-0.0059(13)
CL-10	0.0270(7)	0.2341(3)	0.8355(2)	0.0547(36)	0.0500(35)	0.0359(32)	0.0115(15)	0.0054(14)	-0.0042(13)
CL-11	0.2205(9)	0.6082(4)	0.2113(3)	0.1094(55)	0.1014(52)	0.0578(42)	0.0357(22)	0.0211(20)	0.0200(18)
CL-12	0.2770(8)	0.1289(5)	0.2631(2)	0.0512(41)	0.1526(64)	0.0340(36)	-0.0015(21)	0.0018(16)	-0.0107(19)
N-1	0.3359(23)	0.4299(10)	0.8132(6)	0.0878(138)	0.0433(107)	0.0190(94)	0.0085(50)	-0.0013(46)	0.0009(40)
C-1	0.2800(34)	0.4747(16)	0.7477(10)	0.0964(202)	0.0753(181)	0.0429(151)	0.0240(79)	0.0016(71)	-0.0000(67)
C-2	0.2359(36)	0.3885(16)	0.7007(9)	0.1370(247)	0.1027(208)	0.0380(152)	0.0027(93)	0.0048(78)	-0.0093(72)
C-3	0.4339(31)	0.5582(14)	0.7373(10)	0.0719(176)	0.0479(149)	0.0730(170)	-0.0046(66)	0.0114(70)	0.0104(63)
N-2	0.3403(20)	0.2150(9)	0.9640(6)	0.0459(107)	0.0217(91)	0.0439(104)	-0.0014(40)	0.0070(43)	0.0056(39)
C-4	0.2437(29)	0.1299(14)	0.9936(9)	0.0628(158)	0.0476(146)	0.0485(146)	0.0035(62)	0.0060(63)	0.0002(59)
C-5	0.3756(28)	0.1136(14)	0.0592(9)	0.0522(152)	0.0605(153)	0.0566(149)	0.0051(62)	-0.0023(61)	0.0056(59)
C-6	0.2027(28)	0.0422(13)	0.9500(9)	0.0731(169)	0.0321(129)	0.0694(158)	-0.0022(60)	0.0081(66)	-0.0061(58)
N-3	0.1007(21)	0.2768(10)	0.4413(7)	0.0559(116)	0.0285(97)	0.0518(111)	0.0040(44)	0.0056(46)	-0.0003(42)
C-7	0.1156(34)	0.3794(16)	0.4582(14)	0.0676(192)	0.0536(134)	0.1387(275)	0.0014(75)	0.0051(93)	0.0031(89)
C-8	0.2575(40)	0.4076(17)	0.5205(12)	0.1261(259)	0.1067(231)	0.0971(226)	-0.0007(98)	0.0059(99)	-0.0287(94)
C-9	0.1544(39)	0.4399(15)	0.4007(12)	0.1301(251)	0.0367(157)	0.1275(248)	0.0042(80)	-0.0107(99)	0.0132(78)
N-4	0.0102(22)	0.4119(10)	0.0872(7)	0.0667(125)	0.0344(103)	0.0583(118)	0.0081(46)	0.0173(50)	0.0116(44)
C-10	0.0641(30)	0.3364(14)	0.1305(9)	0.0747(174)	0.0449(147)	0.0545(155)	0.0077(66)	0.0106(66)	0.0066(60)
C-11	0.9712(35)	0.2401(15)	0.0974(10)	0.1281(230)	0.0504(159)	0.0788(181)	0.0106(79)	0.0145(82)	-0.0056(68)
C-12	0.9972(30)	0.3416(15)	0.1929(9)	0.0751(174)	0.1010(191)	0.0382(143)	0.0139(73)	0.0124(65)	0.0011(65)
N-5	0.1215(21)	0.9620(10)	0.6951(6)	0.0431(109)	0.0578(116)	0.0373(100)	0.0013(46)	-0.0030(43)	-0.0082(43)
C-13	0.3060(31)	0.0168(14)	0.7442(9)	0.0859(186)	0.0464(146)	0.0429(144)	0.0096(68)	0.0003(66)	-0.0021(58)
C-14	0.2862(32)	0.1154(15)	0.7499(9)	0.0918(194)	0.0739(179)	0.0599(164)	0.0180(77)	-0.0053(70)	-0.0071(68)
C-15	0.3179(35)	0.9599(15)	0.8032(9)	0.1308(230)	0.0822(185)	0.0288(138)	0.0231(85)	-0.0038(71)	0.0072(62)
N-6	0.3899(21)	0.8696(10)	0.4466(6)	0.0599(119)	0.0523(111)	0.0212(92)	0.0030(47)	0.0031(42)	-0.0072(41)
C-16	0.3615(36)	0.8186(16)	0.3866(11)	0.1071(217)	0.0647(181)	0.0708(190)	0.0197(82)	0.0099(82)	-0.0064(74)
C-17	0.2605(29)	0.8640(15)	0.3309(9)	0.0558(158)	0.1001(193)	0.0341(138)	0.0151(72)	-0.0028(60)	-0.0008(65)
C-18	0.3020(40)	0.7176(16)	0.3944(10)	0.1847(299)	0.0642(182)	0.0428(159)	0.0177(97)	-0.0132(85)	0.0012(68)

[a] Estimated standard deviations are given in parentheses. [b] The U_{ij} are defined by $T = \exp[-2\pi^2\{U_{11}(ha^*)^2 + U_{22}(kb^*)^2 + U_{33}(lc^*)^2 + 2U_{12}(ha^*kb^*) + 2U_{13}(ha^*lc^*) + 2U_{23}(hb^*lc^*)\}]$.

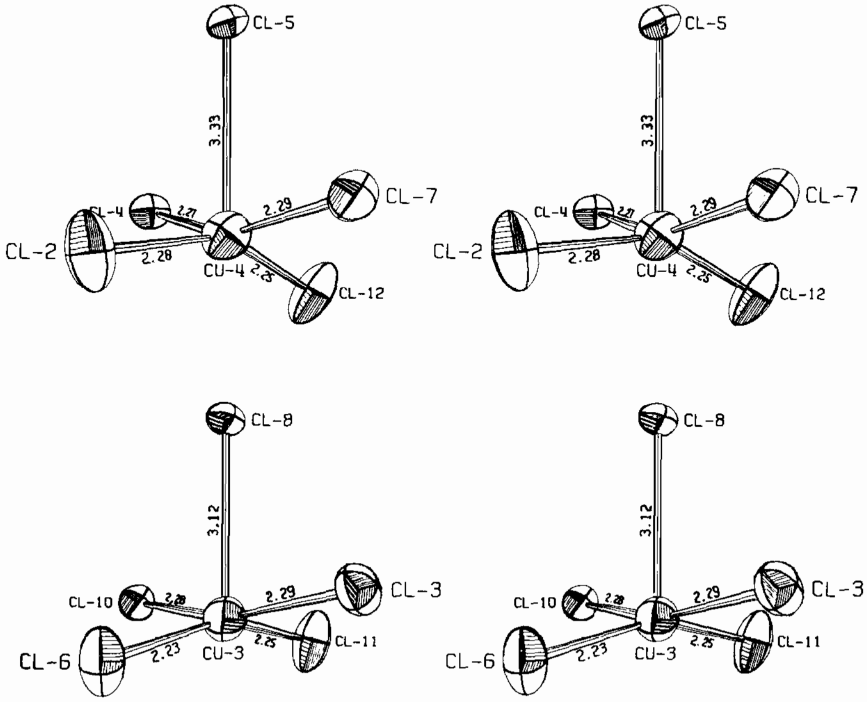

Figure 2. Copper coordination at the edges of the Cu–Cl ribbon in $[(CH_3)_2CHNH_3]_2CuCl_4$ (green – low temperature phase). The upper stereo pair illustrates the coordination found in the Cu(2) ribbon, and the lower pair pictures the conformation found along the edges of the Cu(1) ribbon.

TABLE II. Bond distances and angles for $[(CH_3)_2CHNH_3]_2CuCl_4$.[a]

Atoms	Distance[b] (Å)	Atoms	Angle[b] (°)
Centered copper coordinations			
$Cu_1-Cl_8^{2}$	2.264(11)	$Cl_8^{2}-Cu_1-Cl_1$	89.59(39)
Cu_1-Cl_1	2.300(10)	$Cl_8^{2}-Cu_1-Cl_3$	88.78(31)
Cu_1-Cl_3	3.103(10)	$Cl_1-Cu_1-Cl_3$	92.35(21)
$Cu_2-Cl_5^{3}$	2.264(9)	$Cl_5^{3}-Cu_2-Cl_9$	90.19(37)
Cu_2-Cl_9	2.322(10)	$Cl_5^{3}-Cu_2-Cl_7$	89.73(26)
Cu_2-Cl_7	3.071(12)	$Cl_9-Cu_2-Cl_7$	91.19(32)
Non-centered copper coordination			
Cu_3-Cl_6	2.233(10)	$Cl_6-Cu_3-Cl_{11}$	155.38(30)
Cu_3-Cl_{11}	2.247(10)	$Cl_6-Cu_3-Cl_{10}^{5}$	92.68(31)
$Cu_3-Cl_{10}^{5}$	2.279(8)	$Cl_6-Cu_3-Cl_3$	92.27(26)
Cu_3-Cl_3	2.290(8)	$Cl_6-Cu_3-Cl_8^{5}$	104.04(38)
$Cu_3-Cl_8^{5}$	3.123(17)	$Cl_{11}-Cu_3-Cl_{10}^{5}$	91.73(32)
		$Cl_{11}-Cu_3-Cl_3$	90.52(26)
		$Cl_{11}-Cu_3-Cl_8^{5}$	100.55(38)
		$Cl_{10}^{5}-Cu_3-Cl_3$	162.97(23)
		$Cl_{10}^{5}-Cu_3-Cl_8^{5}$	82.40(26)
		$Cl_3-Cu_3-Cl_8^{5}$	80.59(29)
Cu_4-Cl_{12}	2.250(11)	$Cl_{12}-Cu_4-Cl_4^{1}$	94.39(33)
$Cu_4-Cl_4^{1}$	2.267(8)	$Cl_{12}-Cu_4-Cl_2^{1}$	147.77(35)
$Cu_4-Cl_2^{1}$	2.278(11)	$Cl_{12}-Cu_4-Cl_7$	93.18(36)
Cu_4-Cl_7	2.88(10)	$Cl_{12}-Cu_4-Cl_5^{1}$	117.13(32)
$Cu_4-Cl_5^{1}$	3.326(14)	$Cl_4^{1}-Cu_4-Cl_2^{1}$	94.17(33)
		$Cl_4^{1}-Cu_4-Cl_7$	155.62(26)
		$Cl_4^{1}-Cu_4-Cl_5^{1}$	78.55(30)
		$Cl_2^{1}-Cu_4-Cl_7$	91.67(33)
		$Cl_2^{1}-Cu_4-Cl_5^{1}$	95.00(31)
		$Cl_7-Cu_4-Cl_5^{1}$	77.37(27)
$(CH_3)_2CHNH_3^+$ Ion distances and angles			
C_1-N_1	1.55(2)	$N_1-C_1-C_2$	102.8(1.6)
C_1-C_2	1.58(3)	$N_1-C_1-C_3$	112.2(1.8)
C_1-C_3	1.48(3)	$C_2-C_1-C_3$	115.4(2.0)
C_4-N_2	1.46(2)	$N_2-C_4-C_5^{6}$	110.4(1.6)
$C_4-C_5^{6}$	1.57(2)	$N_2-C_4-C_6$	109.8(1.6)
C_4-C_6	1.56(2)	$C_5^{6}-C_4-C_6$	109.4(1.7)
C_7-N_3	1.53(2)	$N_3-C_7-C_8$	110.6(2.1)
C_7-C_8	1.50(3)	$N_3-C_7-C_9$	107.1(2.1)
C_7-C_9	1.53(3)	$C_8-C_7-C_9$	117.4(2.2)
$C_{10}-N_4$	1.48(2)	$N_4-C_{10}-C_{11}^{4}$	109.1(1.7)
$C_{10}-C_{11}^{4}$	1.53(2)	$N_4-C_{10}-C_{12}^{4}$	109.7(1.6)
$C_{10}-C_{12}^{4}$	1.56(2)	$C_{11}^{4}-C_{10}-C_{12}^{4}$	111.9(1.8)
$C_{13}-N_5^{3}$	1.56(2)	$N_5^{3}-C_{13}-C_{14}$	107.7(1.7)
$C_{13}-C_{14}$	1.50(2)	$N_5^{3}-C_{13}-C_{15}^{3}$	106.8(1.7)
$C_{13}-C_{15}^{3}$	1.49(3)	$C_{14}-C_{13}-C_{15}^{3}$	116.0(1.8)
$C_{16}-N_6$	1.48(2)	$N_6-C_{16}-C_{17}$	113.0(1.8)
$C_{16}-C_{17}$	1.48(3)	$N_6-C_{16}-C_{18}$	111.3(2.0)
$C_{16}-C_{18}$	1.44(3)	$C_{17}-C_{16}-C_{18}$	120.0(2.1)
Copper-copper distances			
Cu_1-Cu_3	5.39(2)		
Cu_2-Cu_4	5.35(2)		
Cu_1-Cu_2	13.48(5)		

