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The crystal structure of $LiCuCl_3 \cdot 2H_2O$*

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Abstract

$LiCuCl_3 \cdot 2H_2O$ forms garnet-red, monoclinic crystals, a = 6.078, b = 11.145, c = 9.145Å (all ±0.003), β = 108°50', space group $P2_1/c$, Z = 4. The structure contains planar $Cu_2Cl_6^=$ ions joined by longer Cu···Cl links to form chains. Oxygen positions were found; half of the water molecules are coordinated to copper. Lithium and hydrogen positions were not revealed by this three-dimensional determination.

A final refinement using the Levy-Bussing anisotropic temperature factor treatment and least squares program achieved a discrepancy factor, R, of 10.5% for our visually determined intensities. Standard deviations as determined from least squares are about 0.007Å for oxygen parameters, less for others, while important interatomic distances have been determined with standard deviations of ~0.0025Å.

The structure has very interesting magnetic properties, reported elsewhere. Because of this, a neutron diffraction study is underway at Brookhaven.

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DISCLAIMER

An interesting correlation between structure and color of copper chlorides is noted.

Introduction

The garnet-red crystals of $LiCuCl_3 \cdot 2H_2O$ were first reported by Chassevant (1891), but the composition was settled by Meyerhoffer (1892). Attempts to interpret the formula and discuss the color in terms of complex ions by Donnon (1905), Werner (1911) and Getman (1922) did not settle the nature of this double salt, and when our preliminary study revealed the possibility of the hitherto unknown $Cu_2Cl_6^=$ ion, complete structural work was undertaken. Simultaneously this ion was found in $KCuCl_3$ (Dwiggins, 1958).

Preparation and Properties

$LiCuCl_3 \cdot 2H_2O$ was prepared by the method of Getman (1922). The prismatic, monoclinic crystals are elongated along what we have chosen as the a-axis. The most prominent face is (011), with (001) and (010), and a complex set of end faces. The garnet-red crystals are pleochroic; when viewed through the (011) face thin crystals appear wine red with the electric vector at 66° to a, green-yellow with the electric vector normal to this direction.

The crystal density, determined by flotation, is 2.36 g/cc., In all but very dry air the crystals are deliquescent, forming a green surface quickly. Upon further standing in moist air the crystals dissolve.

X-ray Study

X-ray data—Single crystals were mounted in thin-walled capillary tubes, inevitably with the long axis of the crystal, a, parallel to the capillary axis. Weissenberg, oscillation and precession photographs showed C_{2h} Laue symmetry. Lattice constants determined by the back reflection Weissenberg technique (Buerger, 1942) were: a = 6.078, b = 11.145, c = 9.145±0.0003Å, β = 108°50'. The X-ray density for Z = 4 is 2.39 g/cc, in good agreement with the observed density, above.

Reflections {h0ℓ} were observed only with ℓ even; {0k0} reflections were observed only for k even. The space group appears, then, to be $P2_1/c$, which the structure confirms.

Though a variety of data were used in the preliminary stages, subsequently three dimensional data were taken with an equi-inclination Weissenberg camera, and filtered MoKα radiation, with intensities visually estimated from a combination of timed exposure and multiple film methods and a standard set of diffraction maxima.

Structure determination—The structure determination proceeded through Patterson projections to find copper positions and a clue as to chlorine positions, and thence through Fourier projections to a rough structure. Oxygen positions appeared on the earliest Fouriers, and it seems unnecessary to record the course of the determination in more detail here.

Patterson and Fourier projections were computed by means of the "TDF40-80 Program for the IBM-650" written here by Dr. D. R. Fitzwater

(unpublished, but a later version T.D.F. 2 available upon request). Refinement procedures, first two dimensional and later three dimensional, were made using the least squares program for the IBM-650 written by Drs. M. E. Senko and D. H. Templeton. This program is limited to isotropic temperature factors, and in a final refinement the full matrix program of Busing and Levy, with anisotropic temperature factors, was used on the MURA IBM-704 at Madison, Wisconsin. Final parameters, Tables I, II and III, are from this program, which gave positional parameters in quite excellent agreement with those of the isotropic refinement. Since there has been some interest in the agreement between the two treatments, both sets of positional parameters are given. The structure factor agreement is given in Table IV.

Throughout this work, the scattering factors used were those of Berghuis et al. (1955). Corrections for anomolous dispersion were made, following Templeton and Dauben (1955).

Discussion of the Structure

General description—$LiCuCl_3 \cdot 2H_2O$ is made up of nearly planar $Cu_2Cl_6^=$ of approximately D_{2h} symmetry. The Cu-Cl distances within the ion are ~2.3Å, and the ions are connected into $(Cu_2Cl_6^=)_X$ chains through two Cu···Cl links of about 2.9Å, to the ion above, and two others to the ion below, as shown in Fig. 1. Including only the closest chlorine neighbors, the configuration about each Cu II is approximately square planar, but in addition each copper atom has a chlorine atom above the plane at 2.9Å, and a water molecule (OI) below at 2.6Å, so that

the over-all configuration about Cu II is approximately a tetragonally deformed octahedron, a predominant feature of Cu II crystal chemistry.

Half the water molecules are bound to Cu II, and half appear between chains, grouped in pairs which suggest that they form part of a polyhedron about the lithium ion. The X-ray data do not seem to be sufficient to locate the lithium ion, although we did not obtain a full three-dimension Fourier for the structure, since a neutron diffraction investigation by Dr. Sidney Abrahams, underway at Brookhaven, should provide an unambiguous position.

An examination of the structure shows that the chlorine ions and water molecules are nearly resolvable into close-packed planes parallel to (010). These are warped enough by the interactions with Cu^{++} and Li^{+} ions so that no very long range cubic or hexagonal arrangement of the layers is maintained. A complete list of interatomic distances is given in Table V; a comparison of bond distances, averaged over thermal motion, is given in Table VI. It is interesting to note that the averages in the case of independent motion differ by more than three standard deviations from the nonindependent averages.

The $Cu_2Cl_6^{=}$ ion—In the crystal this ion is required to have a center of symmetry, and it deviates a small but significant amount from D_{2h} symmetry. There are three crystallographically distinct Cl^{-} ions. If we let normals to the planes containing ClI-Cu-Cu, ClII-Cu-Cu and ClIII-Cu-Cu be denoted by N_1, N_2 and N_3 the angle between N_1 and N_2 is 1.7°, that between N_1 and N_3 is 5.05° and that

between N_2 and N_3 is 6.75°. Cl I forms an external Cu-Cl bond of 2.258Å within the $Cu_2Cl_6^=$ ion and a weaker bond of 2.922Å to the copper of a neighboring $Cu_2Cl_6^=$. Cl II forms an exterior Cu-Cl bond of 2.284Å with no further bond to copper. Standard deviations of 0.0025Å indicate that the difference between these two Cu-Cl bonds is real, and since this is in the opposite direction expected, we expect that Cl II is more strongly hydrogen bonded than Cl I. There are two crystallographic Cu-Cl III bridge bonds of 2.300 and 2.306Å. The difference is of doubtful significance. Bond angles are given in Fig. 1a. They deviate significantly from the right angles expected for most descriptions of the bonding to Cu II, but probably these deviations are no greater than to be expected from the varying environments of the crystallographically different chlorine atoms. The difference in bond distances of bridged and exterior chlorines is surely significant, and in agreement with those reported for $CuCl_2 \cdot 2H_2O$ (Peterson and Levy, 1957) for non-bridged Cu-Cl bonds (2.275Å) and bridges in $CuCl_2$ (Wells, 1947a) (2.3Å).

Lithium position and hydrogen bonding—Two O_{II} oxygens are separated by only 2.8Å, and are related by a center of symmetry. Because of this relationship they cannot be hydrogen bonded unless there is a statistical disorder in the structure. Holes on either side of this oxygen pair, and the arrangement of chlorines about these holes lead us to expect that each O_{II} is coordinated to two lithium ions, Fig. 1b. On this basis we were able to arrive at a satisfactory hydrogen bonding scheme for the crystal.

Unfortunately when a lithium ion was placed in the expected position and least-squares refinement cycles were carried out using the Levy-Busing 704 program, the temperature factors for the lithium ion increased rapidly and unreasonably leading us to discard this approach. We have now decided to await the neutron diffraction solution to the lithium position and hydrogen bonding, as these two problems are related.

Color and structure—As noted above, $LiCuCl_3 \cdot 2H_2O$ is red brown. There are a number of such copper chlorides, and upon examination it was noted that for all those whose structure is known there are $Cu\overset{Cl}{\diagdown\diagup}Cu$ bridges where the bridge angle is ~90° and where both bridge bonds are ~2.3Å. These include $CuCl_2$ (anhyd.) (Wells, 1947a), $CsCuCl_3$ (Wells, 1947b), $KCuCl_3$ (Dwiggins, 1958). NH_4CuCl_3 appears to be isomorphous with $KCuCl_3$ and is red. It is also worth noting that in all of these compounds the four nearest neighbors to Cu II are chlorine. If in all of the $Cu\overset{Cl}{\diagdown\diagup}Cu$ bridges, there is one long bond ~2.9Å, then the color is blue. A further study of the colors of Cu II compounds is underway, but the preliminary data on the pleochroism in $LiCuCl_3 \cdot 2H_2O$ and $CuCl_2$ suggests that for maximum absorption of visible light the electric vector is along the line of centers of the closely bridged copper ions.

Magnetic properties—$LiCuCl_3 \cdot 2H_2O$ remains paramagnetic to about 5.9°K, where magnetic ordering, presumably antiferromagnetic, takes place (Vossos, Jennings and Rundle, 1960). The ground state for the $Cu_2Cl_6^{=}$ ion is apparently a triplet in agreement with a theory of magnetic interaction of bridged transition metal halides (Rundle and Vossos, 1959). The magnetic ordering is also receiving attention in the neutron diffraction study at Brookhaven.