[a] The subscript refers to the atoms as numbered in Table I. The superscript (if present) refers to the following translations of those values:

1: x–1, y–1, z–1
2: x, y, z–1
3: x, y–1, z
4: x–1, y, z
5: –x, 1–y, 1–z
6: x, y, 1+z
7: 1–x, 2–y, 1–z.

[b] Estimated standard deviations in the last figures given are reported in parentheses.

Determination of Structure

An E-map calculated from the most probably set of signs produced by the University of Chicago symbolic addition programs[6] provided locations for all the copper and chlorine atoms. Refinement of these positions to a residual index of 0.26 ($R=\Sigma|\Delta F|/\Sigma|F|$) produced several trial positions for nitrogen and carbon from a difference Fourier. Refinement of the light atoms did not proceed satisfactorily, so the copper and chlorine atom parameters only were refined with their isotropic temperature factors to an R of 0.23. At this point, a β-synthesis[7] provided sufficient peaks for all the remaining atoms (except hydrogen). This is similar to a conventional electron density map except the coefficients are $|F_{obs}|^2/|F_{calc}|$. This emphasizes the unknown atoms at the expense of the known atoms. All except one of these positions were refined successfully. The last carbon atom was located on a difference Fourier map calculated when R = 0.12. Temperature factors were gradually changed to anisotropic over the range R = .16– .08. The unobserved reflections were omitted from the final three cycles of full-matrix least squares refinement in which all parameters were varied simultaneously.[8] A final value of R = 0.073 was obtained. The largest peak remaining on the difference map after refinement was 0.7 e/Å^3. Final parameters are listed in Table I. Bond distances and angles were computed with the ORFFE program[9] and may be found in Fig. 2 and in Table II. The potential N–H...Cl interactions are listed in Table III.

TABLE III. Potential N–H...Cl interactions in the green (low temperature) phase of $[(CH_3)_2CHNH_3]_2CuCl_4$. All distances below 3.75Å are listed.[a]

Atoms[b]	Distance[c] (Å)	Angle[c] (°)	Atoms[b]	Distance[c] (Å)	Angle[c] (°)
N_1–Cl_3^1	3.23	148	N_4–Cl_8^5	3.29	156
N_1–Cl_{10}	3.24	114	N_4–Cl_3	3.33	123
N_1–Cl_1^1	3.34	106	N_4–Cl_8^2	3.34	109
N_1–Cl_8	3.56	138	N_4–Cl_1^4	3.37	106
N_1–Cl_{11}	3.56	95			
N_2–Cl_3^1	3.20	161	N_5–Cl_{12}^5	3.18	120
N_2–Cl_{10}	3.21	104	N_5–Cl_7^5	3.20	165
N_2–Cl_8	3.30	121	N_5–Cl_4	3.25	99
N_2–Cl_6^1	3.30	106	N_5–Cl_5	3.28	108
N_2–Cl_1^6	3.52	107			
N_3–Cl_4^5	3.22	104	N_6–Cl_5^7	3.26	102
N_3–Cl_9	3.26	113	N_6–Cl_5	3.26	155
N_3–Cl_7	3.31	155	N_6–Cl_7^1	3.40	136
N_3–Cl_2^1	3.43	98	N_6–Cl_9^5	3.41	98
N_3–Cl_5^5	3.58	136	N_6^3–Cl_7	3.62	110
			N_6–Cl_9	3.65	62

[a] The angles included are those with the listed nitrogen as vertex, the listed chlorine as one leg, and the carbon bonded to the nitrogen as the second leg. [b] The subscript refers to the atoms as numbered in Table I. The superscript (if present) refers to the following translations of those values:

1: x–1, y–1, z–1
2: x, y, z–1
3: x, y–1, z
4: x–1, y, z
5: –x, 1–y, 1–z
6: x, y, 1+z
7: 1–x, 2–y, 1–z.

[c] Estimated standard deviations for all distances and angles are ca. 0.02Å and ca. 2°, respectively.

The Structure

The basic feature of the structure is a pair of crystallographically independent copper–chlorine "ribbons" extending parallel to the a-axis. Cu(1), Cu(3), Cl(1), Cl(3), Cl(6), Cl(8), Cl(10), and Cl(11) make up one ribbon as shown in Figure 3. The second ribbon contains Cu(2), Cu(4), Cl(2), Cl(4), Cl(5), Cl(7), Cl(9), and Cl(12). As may be noted in the schematic diagram of Figure 4, these ribbons (numbered for the centered copper that they contain) are placed diagonally across the ab and ac faces of the unit cell. The ribbons may be viewed as cut from the planar Cu–Cl sheets present in $(C_2H_5NH_4)_2CuCl_4$ as suggested by the curved lines of Figure 1. To attain the current structure, these ribbons then orient themselves at nearly right angles and relax the rigid square planar conformation for the "edge" chlorine atoms.

There are four crystallographic independent copper atoms in the unit cell. Cu(1) and Cu(2) are located at centers of symmetry and have a planar configuration with Cu–Cl bond distances of 2.26–2.35Å. In the pseudo-octahedral positions two additional chlorine atoms are situated at either 3.10Å [in Cu(1) chain] or 3.07Å [in the Cu(2) chain]. The coordination geometries of Cu(3) and Cu(4) have slight tetrahedral distortion superimposed on the basic square planar conformation, as shown in Figure 2. In both Figures 2 and 3, these non-centered copper atoms may be seen to have only one of their two octahedral "holes" occupied by chlorine atoms coordinated to the copper atoms at the center of symmetry. The Cu–Cl distances are 3.12 and 3.33Å, respectively. This completes the chain or ribbon, although the isopropylammonium ions must be added to "flesh out" the ribbon. As may be noted after careful examination of Figure 5, these ribbons, after the addition of the cations on each face, actually resemble rectangular columns.

The nitrogen atoms of the isopropylammonium groups extend into the layer of chlorine atoms that protrudes from each face of the ribbon. These nitrogen atoms each have at least four chlorine atoms below the upper limit for H-bond distances (see below). N(4) is situated *ca.* halfway between the Cl(1) in adjacent cells [and also between the Cu(1)]. It fills the "hole" (as seen in Figure 3) that occurs once each cell unit along the <100> direction in the face of the Cu(1) ribbon. N(6) fulfills the same service for

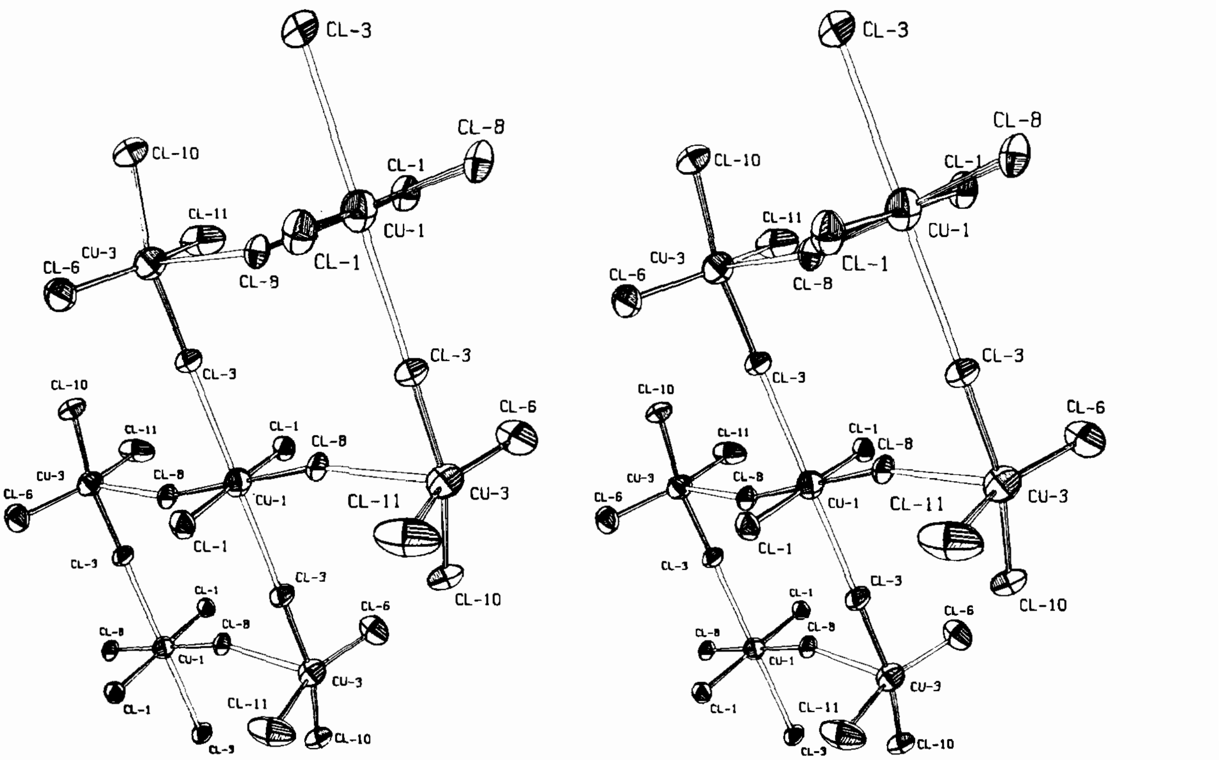

Figure 3. The structure of the Cu(1) ribbon in $[(CH_3)_2CHNH_3]_2CuCl_4$ (green – low temperature phase). Copper(1) from three-unit cells in the <100> direction are shown.

the Cu(2) ribbon. The remaining four nitrogen atoms are at close hydrogen bond distances (3.18–3.23 Å) to the chlorine atoms which comprise the ribbon edges. These have their associated isopropyl groups tilted out away from the center of the ribbon as one might well expect by considering the steric crowding on each face (see Figure 5). It is this tilting of the isopropyl groups which prevents the lateral extension of the ribbons into the two-dimensional sheets found in the high temperature phase of $(C_2H_5NH_3)_2CuCl_4$ and related compounds.

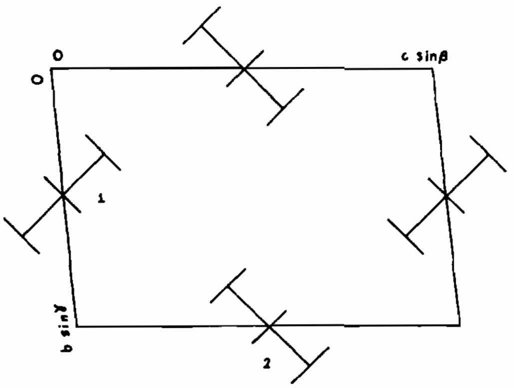

Figure 4. Schematic view of the unit cell of $[(CH_3)_2CHNH_3]_2CuCl_4$ (green – low temperature phase) parallel to the <100> direction. The copper-chlorine ribbons extend parallel to the a-axis.

Hydrogen Bonding

This structure presents some interesting structural questions in interpreting N–H...Cl hydrogen bond distances. As can be seen from Table IV, the isopropylammonium groups approach the Cu–Cl layers so that the ammonium group forms an "umbrella" over one of the chloride ions, leading to C–N–Cl angles intermediate between tetrahedral and linear (range, 148–165°). Although van der Waals' radius is not well defined for the ammonium ion, Pimentel and McClellan[10] favor a value of 3.45 Å for the N–Cl distance. Since the N–Cl distances corresponding to the nearly linear C–N–Cl angles are all ≤ 3.31 Å, these must be considered hydrogen bonds although they do not fit in the familiar pattern of linear N–H...Cl bonds (the latter would lead to a C–N–Cl angle of 109°). In addition to this, there are (with one exception) three other N–Cl distances less than 3.45 Å for each isopropylammonium ion. Examination of the structure reveals that these are not ideally situated for the hy-

TABLE IV. The observed and calculated structure factors for $[CH_3)_2CHNH_3]_2CuCl_4$. The values listed under FO and FC are 10|

K	L	FO	FC
H = 0			
0	2	1261	1124
0	3	95	54
0	4	189	-234
0	6	1033	-902
0	7	235	244
0	8	886	-707
0	9	349	335
0	10	338	-338
0	11	177	145
0	12	535	516
0	13	376	-368
0	14	777	731
0	16	666	683
0	17	255	-297
0	21	292	-326
1	0	137	146
1	1	1939	-1866
-1	1	1509	-1794
1	2	1913	1817
-1	2	1602	-1822
1	3	368	311
-1	3	55	-131
1	4	116	-166
-1	4	287	275
1	5	71	-62
-1	5	163	-162
1	6	157	88
-1	6	308	-265
1	7	642	544
-1	7	94	83
1	8	334	370
-1	8	702	-614
1	9	275	215
-1	9	514	-492
1	10	408	-392
-1	10	553	-571
1	11	230	214
-1	11	526	-529
1	12	298	-301
-1	12	775	778
1	13	691	-688
-1	13	309	-313
1	14	129	113
1	15	649	-653
-1	15	164	-163
1	16	349	387
1	17	332	-366
1	18	343	371
1	19	-295	329
-1	19	-284	-262
-1	20	-322	371
2	0	377	-440
2	1	-726	-776
-2	1	621	720
2	2	525	599
-2	2	301	403
2	3	778	696
-2	3	639	-634
2	4	1719	1561
-2	4	2176	2154
2	5	735	672
-2	5	165	-105
2	6	862	-920
-2	6	241	232
2	7	290	-234
-2	7	262	-234
2	8	221	-139
-2	8	336	302
2	9	733	-735
-2	9	113	126
2	10	-495	496
-2	10	863	880
2	11	296	-299
-2	11	559	536
2	12	-409	421
-2	12	-394	376
2	13	184	187
-2	13	302	-297
2	14	729	712
-2	14	-492	-480
-2	15	-110	109
2	16	355	390
-2	16	-121	-140
2	17	179	-166
-2	17	162	-143
2	18	126	113
-2	18	162	126
2	19	-271	277
-2	19	-215	-248
-2	20	588	603
3	0	167	-182
3	2	334	-289
-3	2	583	664
3	3	-2275	-2053
-3	3	1009	-1080
3	4	395	427
-3	4	-608	-663
3	5	-230	-293
-3	5	858	-944
3	6	288	312
-3	6	694	-791
3	7	-977	930
-3	7	806	-801
3	8	-1035	-911
-3	8	-449	462
3	9	119	-111
3	10	-772	735
-3	10	181	235
3	11	798	-770
-3	11	926	-935
3	12	305	-291
-3	12	532	-519
3	13	-421	-413
3	14	-174	211
3	15	-256	-251
-3	16	266	262
3	17	-226	-236
-3	17	-214	-226
3	18	237	-274
-3	18	180	151
3	19	431	-425
-3	19	-270	-272
3	20	241	-283
-3	20	148	-122
4	0	756	-711
4	1	315	-317
-4	1	90	-145
4	2	227	-211
-4	2	287	-238
4	3	576	-585
-4	3	249	267
4	4	996	971
-4	4	1038	-996
4	5	-1370	-1369
-4	5	1193	1233
4	6	1391	1371
-4	6	1604	1666
4	7	-288	-238
-4	7	-1469	1419
4	8	309	297
-4	8	1367	1346
4	9	866	877
-4	9	845	-814
4	10	177	132
-4	10	471	457
4	11	180	-163
-4	11	497	-493
-4	12	-147	161
4	14	383	-367
-4	15	373	-363
4	16	312	352
-4	16	293	257
4	17	236	240
4	18	587	620
-4	19	209	235
4	20	-318	354
5	0	693	643
5	1	265	241
-5	1	645	528
5	2	628	548
-5	2	798	-751
5	3	181	-178
-5	3	-898	903
-5	4	198	193
5	5	1483	-1372

K	L	FO	FC
H = 0			
-5	5	92	-22
5	6	-1109	1012
5	7	-2213	-2149
-5	7	-1897	-1831
-5	8	945	-915
-5	9	1594	-1503
5	10	325	-321
-5	10	-369	328
5	11	319	328
5	13	399	390
5	14	-402	-435
-5	14	-423	417
5	15	-366	-389
-5	15	-519	-498
5	16	593	-659
-5	16	198	-114
5	17	364	-385
-5	17	-144	-150
-5	18	-271	-298
5	19	341	-356
6	0	-187	-167
6	1	-719	-712
6	2	405	424
-6	2	86	7
6	3	-226	-228
-6	3	567	609
6	4	271	241
-6	4	94	147
6	5	653	663
-6	5	769	-719
6	6	1049	999
-6	6	245	-225
6	7	125	-164
6	8	-1404	1365
-6	8	281	291
-6	9	414	382
6	10	423	-412
-6	10	258	260
6	11	229	201
-6	11	320	293
6	12	132	-124
-6	12	377	365
6	13	258	227
-6	13	408	-360
6	14	378	382
-6	14	-643	619
6	15	278	327
6	16	267	299
-6	16	-427	488
6	17	154	-168
-6	17	-509	511
-6	18	-343	311
-6	19	-135	-99
7	0	598	559
7	1	-453	-490
7	2	619	671
-7	2	-131	-149
7	3	494	-524
-7	3	732	-751
7	4	577	525
-7	4	508	-503
7	5	-196	-252
-7	5	-593	-580
7	6	-663	-679
-7	6	-114	-99
7	7	441	-425
-7	7	-551	517
7	8	211	222
-7	8	124	145
7	9	-277	-301
-7	9	-194	137
7	10	217	-267
7	11	153	-163
-7	11	308	-247
7	12	598	-602
-7	12	-293	242
7	13	-150	-121
-7	13	-876	-766
7	14	157	-204
-7	14	164	109
-7	15	-150	104
7	16	-548	590
7	17	268	-276
-7	17	400	-381
8	0	-282	264
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-8	1	170	-129
8	2	-341	343
-8	2	-109	94
8	3	-268	283
-8	3	-442	-444
8	4	988	937
-8	4	624	617
8	5	-254	-264
-8	5	227	-211
8	6	108	112
-8	8	-236	-231
8	10	717	723
8	11	366	384
-8	11	190	-167
8	12	393	367
-8	12	-859	759
8	13	278	313
-8	13	664	603
8	14	389	-405
-8	14	533	492
-8	15	-165	170
8	16	-135	90
-8	17	-290	-266
9	0	-455	-445
9	1	390	-389
-9	1	632	-629
9	2	-955	-924
-9	2	-117	134
9	3	111	134
-9	3	528	-508
-9	4	-523	439
9	5	199	217
9	6	-437	436
-9	6	-273	255
9	7	-126	94
-9	7	347	330
-9	8	-415	357
9	9	-581	-589
-9	9	-211	-199
9	10	122	-79
-9	10	325	275
9	11	917	-957
-9	11	184	164
9	12	474	505
9	13	330	-373
-9	13	345	-372
-9	14	702	-665
-9	15	561	-533
10	0	-687	644
10	1	165	154
-10	1	-284	295
10	2	151	144
-10	2	638	590
10	3	199	192
10	4	-413	-410
-10	4	275	251
10	6	194	199
10	7	-148	195
-10	7	-493	-511
10	8	506	530
-10	8	-421	338
10	9	-238	281
-10	9	-270	-295
10	10	-205	198
-10	10	-183	162
10	11	336	-355
10	12	379	433
-10	12	398	-335
10	13	-221	-232
-10	13	161	-118
10	14	-379	408
-10	14	211	153
11	0	392	-406
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-11	1	484	-498
-11	2	383	-324
11	4	248	-245
-11	4	175	-165
11	5	-256	-209