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Table I: Refined positional parameters

Atom	Parameter	IBM 650 with unobserved F*	σ	IBM 704 without unobserved F**	σ
Cu	X	0.8251	0.0003	0.82476	0.00020
	Y	0.0070	0.0001	0.00697	0.00011
	Z	0.1119	0.0002	0.11177	0.00013
Cl I	X	0.5332	0.0006	0.53272	0.00040
	Y	0.1295	0.0003	0.12956	0.00020
	Z	0.1194	0.0003	0.11942	0.00028
Cl II	X	0.2012	0.0006	0.20108	0.00039
	Y	0.3981	0.0003	0.39791	0.00021
	Z	0.1827	0.0004	0.18280	0.00026
Cl III	X	0.8913	0.0005	0.89126	0.00039
	Y	0.3809	0.0003	0.38142	0.00020
	Z	0.4186	0.0003	0.41853	0.00026
O I	X	0.1568	0.0020	0.15507	0.00137
	Y	0.1321	0.0009	0.13108	0.00073
	Z	0.3062	0.0011	0.30435	0.00082
O II	X	0.6466	0.0019	0.64661	0.00107
	Y	0.3954	0.0009	0.39556	0.00065
	Z	0.0350	0.0011	0.03522	0.00081

* Isotropic thermal parameters

** Anisotropic thermal parameters

Table II: Scale factors

Layer	Scale factor	σ
0	0.2419	0.0033
1	0.2411	0.0021
2	0.2408	0.0020
3	0.2408	0.0022
4	0.2369	0.0021
5	0.2310	0.0023
6	0.2285	0.0024
7	0.2183	*

* Not varied in anisotropic cycles

Table III: Anisotropic temperature factors

Atom	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Cu	0.01402	0.00342	0.00607	0.00170	0.00512	0.00110
σ	0.00029	0.00009	0.00013	0.00011	0.00014	0.00009
Cl I	0.01540	0.00330	0.00764	0.00124	0.00573	0.00064
σ	0.00056	0.00015	0.00026	0.00021	0.00029	0.00016
Cl II	0.01442	0.00390	0.00599	0.00056	0.00452	0.00091
σ	0.00055	0.00015	0.00024	0.00021	0.00028	0.00015
Cl III	0.01633	0.00349	0.00659	0.00199	0.00530	0.00127
σ	0.00059	0.00015	0.00027	0.00022	0.00030	0.00016
O I	0.01977	0.00555	0.00626	0.00075	0.00546	0.00044
σ	0.00209	0.00061	0.00082	0.00085	0.00103	0.00059
O II	0.00908	0.00459	0.00734	-0.00074	0.00029	0.00050
σ	0.00161	0.00052	0.00090	0.00066	0.00091	0.00054

Table IV: List of observed and calculated structure factors. The calculated structure factors are scaled to the observed data.
(Continued on pages 14-19)

H	K	L	OBSERVED	CALCULATED
0	0	2	4.920	3.913
0	0	4	24.930	-30.261
0	0	6	7.410	-7.468
0	0	8	3.390	2.617
0	0	10	9.710	9.328
0	0	12	3.490	-1.857
0	0	14	3.920	-3.903
0	1	2	8.180	-7.964
0	1	3	6.220	-7.501
0	1	4	4.970	5.256
0	1	5	27.900	-34.165
0	1	6	3.010	3.440
0	1	7	2.440	2.318
0	1	8	4.160	-3.865
0	1	9	13.440	12.472
0	1	10	3.920	-3.306
0	2	2	3.390	3.782
0	2	3	4.350	3.470
0	2	4	17.510	-17.941
0	2	5	10.330	8.768
0	2	6	4.590	-5.629
0	2	7	9.710	8.858
0	2	8	6.410	5.907
0	2	9	7.080	-6.816
0	2	10	4.880	5.097
0	2	11	4.540	-4.321
0	3	1	9.140	9.643
0	3	2	10.530	-10.797
0	3	3	10.050	-10.916
0	3	4	7.610	7.811
0	3	5	2.100	-1.365
0	3	8	4.780	-4.622
0	3	9	5.830	4.791
0	3	10	3.110	-2.774
0	3	13	4.590	-4.129
0	4	0	20.100	-20.366
0	4	1	6.650	6.095
0	4	2	2.530	3.082
0	4	4	6.740	-6.510
0	4	6	4.020	-4.541
0	4	7	4.060	4.566
0	4	8	11.100	10.633
0	5	1	12.490	12.633
0	5	3	11.530	-12.469
0	5	5	3.580	3.130
0	5	6	3.350	-2.961
0	5	7	2.630	2.599
0	5	8	2.820	1.825
0	5	9	3.010	2.370
0	5	13	5.740	-4.981
0	6	0	8.850	8.849
0	6	1	4.690	-3.817
0	6	2	3.300	3.311
0	6	3	5.740	-5.891
0	6	4	13.300	-13.271
0	6	5	3.870	-4.408
0	6	6	7.170	-7.351
0	6	7	3.490	-2.663
0	6	8	9.230	9.483
0	6	9	4.400	4.235
0	7	1	18.710	19.675
0	7	3	9.710	-9.334
0	7	4	9.420	-7.750
0	7	5	15.360	-16.436
0	7	6	4.300	4.040
0	7	8	5.400	4.769
0	7	9	6.840	6.321
0	8	0	29.480	32.353
0	8	1	13.110	-11.936
0	8	2	3.920	3.583
0	8	3	5.790	-5.550
0	8	4	16.030	-16.609
0	8	5	2.150	3.773
0	8	6	6.940	-7.398
0	8	8	4.490	3.275
0	8	10	5.880	6.115
0	9	1	12.490	11.474
0	9	2	3.250	-4.149
0	9	3	2.820	-2.904
0	9	4	2.630	-2.185
0	9	5	16.560	-17.950
0	9	6	8.900	9.240
0	9	9	8.080	7.243
0	9	10	5.880	-5.529
0	10	0	16.360	16.256
0	10	1	3.920	-4.768
0	10	4	6.840	-7.109
0	10	5	7.510	6.781
0	10	7	3.150	3.945
0	10	9	3.780	-3.793
0	10	10	3.390	4.014
0	11	2	4.540	-4.764
0	11	4	3.730	4.010
0	11	5	4.160	-3.936
0	11	6	3.540	2.404
0	11	9	4.590	3.937
0	11	10	3.730	-3.071
0	12	1	3.730	3.490
0	12	7	4.350	3.896
0	13	2	4.300	-3.752
0	13	3	3.150	-2.721
0	14	4	4.690	-3.964
0	14	8	4.880	4.094
0	15	1	6.980	6.641
0	15	2	3.440	-3.782
0	15	3	4.830	-4.163
0	15	4	3.580	-2.366
0	15	5	4.060	-3.251
0	16	0	5.980	5.767
0	16	1	5.550	-4.937
0	16	4	4.730	-4.559
0	17	6	5.500	4.695
1	0	2	11.230	10.141
1	0	4	5.050	4.089
1	0	6	15.490	-15.408
1	0	8	7.270	-7.411
1	0	-8	2.240	-1.342
1	0	-10	7.000	-6.920
1	1	2	23.190	26.080
1	1	3	12.350	14.330
1	1	-3	4.260	-3.740
1	1	4	4.920	3.473
1	1	-4	9.740	-9.545
1	1	5	16.060	-19.068
1	1	-5	4.890	4.150
1	1	6	8.720	-8.214
1	1	-6	4.980	-4.381
1	1	7	8.620	-8.964
1	1	-7	6.310	5.410
1	1	-8	7.460	6.715
1	1	9	2.040	1.075
1	1	-9	1.910	1.785
1	1	-10	2.640	-2.253
1	1	-11	5.250	-4.620
1	1	-13	2.510	-.874
1	1	-15	2.770	2.792
1	2	2	16.520	17.030
1	2	3	4.620	-3.659
1	2	-3	24.710	-33.928
1	2	-4	14.700	-18.971
1	2	5	1.480	-1.569
1	2	-5	5.550	4.726
1	2	6	12.950	-12.375
1	2	-6	7.600	8.902
1	2	7	9.050	-9.056
1	2	-7	2.240	1.946
1	2	8	1.910	-1.520
1	2	-8	9.610	9.406
1	2	9	3.270	-3.014
1	2	-9	1.910	1.675
1	2	10	6.640	6.274
1	2	-10	2.540	-2.753