K	L	FO	FC
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-11	6	201	176
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-11	7	311	-235
11	8	439	468
-11	8	-388	351
-11	9	513	-492
11	10	319	353
-11	10	328	-277
-11	11	364	-313
-12	1	296	275
-12	3	272	220
12	4	262	290
-12	4	141	77
12	5	203	184
12	6	179	146
-12	6	504	410
12	7	345	-335
-12	7	228	-171
-12	8	160	194
12	9	411	-471
12	10	287	268
-12	10	295	256
13	0	145	153
13	1	124	-79
-13	1	183	147
13	3	547	-538
13	4	-120	-91
13	5	193	-170
-13	5	602	-500
-13	6	304	-259
-13	7	284	-234
-13	8	226	-205
-14	1	173	-155
H = 1			
0	0	263	-291
0	1	395	-468
0	2	611	-695
0	3	2720	-2279
0	4	218	185
0	5	83	43
0	6	416	372
0	7	1899	1768
0	8	200	151
0	9	299	-305
0	10	413	426
0	11	800	-792
0	14	232	235
0	15	727	-767
0	16	239	-307
0	17	293	-302
0	19	171	-171
0	20	262	-303
1	0	839	939
1	1	683	1144
-1	1	708	-896
1	-1	353	-397
1	2	232	294
-1	2	1278	1283
1	-2	375	523
1	3	84	79
1	-3	585	-749
1	4	1178	-1035
1	-4	299	379
1	5	1472	-1366
1	-5	396	-411
1	-6	255	237
1	7	97	136
1	-7	289	-327
1	8	545	-505
1	-8	88	141
1	9	607	589
1	-9	353	299
1	10	1114	1068
1	-10	467	483
1	11	703	-662
1	-11	179	170
1	12	732	700
1	-13	1294	1323
1	14	789	819
1	-14	216	285
1	15	362	380
1	16	435	460
1	-16	735	775
1	-17	404	-434
1	18	183	172
1	-18	193	240
1	-19	-408	-480
1	-20	-212	-280
1	-21	-189	-268
2	0	636	-673
2	1	-548	-546
-2	1	-394	-624
2	-1	2275	-2212
2	2	935	827
-2	2	735	819
2	-2	424	509
2	3	-1329	1168
-2	3	555	535
2	-3	197	199
2	4	424	-374
-2	4	105	87
2	-4	353	352
2	5	689	-666
-2	5	649	605
2	-5	468	-458
2	6	733	634
-2	6	1217	-1096
2	-6	694	705
2	7	1071	-1054
-2	7	1093	-1090
2	-7	891	-891
2	8	-637	-626
-2	8	772	718
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2	9	-368	320
-2	9	-193	110
2	-9	948	-1016
2	10	253	-234
-2	10	-134	114
2	11	513	-471
-2	11	-144	-193
2	-12	-865	-849
2	13	750	-733
-2	13	757	-776
2	-13	-264	297
2	14	-370	-371
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2	15	-790	-823
-2	15	-226	-223
2	-15	-530	-555
2	16	-133	-135
-2	16	-148	138
2	-17	321	-345
2	18	167	156
-2	18	145	-150
2	-18	247	-274
2	19	-228	-248
2	-19	263	-294
-2	20	-271	-309
2	-20	-312	351
3	0	-113	-49
-3	1	-295	312
3	-1	-248	278
3	2	555	-515
-3	2	478	-507
3	-2	496	561
3	3	-237	197
-3	3	807	869
3	-3	239	-178
3	4	885	747
3	-4	-302	-280
3	5	-1204	1132
-3	5	519	-517
3	-5	1141	-1181
3	6	1316	1250
-3	6	-913	933
3	-6	-505	547
3	7	1043	-1004
-3	7	516	487
3	-7	-910	-975
3	8	524	511
-3	8	1363	1340

K	L	FO	FC
H = 1			
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3	9	139	-135
-3	9	-396	-326
3	-9	730	780
3	10	-163	-161
-3	10	397	-355
3	-10	336	356
3	11	432	393
-3	11	905	-904
3	-11	895	940
3	12	134	143
-3	12	134	99
3	-12	263	-264
3	13	270	243
-3	13	409	-380
3	14	-578	574
3	-14	-660	703
-3	15	-298	316
3	16	206	204
-3	17	309	363
-3	18	121	-146
3	-18	403	451
3	19	215	-257
3	-20	379	404
4	0	1077	1000
4	1	-417	425
-4	1	-1382	1438
4	-1	-477	-436
4	2	392	353
-4	2	585	-669
4	3	765	-778
-4	3	500	-534
4	-3	967	-965
4	4	473	-486
-4	4	373	381
4	-4	441	-462
4	5	175	146
-4	5	855	-858
4	-5	1294	-1432
4	-6	190	244
4	7	-236	-192
-4	7	828	-829
4	-7	150	178
4	8	180	193
-4	8	738	-762
4	9	1048	-1066
-4	9	945	-962
4	-9	449	504
4	10	179	-154
4	-10	430	-444
4	11	379	-399
-4	11	611	-565
4	12	415	-428
-4	12	767	781
4	-12	270	268
-4	13	483	457
4	-13	608	-587
4	14	165	-184
4	-14	177	183
4	15	374	-377
-4	15	-291	260
4	-15	-272	-304
4	16	422	444
-4	16	208	-193
4	-16	210	-219
4	-17	268	-268
4	18	153	-152
-4	18	151	-179
4	-18	137	176
-4	19	135	-92
4	-19	533	-542
4	-20	259	-299
5	0	95	114
5	1	-280	-248
-5	1	705	943
5	-1	1068	-1092
5	2	762	776
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5	-2	460	-517
5	3	177	-193
-5	3	347	296
5	-3	267	-313
5	4	1022	1010
-5	4	-1086	1137
5	-4	-733	810
5	5	154	-153
-5	5	336	318
5	-5	435	462
5	6	-115	55
-5	6	342	-359
5	-6	794	830
5	7	-1260	1212
-5	7	-303	-264
5	-7	921	928
5	8	-828	838
-5	8	-450	430
5	-8	-689	-696
5	9	-614	615
-5	9	-378	-363
5	-9	-105	-95
5	10	541	630
-5	10	593	1005
5	-10	157	184
5	11	109	110
-5	11	160	-132
5	-11	497	-505
-5	12	-501	486
5	-12	-490	489
5	13	122	145
-5	13	164	137
5	-13	-300	-294
5	14	-372	-442
-5	14	-363	-361
5	-14	-293	313
5	15	378	-411
-5	15	138	-184
5	-15	143	135
5	16	264	309
-5	16	297	-342
5	-16	409	414
5	17	-257	-330
-5	17	-243	230
5	-17	-186	-150
5	18	-381	384
-5	18	-283	284
5	-18	-346	354
5	-19	380	440
6	1	-689	-670
-6	1	178	-175
6	-1	286	-333
6	2	429	-443
6	-2	171	203
6	3	608	-594
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6	-4	1072	1085
6	5	-659	-644
-6	5	-344	-374
6	-5	210	158
6	6	248	-255
-6	6	130	-176
6	-6	971	-992
6	7	-584	-622
-6	7	536	-539
6	8	713	-720
-6	8	849	803
6	-8	393	-427
6	9	211	-241
-6	9	-530	-534
6	-9	112	-133
-6	10	463	473
6	-10	655	625
6	11	123	-112
-6	11	475	-485
6	12	431	437
-6	12	380	-383
6	-12	226	209
6	13	-145	160
-6	13	-371	-349
-6	14	-411	-416
6	15	311	354
6	-15	-414	-382
6	16	165	217
6	-16	-328	314

K	L	FO	FC
H = 1			
6	17	-473	-543
6	-17	336	-294
7	0	-923	902
7	1	467	-444
-7	1	-186	-263
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4	6	312	247
-4	6	-235	219
4	-6	251	280
-4	7	-170	-157
4	-7	-704	-705
-4	8	-150	162
4	-8	-606	-605
4	9	-169	-153
-4	9	-297	314
4	-9	-482	-520
-4	10	281	-312
4	11	155	167
4	-11	597	-616
-4	12	127	-170
4	-12	339	312
-4	13	305	-343
4	-13	309	-295
-4	14	-288	-321
4	-14	165	-214
4	15	-444	-497
-4	15	240	-312
4	-15	-256	-284
-4	16	164	-204
4	-16	154	-130
4	-17	-303	299
5	0	-143	139
5	1	206	218
-5	1	-93	-75
5	-1	691	715
5	2	769	721
-5	2	-825	916
5	3	938	-919
-5	3	489	-541
5	-3	210	210
-5	4	573	598
5	-4	225	250
5	5	-278	-267
5	-5	230	-274
5	6	163	196
-5	6	707	712
5	7	152	107
-5	7	635	657
5	9	331	285
-5	8	218	-243
5	-8	-339	351
5	-10	589	570
5	-11	259	-205
5	-12	-211	185
5	13	-222	224
5	14	-375	429
-5	14	-166	202
-5	15	185	190

K	L	FO	FC
H = 3			
5	-15	-306	279
-5	16	563	615
5	-17	-296	281
5	-18	200	153
6	0	332	-305
6	1	605	575
-6	1	826	-888
6	-1	132	-117
6	2	383	379
-6	2	369	-418
6	3	127	178
-6	3	489	-539
6	-3	732	-728
6	4	432	416
-6	4	-449	459
6	-4	-289	-304
6	5	-388	-369
-6	5	442	506
6	-5	545	-579
6	6	377	-346
-6	6	259	-267
6	7	-239	-189
-6	7	167	139
6	-7	488	-505
-6	8	-129	-120
6	9	170	-174
-6	9	-418	-454
6	-9	418	-406
6	10	157	155
-6	10	155	159
6	11	472	-520
-6	11	131	-120
6	-11	157	-149
6	12	249	-272
6	-12	227	-224
6	13	-205	-226
-6	13	-186	-192
6	-13	-169	164
6	-14	162	-209
-6	15	-403	-429
6	-17	498	-467
7	0	237	-221
7	-1	-656	-667
7	2	-615	-630
-7	2	-779	819
7	-2	434	412
7	3	162	144
-7	3	571	545
7	4	411	425
-7	4	116	108
7	-4	445	404
7	6	232	221
-7	6	651	-625
7	-6	364	405
-7	7	-307	-296
7	-7	160	-127
-7	8	157	161
7	-8	-137	105
7	9	-137	168
-7	9	-219	-236
7	10	436	465
-7	10	185	182
-7	11	171	186
7	-11	-299	267
-7	12	379	391
-7	13	154	-129
7	-13	370	382
-7	14	-432	414
7	-14	-125	128
-7	15	140	-131
7	-16	214	203
8	0	-303	300
8	2	-353	-352
-8	2	-250	277
8	-2	145	94
8	3	132	163
-8	3	258	-263
8	4	137	-135
-8	4	-674	-670
8	5	194	-244
-8	5	192	-215
8	-5	525	-490
8	6	251	267
-8	6	-121	-140
8	-6	-192	193
8	7	379	-409
8	-7	-168	-134
-8	8	239	246
8	-8	362	379
8	9	-501	-560
-8	9	277	268
8	10	408	-424
-8	11	-166	-151
-8	12	254	291
8	-12	232	-175
-8	13	602	-577
8	-13	129	-95
-8	14	244	232
8	-14	-253	-268
9	0	279	245
9	1	264	298
-9	1	336	-321
9	-1	196	239
-9	2	-484	-454
9	-2	-134	-91
9	3	125	152
-9	3	-239	-242
9	-3	-173	-161
9	4	143	-159
-9	4	267	-296
9	-4	386	396
-9	5	-152	118
9	-5	-248	-284
9	6	-207	225
-9	6	-304	315
9	-6	-573	572
-9	7	333	319
9	8	-694	730
9	-8	-222	163
-9	9	-184	175
9	-10	161	-138
-9	11	-275	-319
-9	12	614	606
9	-12	-167	-213
10	0	213	-149
10	1	-207	-222
-10	1	-339	-368
10	-1	241	-249
-10	3	347	388
10	4	138	-169
-10	4	-245	247
10	-4	606	615
10	5	-118	-138
-10	5	-147	99
10	-6	133	65
-10	8	364	-328
10	-8	197	-182
-10	9	503	-476
-10	10	282	245
10	-10	340	-355
-10	11	319	-292
-10	12	223	223
11	0	276	264
-11	1	214	197
11	-1	132	85
-11	2	423	400
11	-2	335	326
-11	4	195	184
-11	8	451	408
-11	10	545	492
-12	1	177	-145
-12	2	189	171
-12	3	-173	-117
-12	4	310	-263
-12	7	153	-120
-12	8	329	295
-13	1	254	284
-13	3	-447	451
-13	5	219	197
-13	6	633	580
-14	2	321	-334

and 10 | F_{calc} |, respectively. A negative sign preceding the value of 10 F_{obs} denotes a reflection with $I>2\sigma_I$.

H = 4

K	L	FO	FC
0	0	1282	1208
0	1	188	206
0	4	426	-387
0	5	787	-725
0	7	118	-115
0	9	341	347
0	10	320	312
0	11	209	208
0	12	554	575
0	13	217	-247
0	14	174	208
1	0	253	-181
1	1	729	-684
-1	1	308	-255
1	-1	255	-298
1	2	602	542
-1	2	458	-441
1	-2	340	-322
1	3	499	459
-1	3	340	-359
1	-3	256	298
1	4	125	71
-1	4	202	188
1	5	138	154
1	-5	377	-433
1	6	177	134
-1	6	131	-111
1	7	434	-390
-1	7	608	602
1	-7	966	-998
1	-8	152	-176
1	9	318	-295
1	-9	470	-503
1	10	211	-168
-1	10	139	-178
1	11	125	-70
-1	11	434	-420
1	-11	158	160
-1	12	332	410
1	-12	341	360
1	13	197	-230
-1	13	437	-479
1	14	142	158
-1	14	184	208
1	-14	187	-205
1	-15	246	-203
1	-17	209	225
1	-19	-198	-190
2	0	167	155
2	1	511	-493
-2	1	221	-188
2	-1	472	468
2	2	809	778
2	3	688	-643
-2	3	-223	-231
2	4	354	350
-2	4	182	167
2	-4	129	-169
2	5	157	109
-2	5	733	718
2	6	157	197
-2	6	431	-450
2	-6	184	-237
-2	7	338	313
2	8	-176	123
2	-8	587	600
-2	9	199	-183
2	-9	854	913
-2	10	190	164
2	-10	720	738
-2	11	174	-147
2	12	136	-168
-2	12	-405	426
2	-12	-344	332
2	13	198	196
-2	13	209	-255
2	-13	343	-356
2	-14	-269	286
2	-19	-300	-294
3	0	131	-111
-3	1	749	-731
3	-1	239	245
3	2	-609	593
-3	2	410	422
3	-2	-190	196
3	3	1165	-1107
-3	3	-379	-411
3	4	-462	438
-3	4	-204	-194
3	-4	455	-501
3	5	-555	-522
-3	5	132	148
3	-5	205	249
-3	6	-731	-736
-3	7	541	-528
3	-7	134	76
3	8	167	-214
3	-9	529	-545
-3	10	218	215
3	-10	232	-263
3	-11	1130	-1159
3	12	528	-629
-3	12	-130	159
3	-13	-231	-237
3	-14	-122	127
3	-17	218	-191
3	-18	-195	192
4	0	277	-274
4	1	-258	287
4	-1	509	-533
4	2	339	358
4	-2	224	-219
-4	3	302	305
4	-3	349	-368
4	4	1008	983
-4	4	184	-214
4	-4	-148	-203
4	5	134	-138
-4	5	164	145
4	-5	-200	188
4	6	517	504
-4	6	341	325
4	-6	320	369
-4	7	-151	158
4	8	142	-151
-4	8	514	538
4	9	-154	125
4	-9	-219	-196
-4	10	231	-240
4	-10	449	417
4	11	-136	158
-4	11	349	-365
4	-11	232	252
4	12	155	116
-4	12	153	-184
4	-12	298	275
4	-13	232	190
4	-14	137	-157
4	-15	295	-272
4	-16	155	164
4	-17	337	-325
5	0	-199	181
5	1	258	-252
5	-1	372	-341
5	2	-419	-383
-5	2	753	-755
5	-2	543	585
5	3	430	-416
-5	3	464	-455
5	-3	222	226
5	4	380	-382
-5	4	-541	-558
5	-4	-354	401
5	5	396	-379
-5	5	442	-473
5	6	137	107
-5	6	-351	376
5	-6	146	-151
5	7	293	-305
-5	7	495	-487
5	-7	-243	-289
-5	8	-212	-218
5	-8	-295	-336
-5	9	407	-433
5	-9	142	-90

H = 4

K	L	FO	FC
5	10	302	-319
5	11	-136	-144
-5	12	-161	162
5	-12	499	-473
5	-13	272	-191
5	-14	130	153
5	-15	-510	-464
5	-16	270	280
6	0	-484	467
-6	1	267	269
6	2	190	146
-6	2	-160	-173
6	-2	-201	212
-6	3	-659	700
-6	4	928	950
-6	5	154	188
6	-5	201	-221
6	6	118	90
-6	6	-541	565
-6	7	440	-467
6	8	470	473
-6	8	179	152
6	-8	203	185
6	9	162	173
-6	10	298	318
6	-10	238	-217
-6	12	302	290
6	-13	333	-299
6	-14	511	456
6	-15	151	151
7	0	147	-134
-7	1	379	425
7	-1	116	-51
-7	2	168	178
7	-2	270	-254
-7	3	147	-106
7	-3	246	-243
-7	4	280	-306
7	5	135	-178
-7	5	-857	-873
7	-5	-283	-254
7	6	283	-276
-7	6	155	-163
7	-6	292	306
7	7	545	-573
-7	7	220	-197
7	-7	208	-191
7	8	-130	144
-7	8	-218	234
7	-8	-154	164
-7	10	218	208
-7	11	-247	-275
7	-12	-381	356
-7	13	432	-463
8	0	110	126
8	1	-194	238
8	2	127	-179
-8	2	211	-226
8	-2	302	290
8	3	135	159
-8	3	-371	-395
8	-3	-196	238
8	4	183	172
-8	4	159	-170
8	-4	463	453
-8	6	187	189
8	-6	213	213
-8	7	195	168
8	-7	-179	-170
-8	8	466	469
8	-8	152	-151
-8	9	162	200
8	-9	132	-196
-8	10	408	389
-8	11	-262	-278
8	-11	-225	-276
-8	12	277	323
-9	1	-550	-591
9	-1	-166	-199
9	-2	-189	-252
-9	3	232	233
9	-3	422	-440
-9	4	319	342
9	-4	302	-337
-9	5	-376	390
9	-5	-235	-247
-9	6	239	265
9	-6	-238	-234
9	-8	-145	112
-9	9	-591	-526
-9	10	238	-272
-9	11	280	-300
-10	2	-264	263
-10	6	166	-181
-10	7	289	-268
-10	10	353	333
-11	1	182	-204
-11	2	161	147
-11	4	273	290
-11	5	243	-189
-11	7	171	-194
-11	8	179	203
-12	2	128	132
-12	3	184	-178
-12	5	-285	-325
-12	6	289	271
-13	2	121	-170
-13	3	-279	-238

H = 5

K	L	FO	FC
0	0	129	-144
0	1	242	241
0	2	165	175
0	3	253	-212
0	4	151	-141
0	9	336	-348
0	11	510	-535
1	0	261	-244
1	1	248	228
-1	1	463	-433
1	2	392	377
-1	3	254	-244
1	4	144	81
-1	4	234	-224
1	-4	599	632
1	5	416	-408
-1	5	293	305
-1	6	303	295
1	-6	220	287
-1	7	121	146
1	-7	290	-339
-1	8	347	327
1	-8	301	-309
1	9	348	374
-1	9	294	-339
1	-9	397	-393
1	10	465	487
-1	10	163	164
-1	11	134	134
1	-11	306	-300
1	-13	616	621
1	-16	305	353
2	0	293	-290
2	1	168	-136
-2	1	648	-596
2	2	-214	-155
-2	2	238	223
2	-2	-471	524
-2	3	-432	425
2	4	163	99
-2	4	178	198
2	-4	120	103
2	5	274	-236
-2	5	324	389
2	-5	362	-407
2	6	231	202
2	-6	120	-126
2	7	535	-559
-2	7	394	-359
2	-7	275	-294
2	8	-246	-260
-2	8	-173	-129
2	-9	326	-295
2	-10	-219	202