1	2	11	3.760	3.840
1	2	-11	5.410	4.850
1	2	-12	4.290	-3.699
1	2	-15	2.770	.852
1	3	1	18.010	22.802
1	3	-1	5.710	-4.851
1	3	2	19.100	24.198
1	3	-2	5.180	3.960
1	3	3	4.260	5.186
1	3	-3	28.120	-32.866
1	3	4	5.410	4.497
1	3	-4	10.240	-11.401
1	3	5	6.140	-6.553
1	3	-5	5.840	-5.663
1	3	6	9.250	-8.980
1	3	-6	7.170	-7.303
1	3	7	4.690	-4.611
1	3	-7	16.020	16.058
1	3	-8	9.150	8.468
1	3	9	4.260	4.468
1	3	-9	7.270	7.642
1	3	-10	2.110	-1.946
1	3	11	2.670	2.449
1	3	-11	5.410	-5.038
1	3	-13	5.750	-4.821
1	3	-14	2.670	1.056
1	4	0	8.420	9.056
1	4	1	5.380	3.328
1	4	-1	2.440	3.209
1	4	2	20.150	25.594
1	4	-2	16.650	-19.796
1	4	3	8.920	-8.483
1	4	-3	5.710	-4.820
1	4	4	6.440	-6.592
1	4	-4	12.850	-15.509
1	4	6	8.550	-7.993
1	4	-6	7.460	8.166
1	4	8	3.370	3.464
1	4	-8	18.070	18.870
1	4	9	2.370	-1.708
1	4	-10	3.200	2.457
1	4	11	2.410	.792
1	4	-11	3.100	2.640
1	4	-12	9.510	-8.995
1	4	-14	3.300	-2.065
1	5	0	1.680	1.809
1	5	1	11.030	11.394
1	5	-1	2.140	-2.638
1	5	2	16.350	-16.615
1	5	-2	10.040	9.227
1	5	3	7.630	7.581
1	5	-3	24.250	-32.524
1	5	4	2.540	-3.066
1	5	-4	2.540	2.506
1	5	-5	6.310	-6.413
1	5	6	6.310	5.783
1	5	-6	2.470	-2.154
1	5	7	7.270	-7.027
1	5	-7	16.350	17.841
1	5	8	2.670	2.816
1	5	9	4.560	4.795
1	5	-9	3.600	3.917
1	5	-10	2.670	2.540
1	5	11	3.000	2.767
1	5	-11	4.560	-4.168
1	5	-13	3.990	-3.816
1	6	0	4.620	4.833
1	6	1	12.290	-12.662
1	6	-1	4.980	5.814
1	6	2	17.970	21.419
1	6	-2	16.290	-17.272
1	6	3	5.880	-5.833
1	6	-3	15.920	18.844
1	6	4	4.390	-3.817
1	6	-4	1.520	-1.881
1	6	-5	5.180	-5.853
1	6	6	8.720	-8.366
1	6	-6	5.840	5.393
1	6	7	10.040	9.985
1	6	-7	2.510	-1.763
1	6	-8	8.360	8.106
1	6	9	2.940	2.891
1	6	11	3.630	-3.673
1	6	-11	3.100	-2.659
1	6	-12	6.170	-6.012
1	7	0	4.820	4.682
1	7	1	8.390	7.974
1	7	-1	3.070	-2.591
1	7	2	16.450	-17.659
1	7	-2	1.980	1.075
1	7	3	10.730	10.829
1	7	-3	9.680	-9.715
1	7	4	7.500	-8.455
1	7	-4	3.990	4.260
1	7	5	6.170	-6.165
1	7	6	8.260	8.531
1	7	-6	2.540	2.524
1	7	7	9.740	-9.989
1	7	-7	7.790	7.097
1	7	-8	4.520	-4.353
1	7	-9	3.130	-2.509
1	7	10	2.410	.193
1	7	-10	3.330	3.142
1	7	11	4.820	4.890
1	7	-11	3.600	-2.953
1	8	0	6.010	5.451
1	8	-1	4.420	4.602
1	8	2	9.940	9.197
1	8	-2	8.290	-7.864
1	8	3	2.340	2.047
1	8	-3	4.320	4.053
1	8	-4	3.600	-3.215
1	8	5	3.330	-2.736
1	8	-5	5.280	-6.136
1	8	6	10.310	-9.948
1	8	-6	4.360	3.923
1	8	7	3.460	2.786
1	8	8	4.290	-4.674
1	8	-8	2.080	-1.301
1	8	9	3.500	4.204
1	8	10	6.110	6.002
1	8	-10	3.600	-3.354
1	8	11	3.300	-2.089
1	8	-11	3.370	-3.046
1	9	0	6.540	7.072
1	9	1	13.020	13.340
1	9	-1	3.290	-2.965
1	9	2	4.790	4.851
1	9	-2	4.820	-4.984
1	9	3	5.020	4.606
1	9	-3	1.750	-1.568
1	9	4	4.420	-5.003
1	9	-4	6.270	-5.767
1	9	5	11.070	-10.745
1	9	-5	1.880	1.322
1	9	7	4.850	-4.318
1	9	-8	2.970	2.200
1	9	-9	2.280	1.750
1	9	-11	3.100	-2.835
1	10	0	7.830	7.244
1	10	1	10.010	8.983
1	10	-1	2.870	3.261
1	10	2	2.800	2.673
1	10	-2	4.030	-3.426
1	10	-3	10.900	-9.865
1	10	-4	13.440	-13.103
1	10	5	2.310	-2.875
1	10	-5	3.960	-4.424
1	10	6	6.770	-6.731
1	10	-6	4.260	4.139
1	10	7	3.270	-3.385
1	10	-8	4.360	4.103