H = 5

K	L	FO	FC
2	-12	-442	-467
2	-15	384	-359
2	-17	197	-221
3	0	-554	531
3	1	-129	138
-3	1	-120	120
-3	2	252	239
3	-2	-360	351
-3	3	-544	551
3	-3	359	-374
3	4	-185	174
3	-4	-206	-220
3	5	326	371
-3	5	291	-291
3	-5	269	-259
3	6	-362	330
3	8	-250	253
3	-8	244	236
-3	9	205	197
3	-9	-192	192
3	-10	163	-194
-3	11	384	-440
3	-11	294	276
3	-12	194	-161
3	-13	-220	-198
3	-14	-541	516
3	-15	-240	-217
3	-16	-233	200
4	0	283	253
4	1	-283	-221
-4	1	-316	349
4	-1	-550	-576
4	2	-136	120
-4	2	304	-340
4	3	305	-345
-4	3	575	-593
4	-3	221	-244
4	4	307	-312
-4	4	237	-254
4	5	255	-248
-4	5	551	-581
4	6	422	-435
4	-6	-143	173
4	7	157	-132
-4	7	149	155
4	-8	209	-203
-4	9	-172	-140
-4	10	185	207
4	-10	518	-497
4	11	310	-295
4	-11	136	129
4	-12	408	404
4	-13	259	-207
4	-14	464	441
5	0	218	225
5	1	129	-100
5	-1	217	-263
5	2	368	303
5	3	281	321
-5	3	-294	-298
5	4	-400	417
-5	4	-525	545
5	-4	-367	390
5	5	326	318
-5	5	-251	249
5	-6	143	141
5	7	252	-262
5	-7	137	159
5	9	391	-266
-5	9	392	-381
-5	10	120	99
5	-10	206	185
5	-12	378	331
5	-13	-281	-289
6	1	361	-387
-6	1	543	-592
6	-1	134	-157
6	2	154	-158
-6	2	-146	135
6	-2	-243	266
6	3	-248	-234
6	-3	-249	-256
6	4	144	-133
-6	4	275	-302
6	-4	262	250
-6	5	-160	-131
6	-5	-282	-229
6	-6	-350	-350
-6	7	-502	-507
-6	8	290	311
6	-8	137	-158
-6	9	186	-163
6	-9	159	158
-6	10	332	365
6	-11	261	-244
7	0	252	266
-7	1	228	214
7	-1	117	105
7	-2	354	335
-7	3	205	237
7	-3	156	-105
-7	4	220	-253
7	-5	-328	307
-7	6	477	498
-7	7	311	-343
7	-7	336	331
-7	8	-535	538
7	-8	-205	182
-7	10	212	220
-8	1	197	-211
-8	2	-322	-298
-8	3	139	172
-8	4	-232	236
-8	5	215	-264
-8	6	-504	497
-8	7	227	-235
-8	9	-313	-317
-9	1	-423	435
-9	2	-298	321
-9	4	-414	393
-9	5	-196	-207
-9	6	-217	172
-10	2	169	171
-10	3	-420	-435
-10	5	236	-219
-10	6	-170	-159
-11	1	456	-447
-11	2	161	118
-11	3	287	-286
-11	4	182	213
-12	1	351	-314

H = 6

K	L	FO	FC
0	1	523	545
0	6	507	499
1	0	201	-247
1	1	125	-86
1	-1	631	-650
1	2	157	-191
-1	2	195	-171
1	-2	415	-411
-1	3	149	-138
1	-3	265	-283
1	5	162	-110
-1	5	273	-257
-1	6	252	280
1	-6	363	411
1	-8	350	345
1	-10	197	-164
1	-12	168	-173
1	-13	402	-421
1	-14	141	112
2	0	312	274
2	1	187	-153
2	2	194	149
-2	2	-216	201
2	-2	190	177
2	3	-176	148
-2	3	226	201
2	-3	362	372
2	4	127	114
-2	4	323	311
2	-4	319	352
-2	6	205	228

H = 6

K	L	FO	FC
2	-5	233	-230
2	-11	188	-194
2	-12	411	403
2	-13	-155	-122
3	1	-437	-420
3	2	-178	-200
-3	2	-202	181
-3	3	222	-199
3	-3	235	-246
-3	4	-145	-149
3	-4	-166	182
-3	5	459	-484
3	-5	314	-331
-3	6	-201	-185
3	-6	248	-232
3	-10	164	175
3	-11	179	-122
4	0	243	271
-4	1	-515	-533
-4	2	191	190
4	-2	274	271
-4	3	290	-304
4	-3	419	-461
-4	4	200	215
4	-4	311	327
-4	6	-412	412
-4	7	207	216
4	-7	308	311
4	-8	-321	340
-5	1	367	-401
-5	2	310	346
-5	4	245	269
-5	5	-122	-98
-5	7	188	-192
-6	2	160	166
-6	3	168	-195
-6	4	174	171
-6	5	350	-331
-6	6	130	130
-7	1	-242	-254
-7	3	331	-302
-7	4	-367	382
-8	2	-401	420
-9	1	-136	-121

H = -1

K	L	FO	FC
0	1	128	244
0	2	515	596
0	3	803	-922
0	4	174	-54
0	5	1104	-1013
0	6	750	685
0	7	953	-854
0	8	558	-511
0	9	205	-252
0	10	82	-54
0	11	802	-778
0	12	750	-731
0	13	461	-439
0	14	1015	-1006
0	15	115	122
0	16	474	497
0	17	218	-254
0	18	772	821
0	20	253	328
0	21	214	-216
1	0	170	-206
1	1	290	308
1	2	255	283
1	3	446	488
1	4	2348	2000
1	6	410	428
1	7	682	582
1	8	934	866
1	9	104	-62
1	10	96	-97
1	11	234	-197
1	12	1156	1129
1	14	162	-171
1	16	479	-518
1	18	145	155
1	20	-458	479
2	0	438	564
2	1	1165	-1175
2	2	911	-1034
2	3	276	51
2	4	204	-200
2	5	578	-563
2	6	562	-469
2	7	238	-145
2	8	-361	313
2	9	504	-486
2	10	137	-179
2	11	603	-589
2	12	-293	260
2	13	414	-430
2	14	-731	742
2	15	-216	241
2	16	326	-322
2	17	190	-185
2	18	382	-394
2	20	291	299
2	21	-230	-274
3	0	-2040	2023
3	1	-527	-505
3	2	834	784
3	3	885	832
3	4	256	233
3	5	-73	7
3	6	-1070	980
3	7	-137	20
3	8	1301	1285
3	9	-201	-185
3	10	-685	647
3	12	384	-329
3	13	-685	-675
3	14	-226	-238
3	15	-196	200
3	16	448	563
3	17	-428	467
3	18	163	-206
3	19	119	145
3	21	219	-230
4	0	208	-206
4	1	-1053	-1103
4	2	217	191
4	3	270	244
4	4	-1013	-936
4	5	1146	-1058
4	6	932	-880
4	7	1547	-1467
4	8	196	204
4	10	879	834
4	11	-523	504
4	12	709	722
4	13	412	415
4	15	244	-218
4	16	453	-468
4	19	155	180
4	20	484	-569
5	0	-92	-100
5	1	92	107
5	2	1359	1295
5	3	1000	-911
5	4	420	450
5	5	365	394
5	6	694	608
5	7	-218	-144
5	8	-521	-513
5	9	-859	-856
5	10	227	-165
5	11	617	-631
5	12	282	299
5	13	144	142
5	14	-304	296
5	18	-366	406
5	19	344	383
5	20	-182	215
6	0	-929	-936
6	1	407	403
6	2	461	431
6	3	652	-690
6	4	-587	611
6	5	-1382	-1357

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K	L	FO	FC
6	6	867	829
6	7	-500	526
6	10	385	-422
6	11	510	-774
6	12	521	-543
6	13	-190	-215
6	17	183	-206
6	19	-570	-613
7	1	-547	536
7	2	-213	-187
7	3	675	642
7	4	372	369
7	5	-679	-684
7	7	921	-909
7	9	-676	698
7	10	576	579
7	12	-290	298
7	13	200	-197
7	14	117	131
7	16	-234	254
7	17	172	97
7	18	168	188
8	0	-166	-171
8	1	979	-959
8	3	339	326
8	4	-195	142
8	5	745	720
8	6	774	808
8	7	-203	-249
8	8	-254	-279
8	9	360	-384
8	10	310	-319
8	12	223	261
8	13	-617	-704
8	14	235	-263
8	15	-663	-711
9	0	486	467
9	1	-374	-363
9	3	-612	-578
9	4	-624	-604
9	5	168	152
9	7	235	225
9	8	-920	960
9	9	-109	-130
9	11	294	314
9	12	-439	475
9	13	317	320
9	14	512	548
9	16	169	170
9	17	278	-329
10	1	672	679
10	2	146	149
10	4	328	-355
10	5	183	-185
10	6	528	-514
10	7	-224	-236
10	8	461	473
10	9	-599	-668
10	10	-210	231
10	11	473	-519
10	12	264	-299
10	13	346	-368
11	0	215	-215
11	1	232	258
11	2	197	215
11	3	860	906
11	4	679	678
11	5	180	202
11	7	-169	195
11	9	127	-201
11	10	496	529
11	12	391	388
11	13	125	-141
12	0	422	408
12	1	290	-306
12	2	404	-382
12	3	271	-305
12	5	204	-197
12	7	286	-318
12	8	381	-403
12	9	119	-87
12	11	134	-98
12	12	323	314
13	0	348	326
13	2	287	275
13	5	204	215
13	6	606	663
13	7	220	239
13	8	343	348
14	1	-404	-401
14	2	144	149
14	3	258	-278
14	4	243	-280
14	5	154	-138

H = -2

K	L	FO	FC
0	1	159	-220
0	2	846	947
0	3	758	-705
0	4	1172	-1129
0	5	214	-188
0	6	557	569
0	7	829	-819
0	8	572	505
0	9	159	163
0	10	566	545
0	11	1394	1385
0	12	613	639
0	13	102	115
0	14	248	251
0	15	645	-643
0	17	429	419
0	18	205	225
0	20	203	174
1	1	2246	-2024
1	2	200	165
1	3	2136	-1984
1	4	309	-240
1	5	303	-236
1	6	88	54
1	7	292	-274
1	8	359	299
1	9	488	-519
1	10	291	-227
1	11	320	-315
1	12	636	-622
1	13	759	758
1	14	319	304
1	15	988	-955
1	16	136	-156
1	17	675	-668
1	18	169	-134
1	20	-243	266
2	0	660	-669
2	1	1311	1361
2	2	426	402
2	3	270	-266
2	4	633	-542
2	5	214	212
2	6	896	813
2	7	83	50
2	8	742	744
2	9	-253	-222
2	10	669	647
2	11	-608	-595
2	13	603	616
2	15	588	609
2	16	-893	929
2	17	148	-144
2	19	182	-218
3	0	-248	239
3	1	-483	542
3	2	537	-501
3	3	-1250	1150
3	4	-1316	-1225
3	5	-1061	-1032
3	6	1684	-1573
3	7	1405	-1292
3	10	-949	910
3	11	774	-757
3	12	1160	1151
3	13	-884	-881
3	14	-452	-668
3	17	-145	-175

H = -2

K	L	FO	FC
3	19	139	-135
3	20	298	-301
4	0	-578	588
4	1	-501	480
4	2	-284	-266
4	3	1117	1056
4	4	1390	1378
4	5	2157	2007
4	6	1050	1092
4	7	-86	-107
4	8	-205	-220
4	9	-340	-311
4	11	304	-277
4	12	1222	1200
4	13	635	-628
4	14	-454	464
4	15	-120	115
4	16	227	-222
4	17	271	294
4	18	-248	255
4	19	-176	205
4	20	168	97
5	0	-107	97
5	1	148	-152
5	2	-763	-731
5	3	370	-305
5	4	-1056	-1016
5	5	416	-391
5	6	470	486
5	7	241	251
5	8	-772	746
5	9	1252	-1229
5	10	493	-481
5	11	-278	-251
5	12	-263	239
5	13	339	-327
5	14	-399	377
5	16	206	-207
5	17	-123	142
5	18	-206	-180
5	20	-179	215
6	0	791	890
6	2	-537	574
6	3	119	111
6	4	357	-312
6	5	265	-226
6	6	135	-99
6	8	-1237	1163
6	9	170	165
6	10	1047	1066
6	11	437	-451
6	12	299	-313
6	13	-214	-211
6	14	-135	142
6	16	-134	98
6	17	164	232
6	18	192	-246
6	19	237	253
7	0	-542	-577
7	1	1141	-1150
7	2	-819	817
7	3	324	-315
7	4	269	295
7	5	-305	280
7	6	-594	-625
7	7	317	-333
7	8	875	-869
7	9	364	-381
7	10	-295	272
7	13	-278	-264
7	15	-240	-223
7	16	-308	322
7	17	244	-215
7	18	197	213
8	0	-405	423
8	1	524	-531
8	2	644	657
8	3	1207	-1277
8	4	241	269
8	5	-104	-74
8	7	121	107
8	8	-584	-577
8	9	249	278
8	10	118	-91
8	11	-265	295
8	12	376	395
8	13	145	126
8	14	175	144
8	15	332	-371
8	17	437	-453
8	19	322	345
9	0	539	594
9	1	444	455
9	2	-150	89
9	3	701	-712
9	5	-410	-383
9	6	-270	244
9	8	-160	-137
9	9	-157	161
9	10	296	-322
9	11	242	-227
9	12	122	-144
9	13	298	-285
9	14	-284	323
10	0	250	245
10	1	196	199
10	2	-495	519
10	3	527	522
10	5	-144	-143
10	8	192	-189
10	9	-228	218
10	12	247	229
10	13	285	-330
10	14	525	581
10	15	213	-222
10	16	297	347
11	1	752	-765
11	4	179	189
11	6	114	137
11	7	278	-244
11	13	131	-178
12	3	170	-114
12	4	-193	193
12	5	276	285
12	6	356	362
12	8	-444	432
12	9	327	-337
12	12	171	-189
13	1	184	164
13	3	337	-349
13	5	-306	-331
13	8	-273	283
13	9	195	-223
13	10	272	279
14	4	457	446
14	5	201	-225
14	6	193	195

H = -3

K	L	FO	FC
0	1	547	-549
0	2	566	-612
0	3	820	-917
0	4	643	723
0	5	514	-504
0	6	377	-368
0	7	282	269
0	8	741	-715
0	9	323	-330
0	10	342	320
0	11	284	273
0	12	722	701
0	15	519	-525
0	16	171	-162
0	17	433	-400
0	18	131	116
0	19	188	-202
0	20	164	-180
1	0	1378	1305
1	1	398	387
1	3	120	127
1	4	106	100
1	5	313	-234
1	6	1241	1230
1	7	332	296

H = -3

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1	8	538	-504
1	9	161	203
1	10	674	-627
1	11	983	-965
1	12	193	172
1	14	917	864
1	15	457	416
1	16	290	299
1	17	186	-206
1	18	354	364
2	0	318	344
2	1	412	-442
2	2	-800	757
2	3	210	208
2	4	1075	-991
2	5	942	-919
2	7	397	-445
2	9	953	927
2	12	-327	310
2	13	1008	-971
2	14	-383	379
2	15	548	-533
2	17	231	-245
2	18	211	-245
2	19	375	-414
2	20	-251	-318
3	0	-473	-541
3	1	-716	-737
3	2	885	881
3	3	135	166
3	4	-495	470
3	6	455	-424
3	7	1139	-1098
3	9	104	130
3	11	395	367
3	13	-162	-136
3	14	-735	719
3	15	-453	-408
3	16	618	614
3	17	296	297
3	18	527	537
3	19	157	153
3	21	148	190
4	1	230	-304
4	2	524	-512
4	3	1169	-1207
4	4	397	392
4	5	911	870
4	6	326	267
4	8	-225	241
4	9	-1193	-1140
4	10	157	152
4	11	423	-432
4	12	-412	-396
4	14	-713	-238
4	15	-520	-503
4	17	-513	-512
4	18	283	-302
4	19	-160	-135
5	0	-272	293
5	1	457	505
5	2	381	-405
5	3	820	-810
5	4	516	-472
5	5	-605	-549
5	7	-1061	1012
5	8	1072	1063
5	9	328	296
5	10	-911	881
5	11	178	-111
5	12	582	557
5	13	-467	470
5	14	-249	-250
5	16	260	236
5	17	-152	-116
5	18	-188	152
6	0	277	297
6	1	90	65
6	2	332	328
6	3	206	177
6	4	784	808
6	5	-686	-653
6	6	331	-325
6	7	882	-848
6	8	-226	-196
6	9	211	212
6	10	350	-321
6	11	411	-406
6	13	351	-347
6	14	218	-208
6	15	305	356
6	17	283	-329
6	18	-364	378
7	0	138	103
7	1	465	-534
7	4	403	407
7	5	103	-104
7	6	710	703
7	7	434	-419
7	8	512	485
7	9	-214	203
7	11	856	878
7	12	-536	521
7	14	-241	249
7	15	-241	260
7	16	298	-327
7	17	214	-211
7	19	-422	-487
8	0	-709	764
8	1	654	-664
8	2	-150	-142
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8	4	142	-183
8	6	-493	-524
8	7	-349	-348
8	9	572	-547
8	10	565	-574
8	11	-123	-136
8	12	233	-213
8	13	210	-203
8	14	407	420
8	16	225	224
8	17	280	332
9	0	-846	881
9	2	-1203	1228
9	3	196	-187
9	4	552	566
9	5	-232	254
9	7	316	301
9	8	-165	-210
9	10	-209	200
9	12	308	-337
9	13	190	-215
9	15	375	-418
9	16	-364	389
10	0	581	-586
10	1	-753	-734
10	3	583	-574
10	5	454	-449
10	7	149	157
10	10	135	129
10	11	154	-169
10	12	205	243
10	13	-234	261
10	14	135	-148
10	15	322	-355
10	16	154	-150
11	1	138	140
11	4	419	427
11	5	172	198
11	6	275	254
11	11	540	-591
11	14	-274	314
12	2	179	-189
12	3	395	-419
12	4	-216	-227
12	5	507	-521
12	7	184	-180
12	8	237	244
12	9	242	240
12	10	-276	309
12	11	160	212
13	4	-231	265
13	5	313	-396
13	6	122	134

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13	7	450	-472
13	9	155	170
14	2	151	149
14	3	143	149
14	4	198	234

H = -4

K	L	FO	FC
0	1	132	-160
0	3	525	590
0	4	499	576
0	5	752	789
0	6	517	525
0	7	285	-298
0	8	368	383
0	9	531	-473
0	10	115	-104
0	11	200	-209
0	12	399	416
0	13	250	234
0	14	403	370
0	15	210	234
0	16	195	193
0	18	154	-156
0	19	192	205
1	0	749	667
1	1	1002	-942
1	2	501	478
1	3	1187	-1307
1	4	640	-700
1	5	257	-243
1	6	367	-344
1	7	693	650
1	8	408	384
1	10	244	-230
1	12	244	-232
1	13	551	-570
1	15	119	-82
1	16	289	236
1	17	383	-390
1	18	-146	167
1	19	-135	184
2	1	293	-278
2	2	-2092	2003
2	3	186	166
2	4	1935	1778
2	5	154	-124
2	6	417	-390
2	7	542	515
2	10	218	-234
2	12	-127	-110
2	15	118	-113
2	16	214	172
2	17	238	-205
2	18	-647	610
3	0	338	-416
3	1	-616	-758
3	2	605	-627
3	3	860	-797
3	4	-856	833
3	5	158	-119
3	7	267	219
3	8	-539	-496
3	9	-110	124
3	10	509	483
3	11	153	131
3	13	-274	-265
3	14	-180	161
3	15	-156	-168
3	16	285	-288
3	17	443	-428
3	19	312	-293
3	20	152	155
4	0	648	738
4	1	-355	-340
4	2	170	-140
4	3	399	-387
4	4	525	-478
4	5	670	-601
4	6	618	595
4	7	-579	532
4	8	134	-74
4	9	-450	435
4	12	344	300
4	13	388	-352
4	14	-431	410
4	15	257	-304
4	16	280	295
4	19	154	-140
5	0	428	469
5	2	607	641
5	5	560	-536
5	7	1110	-1065
5	9	114	128
5	10	461	-475
5	11	146	125
5	14	-295	304
5	15	-433	-437
5	18	169	189
5	19	-178	-194
6	0	-592	-620
6	2	-427	457
6	3	-290	-277
6	6	-431	403
6	7	669	-621
6	8	-678	633
6	9	503	-475
6	10	281	215
6	11	474	479
6	13	-295	248
6	16	135	-126
6	19	-166	171
7	0	428	-477
7	1	-215	204
7	3	128	-124
7	4	796	789
7	5	125	-173
7	7	160	-169
7	8	-557	560
7	9	845	-832
7	11	-670	-634
7	12	315	-282
7	13	245	263
7	15	207	210
7	17	171	-140
7	18	-292	-322
8	0	161	155
8	1	324	335
8	2	212	-252
8	3	250	-205
8	4	671	655
8	5	430	-436
8	6	432	428
8	7	-171	213
8	8	252	258
8	9	226	184
8	10	655	668
8	14	-290	-305
8	15	322	333
8	16	363	348
9	0	132	-175
9	1	-266	-335
9	2	-344	-375
9	3	-133	-133
9	5	-596	-603
9	6	-423	440
9	7	313	-267
9	11	-131	137
9	12	-235	195
9	13	-190	-168
9	14	655	-700
9	15	196	-184
9	16	-325	-354
10	0	-403	424
10	1	217	-232
10	3	-283	290
10	5	159	139
10	6	270	265
10	8	-376	377
10	9	272	-271
10	10	133	-121
10	12	421	422
10	13	181	242
10	14	600	601
10	15	220	234

H = -4

K	L	FO	FC
11	0	182	161
11	1	146	-100
11	3	352	-382
11	4	546	-550
11	6	437	-437
11	8	224	227
11	9	143	-150
11	11	196	-222
11	12	199	-203
11	13	424	-442
12	0	125	116
12	1	140	177
12	2	396	394
12	3	294	332
12	4	290	308
12	6	-274	-301
12	9	125	-107
12	10	553	560
13	2	-237	-243
13	7	155	-154
13	8	345	-341