H	K	L	OBSERVED	CALCULATED
1	10	-9	3.430	3.310
1	10	10	5.780	5.543
1	10	-10	2.470	-2.289
1	11	0	4.090	4.199
1	11	1	11.660	11.872
1	11	2	7.600	6.819
1	11	-1	3.270	-2.926
1	11	-2	2.640	2.106
1	11	-3	8.060	-8.077
1	11	-4	8.160	-7.884
1	11	5	7.130	-6.430
1	11	-5	2.080	-2.005
1	11	6	3.000	-3.617
1	11	-6	4.720	-4.618
1	11	-7	4.360	4.343
1	11	-8	5.550	4.968
1	11	-9	6.870	6.804
1	11	-11	2.640	-2.585
1	11	-13	3.600	-3.428
1	12	0	4.130	3.587
1	12	1	2.970	3.196
1	12	-1	3.860	4.213
1	12	2	5.250	5.151
1	12	-2	6.930	-6.275
1	12	3	6.600	-6.760
1	12	-3	3.760	-3.547
1	12	-4	9.780	-9.615
1	12	-5	2.180	-2.119
1	12	6	2.870	-2.445
1	12	-6	3.660	3.651
1	12	-7	2.340	-1.713
1	12	-8	8.120	8.231
1	12	-9	3.200	3.311
1	12	-11	3.330	2.895
1	12	-12	3.560	-3.071
1	12	-13	2.870	-2.057
1	13	1	3.890	3.366
1	13	-1	2.940	-2.431
1	13	2	4.590	-4.405
1	13	-2	8.590	7.905
1	13	3	4.030	4.006
1	13	-3	9.310	-9.277
1	13	-5	2.280	-1.325
1	13	-6	4.850	-4.682
1	13	7	2.510	-2.415
1	13	-7	5.780	6.339
1	13	8	3.430	3.534
1	13	-8	2.510	2.026
1	13	-9	2.610	2.579
1	14	1	3.100	-2.848
1	14	-1	3.830	3.886
1	14	2	7.730	7.333
1	14	-2	6.670	-6.318
1	14	3	7.860	-7.388
1	14	-3	3.730	3.340
1	14	6	2.510	-2.049
1	14	7	5.280	4.891
1	15	1	2.370	-.148
1	15	2	5.150	-5.146
1	15	-2	3.270	2.779
1	15	3	4.590	4.261
1	15	-3	3.830	-3.721
1	15	4	3.300	-3.286
1	15	6	2.610	2.299
1	15	7	4.750	-4.879
1	15	-7	3.330	3.166
1	15	8	2.740	2.788
1	16	-1	2.470	2.018
1	16	2	4.190	4.215
1	16	-2	3.300	-2.083
1	16	6	3.330	-2.968
1	17	0	3.430	3.406
1	17	1	3.200	2.291
1	17	-2	2.900	-2.067
1	17	4	2.700	-2.663
1	18	0	2.700	2.316
1	18	1	2.700	2.104
1	19	0	2.800	2.717
1	19	1	3.560	3.044
1	19	-4	3.460	-2.584
1	19	-5	3.200	-1.072
1	20	-4	2.900	-3.068
1	21	-3	1.020	-1.314
2	0	2	4.650	5.411
2	0	4	2.410	-1.697
2	0	6	9.180	-10.784
2	0	-8	8.390	7.584
2	0	10	2.790	2.067
2	0	-10	13.310	-11.478
2	0	-12	2.900	-2.670
2	0	-14	5.690	5.138
2	1	1	10.520	8.659
2	1	2	4.010	3.419
2	1	3	2.030	3.169
2	1	4	4.010	-3.846
2	1	5	2.090	2.700
2	1	-5	14.730	17.095
2	1	-6	13.980	-13.954
2	1	7	3.220	-2.821
2	1	-7	1.420	2.250
2	1	-8	1.540	-1.216
2	1	-9	7.960	-8.407
2	1	10	2.790	-2.622
2	1	-10	4.180	3.767
2	1	11	3.830	4.166
2	1	-11	4.210	-4.217
2	1	-12	2.700	2.018
2	1	-15	4.590	4.257
2	2	1	4.530	4.237
2	2	2	10.230	11.692
2	2	3	5.580	-5.286
2	2	4	11.850	12.325
2	2	-4	4.760	5.862
2	2	5	6.450	6.863
2	2	-5	4.500	-3.712
2	2	6	5.900	-6.246
2	2	-6	15.110	15.088
2	2	7	6.010	-6.289
2	2	-7	6.830	-7.116
2	2	8	5.900	-5.956
2	2	-8	2.060	1.486
2	2	9	2.150	-2.250
2	2	-9	2.870	-2.879
2	2	-10	9.180	-8.600
2	2	-11	8.160	7.457
2	2	12	2.580	2.248
2	2	-14	3.740	3.467
2	2	-15	2.700	-2.024
2	3	0	5.110	-4.591
2	3	2	7.260	6.682
2	3	-2	4.650	3.822
2	3	3	21.240	25.666
2	3	-3	6.450	-6.499
2	3	4	7.260	-7.345
2	3	5	4.650	5.029
2	3	-5	13.680	15.285
2	3	6	2.840	-2.407
2	3	-6	14.240	-15.335
2	3	7	9.470	-9.911
2	3	-7	10.920	11.481
2	3	8	2.580	2.393
2	3	9	5.340	-5.610
2	3	-9	4.730	-4.586
2	3	10	2.730	-2.359
2	3	-10	5.050	4.625
2	3	11	2.170	1.798
2	3	-11	5.750	-5.622
2	3	12	2.580	2.120
2	3	-12	2.060	.762
2	3	-13	3.570	3.330