H = -5

K	L	FO	FC
0	2	127	-128
0	3	711	-774
0	5	285	-270
0	6	695	725
0	8	148	147
0	11	368	-351
0	12	325	-315
0	13	305	-295
0	14	569	-580
0	16	193	-211
0	17	286	-285
0	18	275	265
1	1	513	490
1	2	257	269
1	4	221	239
1	5	345	-365
1	6	395	343
1	7	300	-284
1	8	649	653
1	9	220	178
1	11	347	349
1	12	190	207
1	13	220	225
1	15	259	275
1	17	371	348
1	18	-374	348
2	0	125	124
2	1	391	-351
2	2	-189	-182
2	5	173	-173
2	6	139	-183
2	7	622	-569
2	8	177	186
2	9	493	-503
2	10	152	-191
2	15	324	-259
2	16	396	-378
2	18	174	-136
3	0	595	584
3	1	426	-427
3	3	-149	-168
3	5	221	186
3	6	-320	266
3	7	370	315
3	8	-365	516
3	10	436	432
3	11	184	208
3	14	-214	189
3	16	340	286
3	17	232	-249
3	18	401	-417
4	0	280	309
4	2	403	455
4	3	138	-83
4	5	378	-369
4	6	592	-578
4	7	381	-344
4	8	187	-152
4	9	-529	-504
4	11	316	-304
4	13	125	-123
4	15	208	227
4	16	343	310
4	17	123	172
4	18	-189	201
5	0	149	-196
5	1	201	231
5	2	216	237
5	3	-117	96
5	4	-506	473
5	5	353	389
5	6	318	330
5	7	272	242
5	8	-116	74
5	9	271	-237
5	10	644	585
5	11	248	-240
5	12	459	414
5	13	-381	-380
5	14	-159	-128
5	15	189	-183
5	16	494	-516
5	18	305	267
6	0	-375	-459
6	2	-313	-321
6	3	207	-203
6	5	-293	-239
6	6	-299	302
6	7	-176	160
6	8	236	-237
6	9	-436	-426
6	11	469	-436
6	12	265	226
6	14	462	436
6	16	-203	-159
7	0	335	368
7	1	207	286
7	3	235	241
7	4	151	196
7	5	-510	-498
7	6	407	384
7	7	247	-225
7	8	354	359
7	9	228	217
7	11	-359	-387
7	12	-388	-387
7	13	160	-109
7	14	-243	209
7	16	-156	148
7	17	169	169
8	0	281	-314
8	1	284	-272
8	2	118	-158
8	3	-123	-113
8	4	225	-229
8	6	377	390
8	7	-519	-474
8	8	-319	306
8	9	144	162
8	10	583	580
8	11	289	309
8	13	326	-321
8	14	-383	-443
8	15	472	-424
9	0	132	160
9	2	-320	320
9	4	-135	123
9	5	-163	159
9	6	123	-150
9	7	-223	-212
9	8	-158	-169
9	9	497	-499
9	11	-274	308
9	12	-461	474
9	13	419	401
9	14	-323	334
10	0	-123	102
10	1	149	137
10	7	322	334
10	8	-194	187
10	11	355	-319

H = -5

K	L	FO	FC
10	12	245	-266
11	1	-168	193
11	3	-267	301
11	5	331	-317
11	7	136	152
11	10	-338	355
12	0	229	236
12	1	235	-239
12	3	497	562
12	5	-136	164
12	6	152	-191
12	7	367	-365
12	8	333	-347

H = -6

K	L	FO	FC
0	1	425	417
0	2	256	279
0	4	132	-135
0	5	169	-164
0	7	519	-549
0	8	306	277
0	9	385	-369
0	10	276	267
0	11	297	313
0	12	159	-132
0	14	127	118
1	0	400	-425
1	4	162	165
1	5	144	-119
1	8	381	242
1	9	385	-392
1	10	355	333
1	13	169	186
1	14	140	-114
1	15	513	-507
2	0	-196	-165
2	3	328	-341
2	4	236	212
2	5	171	-169
2	6	409	393
2	10	125	130
2	11	257	-234
2	13	-534	521
2	14	-163	167
2	15	245	240
3	0	231	237
3	1	457	465
3	2	187	167
3	5	552	-514
3	7	524	-505
3	10	168	-173
3	11	400	-347
3	13	-129	-116
3	14	-200	-210
3	15	-347	383
4	1	-137	-170
4	2	163	-239
4	3	294	338
4	4	130	148
4	5	456	409
4	7	211	-155
4	8	-425	407
4	9	-275	210
4	10	-285	260
4	12	194	161
4	13	441	-420
5	0	305	372
5	1	-162	-190
5	4	-196	-223
5	5	-381	349
5	6	139	-148
5	8	205	-290
5	9	698	-688
5	12	251	226
5	13	176	-190
5	14	-221	196
5	15	463	-412
6	0	-321	373
6	5	170	125
6	7	-562	591
6	8	570	503
6	10	-302	285
6	11	321	-296
6	13	-185	160
6	14	-260	255
7	1	155	-210
7	3	159	-163
7	4	277	-276
7	5	-232	-220
7	6	416	-420
7	10	523	515
7	11	-442	-413
7	13	397	-361
7	14	124	-70
8	2	-333	404
8	3	-163	161
8	4	-317	285
8	6	-129	-129
8	7	-192	-195
8	8	401	-396
8	10	-154	148
8	12	616	605
9	1	-310	-332
9	2	175	-174
9	3	380	-383
9	4	-175	225
9	6	-317	289
9	8	-182	-197
9	10	369	-377
9	11	163	-164
10	0	-481	501
10	1	175	193
10	2	416	443
10	5	194	-188
10	6	-285	270
10	8	-148	110
10	9	128	140

H = -7

K	L	FO	FC
1	3	189	199
1	4	177	207
1	6	330	370
2	1	189	-165
2	4	257	-289
2	5	204	-230
2	7	117	-85
3	1	192	-212
3	2	-476	418
3	4	-143	179
3	8	204	199
3	9	-164	209
4	1	191	-183
4	3	239	-303
4	4	335	315
4	8	-232	-216
5	2	136	-163
5	3	-185	-242
5	5	-203	-205
5	6	-197	152
5	7	139	166
5	8	163	-181
6	4	132	-126
6	8	143	127

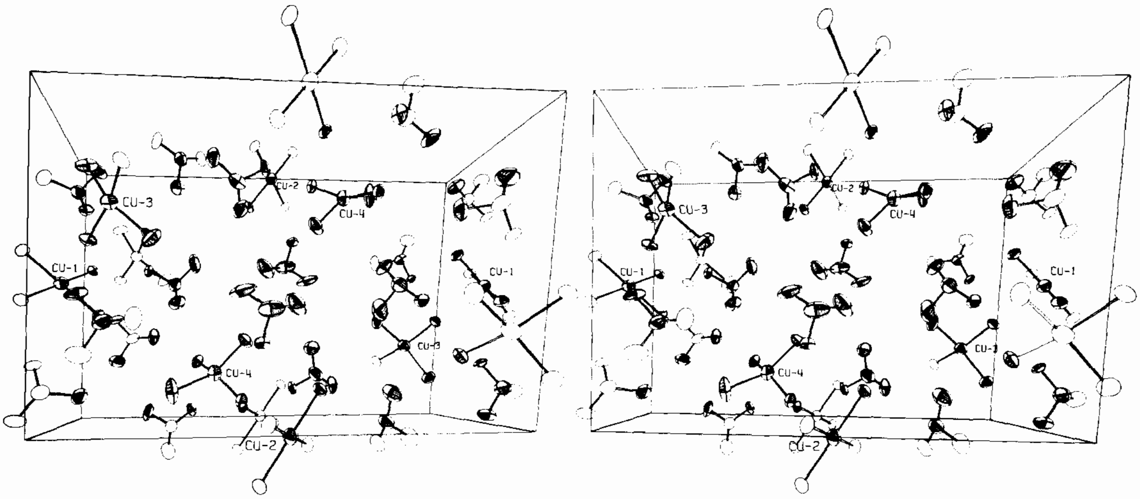

Figure 5. Contents of one unit cell in the structure of $[(CH_3)_2CHNH_3]_2CuCl_4$ (green – low temperature phase). The atoms shown with blank thermal ellipsoids are outside the cell but complete a particular ion started inside.

drogen atoms on the nitrogen. Thus, the hydrogen atoms are probably disordered in this structure.

Geometry of the $CuCl_4^{2-}$ Ion

The $CuCl_4^{2-}$ ion has been found to assume a variety of coordination geometries in various compounds. Ions with geometries approaching square planar have been found only in compounds of the type $(RNH_3)_2CuCl_4$. It is probably hydrogen bonding which accounts for the stabilization of this geometry. Felsenfield[11] has indicated in his calculations on the electronic structure of the $CuCl_4^{2-}$ ion that it is primarily electrostatic repulsions between the chlorine atoms which favor the tetrahedral geometry. Hydrogen bonding will reduce the effective charge on the chlorine atoms, thus allowing the square planar geometry favored by the crystal field stabilization. The $CuCl_4^{2-}$ ions then can pack in the manner shown in Figure 1 or Figure 3, leaving convenient "holes" for the $R–NH_3^+$ groups to pack.

Other compounds containing the $CuCl_4^{2-}$ but without the extensive N–H...Cl hydrogen bonding possibilities show a distinctly different coordination. The compound Cs_2CuCl_4[12, 13] exhibited a distorted tetrahedral configuration with a pair of angles at *ca.* 124°. Even $[(CH_3)_2NH_2]_3Cl(CuCl_4)$[14] has a distorted tetrahedral $CuCl_4^{2-}$ ion with two angles widened to *ca.* 136°. The present compound, with its examples of angles widened to 148–163°, extends this even further. It suggests the probable existence of a continuum of $CuCl_4^{2-}$ ions from nearly tetrahedral geometry to the square planar state, depending on the specific environment. In particular, it should be noted that the greater the potential for hydrogen bonding, the closer the $CuCl_4^{2-}$ ions approach the square-planar coordination.

Thermochromism

This structural study has elucidated the structure of the low-temperature form of one compound of the type $(RNH_3)_2CuCl_4$. The principal features are the breakdown of the two-dimensional sheets and the distortion of some of the $CuCl_4^{2-}$ ions from strict square-planar geometry. Since the formation of the ribbon structure in this structure appears to be related to the bulk of the isopropyl group, it seems unlikely that this breakup of the two-dimensional sheets extends to those compounds with straight-chain organic groups. Indeed, recent studies[15] have shown that the yellow to green thermochromism observed upon cooling several copper chloride salts is due solely to a change in the width of the electronic absorption band and not to a shift in position. The latter would be expected if a change in coordination geometry were to occur.

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5 Reflections were called observed if they were $2\sigma_I$ above background, where σ_I = [total]count + background + $(.01 \times \text{net count})^2 + (.01 \times \text{background})^2]^{1/2}$.
Weights (w) assigned to each $|F_{obs}|$ were ($w = 1/\sigma_F^2$, where $\sigma_F = |F_{obs}|\sigma_I/2I$, and I is the observed diffraction intensity.
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