2	3	-14	2.320	1.630
2	3	-15	2.410	1.540
2	4	0	12.350	-12.689
2	4	1	3.340	4.303
2	4	-1	9.620	9.288
2	4	2	14.530	17.658
2	4	-2	27.780	-36.643
2	4	-3	5.430	-5.882
2	4	4	19.640	22.466
2	4	-4	3.920	4.569
2	4	-5	2.230	-1.652
2	4	6	1.800	1.138
2	4	-6	16.820	20.393
2	4	7	3.130	-2.599
2	4	-7	5.170	4.609
2	4	8	11.530	-12.085
2	4	-8	4.990	-4.956
2	4	9	2.200	1.573
2	4	-9	1.740	-1.490
2	4	-10	4.850	-3.887
2	4	12	4.040	3.945
2	5	0	6.300	5.079
2	5	1	6.360	-5.699
2	5	-1	19.900	-26.769
2	5	2	3.570	2.910
2	5	-2	11.650	-11.006
2	5	3	24.930	25.283
2	5	-3	4.350	-4.337
2	5	4	3.830	-2.840
2	5	-4	2.550	-2.492
2	5	5	2.470	2.931
2	5	-5	8.570	8.474
2	5	6	1.860	-1.784
2	5	-6	9.320	8.811
2	5	7	10.020	-11.085
2	5	-7	13.680	14.885
2	5	8	2.760	2.191
2	5	-8	4.120	4.436
2	5	9	4.210	-4.248
2	5	-9	2.170	-1.925
2	5	10	2.810	2.786
2	5	-10	2.760	-2.043
2	5	-11	6.300	-6.400
2	5	12	2.350	-1.359
2	5	-12	4.120	-4.113
2	5	-13	3.370	3.641
2	6	0	3.050	-3.357
2	6	1	1.910	2.613
2	6	-1	12.750	-13.368
2	6	2	10.630	11.224
2	6	-2	17.580	-20.769
2	6	3	3.020	2.488
2	6	-3	5.170	-5.851
2	6	4	7.120	7.154
2	6	-4	3.630	3.623
2	6	5	6.420	-7.452
2	6	-5	1.420	1.636
2	6	-6	11.240	11.364
2	6	7	3.570	4.218
2	6	-7	9.940	10.028
2	6	8	6.710	-6.336
2	6	-8	1.710	-1.671
2	6	9	3.540	3.656
2	6	-9	3.160	2.860
2	6	-10	3.950	-3.463
2	6	-11	8.020	-7.409
2	6	12	3.480	3.351
2	6	-12	2.960	-2.908
2	6	-13	2.260	-1.859
2	6	-15	2.470	1.829
2	7	0	7.490	6.545
2	7	-1	3.540	-3.271
2	7	2	2.670	-2.648
2	7	-2	5.080	-4.356
2	7	3	5.310	5.223
2	7	-3	3.800	-3.895
2	7	4	2.170	2.658
2	7	-4	5.020	-4.980
2	7	-5	5.900	5.365
2	7	-6	12.990	13.230
2	7	7	4.880	-4.615
2	7	-7	7.030	6.728
2	7	-8	2.670	3.394
2	7	-9	3.690	-3.204
2	7	10	3.220	3.043
2	7	-10	4.560	-4.164
2	7	11	2.290	1.375
2	7	-11	5.460	-5.147
2	7	12	2.700	-2.571
2	7	-12	3.020	-2.571
2	7	-15	2.790	2.609
2	8	0	3.720	-3.402
2	8	1	2.150	2.504
2	8	-1	6.680	-6.995
2	8	2	3.250	2.904
2	8	4	2.760	-2.108
2	8	-4	3.400	3.184
2	8	5	3.740	-3.925
2	8	-5	1.590	-.983
2	8	6	4.500	-4.278
2	8	-6	5.200	4.560
2	8	7	3.480	3.630
2	8	-8	2.520	2.387
2	8	-9	4.760	4.335
2	8	-10	6.590	-6.420
2	8	-11	2.930	-2.606
2	8	-12	3.080	-2.205
2	8	-14	3.100	2.757
2	9	0	5.170	4.696
2	9	1	4.240	3.989
2	9	-1	4.270	-4.368
2	9	2	2.060	-1.436
2	9	-2	5.720	5.718
2	9	-3	4.150	-3.615
2	9	-4	4.350	-5.120
2	9	5	2.030	1.321
2	9	-5	9.760	9.651
2	9	-6	1.940	-2.114
2	9	7	1.970	-1.034
2	9	-9	5.550	-5.236
2	9	11	3.050	3.111
2	9	-11	2.900	-2.754
2	9	-12	2.290	1.552
2	9	-15	3.480	3.151
2	10	0	10.230	-10.275
2	10	1	3.950	4.377
2	10	-1	7.260	7.240
2	10	2	3.800	3.406
2	10	-2	2.410	-1.858
2	10	3	2.230	-1.965
2	10	4	6.910	6.914
2	10	-4	3.310	2.995
2	10	-5	4.880	-4.466
2	10	6	5.840	-5.674
2	10	-6	7.120	6.702
2	10	7	2.060	-1.600
2	10	-7	4.850	-4.127
2	10	8	2.410	-2.224
2	10	-8	2.200	1.786
2	10	-10	6.970	-6.431
2	10	-11	3.080	2.661
2	10	-14	2.810	2.891
2	11	0	4.120	3.872
2	11	1	2.700	2.233
2	11	-1	12.750	-13.642
2	11	2	4.760	4.575
2	11	3	7.990	7.998
2	11	-3	5.020	-4.564
2	11	4	5.520	-5.464
2	11	-4	3.600	-3.404
2	11	5	4.940	4.854
2	11	-5	10.110	9.951
2	11	6	2.290	-2.746

H	K	L	OBSERVED	CALCULATED
2	11	-6	6.620	-6.393
2	11	7	2.900	-2.655
2	11	-7	1.970	1.530
2	11	8	2.200	1.354
2	11	9	4.090	-4.212
2	11	-9	4.010	-3.672
2	11	-10	2.490	1.998
2	11	-13	2.470	.722
2	12	0	8.080	-8.115
2	12	1	4.300	4.928
2	12	-1	6.910	6.890
2	12	2	6.270	5.876
2	12	-2	9.320	-9.501
2	12	-3	5.920	-6.435
2	12	4	9.880	10.461
2	12	5	2.060	-2.515
2	12	-5	2.550	-2.215
2	12	-6	7.320	7.114
2	12	7	3.020	-2.859
2	12	-7	4.670	4.536
2	12	8	5.050	-5.133
2	12	9	3.250	2.510
2	12	-10	3.340	-2.726
2	13	-1	7.900	-8.359
2	13	2	5.260	5.155
2	13	-2	6.130	-6.167
2	13	3	8.280	8.625
2	13	-3	3.720	-3.593
2	13	4	5.310	-5.037
2	13	-4	1.970	-1.763
2	13	5	2.810	2.551
2	13	-5	2.960	2.848
2	13	6	2.470	-2.708
2	13	7	3.600	-3.518
2	13	-7	5.780	5.503
2	13	8	2.610	2.992
2	13	-8	3.830	4.293
2	13	9	3.310	-2.984
2	13	-11	2.440	-2.059
2	13	-12	3.630	-3.524
2	14	1	2.490	2.307
2	14	2	3.890	3.419
2	14	-2	7.140	-7.097
2	14	-3	4.880	-5.309
2	14	4	2.150	2.363
2	14	5	2.200	-2.143
2	14	-6	3.080	3.320
2	14	-7	6.420	6.612
2	14	8	3.080	-2.973
2	14	9	2.760	2.446
2	14	-11	3.400	-3.047
2	14	-12	2.520	-2.151
2	15	-2	3.100	-2.582
2	15	-6	4.380	3.688
2	15	-7	4.620	3.959
2	15	-8	2.640	2.613
2	15	-10	2.760	-.930
2	15	-11	3.220	-2.536
3	0	2	6.560	4.677
3	0	4	9.970	10.143
3	0	6	4.030	4.300
3	0	-6	5.200	4.546
3	0	-8	12.620	-11.183
3	0	-10	13.000	-13.529
3	0	-12	2.050	.557
3	0	-14	6.700	7.268
3	1	1	30.150	-24.537
3	1	2	5.230	5.130
3	1	3	1.970	-1.416
3	1	4	7.350	-6.919
3	1	5	12.940	14.064
3	1	-5	21.910	28.229
3	1	6	4.640	-4.625
3	1	-6	2.880	2.999
3	1	7	3.030	-3.326
3	1	-7	1.910	-2.189
3	1	8	1.940	-.817
3	1	-8	2.410	-2.159
3	1	9	3.640	-3.297
3	1	-9	17.560	-18.529
3	1	-13	5.560	5.318
3	2	1	10.170	8.004
3	2	2	2.700	-3.106
3	2	3	3.700	4.018
3	2	4	8.850	9.367
3	2	-4	17.760	19.277
3	2	5	8.730	-8.421
3	2	-5	11.380	-11.043
3	2	6	4.580	5.109
3	2	-6	2.790	2.840
3	2	7	4.260	-4.378
3	2	-7	2.970	2.577
3	2	8	1.940	-2.354
3	2	-8	9.620	-9.178
3	2	9	5.140	5.407
3	2	-9	3.410	-2.783
3	2	10	3.200	-3.436
3	2	-10	4.670	-4.917
3	2	-11	4.440	-4.920
3	2	-12	2.850	2.547
3	2	-13	4.350	4.318
3	2	-14	3.500	3.602
3	2	-15	2.440	1.587
3	3	0	14.700	13.535
3	3	1	8.350	-7.177
3	3	2	6.580	6.192
3	3	3	6.730	6.739
3	3	-3	12.970	12.324
3	3	4	8.640	-8.924
3	3	-4	2.440	2.095
3	3	5	6.940	6.214
3	3	-5	1.520	1.117
3	3	6	4.230	-4.192
3	3	-6	3.050	3.509
3	3	7	2.050	2.296
3	3	-7	4.730	-4.996
3	3	8	1.970	-1.576
3	3	-8	3.760	-3.581
3	3	9	4.670	-4.987
3	3	-9	2.470	-1.918
3	3	-10	2.080	1.409
3	3	-13	3.760	3.702
3	4	0	1.820	-1.113
3	4	1	3.000	-2.927
3	4	-1	1.730	.776
3	4	2	10.590	-10.977
3	4	-2	4.380	-3.417
3	4	3	3.350	3.821
3	4	-3	1.820	-.817
3	4	4	8.530	8.781
3	4	-4	2.580	-2.033
3	4	-5	3.730	-3.892
3	4	6	4.610	4.897
3	4	-6	3.640	3.405
3	4	7	1.880	-1.995
3	4	-7	2.350	2.475
3	4	8	5.500	-6.321
3	4	-8	6.970	-7.210
3	4	9	2.110	2.266
3	4	-9	2.440	-1.805
3	4	10	2.230	-2.057
3	4	-10	3.550	3.239
3	4	-12	5.580	5.770
3	4	-13	2.500	1.924
3	5	0	7.790	-6.558
3	5	1	2.820	-2.081
3	5	-1	10.760	-10.006
3	5	-2	3.440	-3.700
3	5	3	10.500	10.407
3	5	-3	12.820	13.378
3	5	4	3.290	3.039
3	5	-4	4.850	4.460
3	5	5	3.410	3.145
3	5	6	3.050	3.295
3	5	7	2.440	2.398
3	5	-7	6.060	-6.469
3	5	9	4.550	-4.645
3	5	-13	3.200	3.189
3	6	0	11.350	-10.573
3	6	1	4.320	-4.452
3	6	-1	7.230	+6.811
3	6	2	6.410	-6.889
3	6	-2	3.170	-2.527
3	6	4	8.670	8.531
3	6	-4	8.790	8.113
3	6	5	5.610	5.545
3	6	-5	8.350	8.540
3	6	6	2.850	3.124
3	6	-6	7.610	7.778
3	6	7	1.970	1.577
3	6	8	4.700	-5.416
3	6	-8	7.760	-8.467
3	6	9	3.000	-2.995
3	6	-10	3.500	-3.882
3	6	-12	5.080	5.364
3	6	-13	2.940	-2.536
3	7	0	9.910	-9.603
3	7	1	11.590	-11.496
3	7	-1	12.320	-12.151
3	7	3	4.380	4.537
3	7	-3	10.090	10.099
3	7	4	7.230	7.755
3	7	-4	4.380	-3.426
3	7	5	6.670	6.763
3	7	-5	14.700	16.999
3	7	6	1.910	.287
3	7	-6	1.850	2.830
3	7	-7	3.640	-3.918
3	7	-8	4.640	4.613
3	7	9	2.820	-2.397
3	7	-9	9.440	-10.175
3	7	-10	4.110	-4.083
3	7	-13	3.610	3.681
3	8	0	17.620	-18.406
3	8	1	8.610	8.399
3	8	-1	5.880	-5.940
3	8	2	1.640	-1.427
3	8	-2	1.550	1.312
3	8	-3	6.320	-5.549
3	8	4	5.970	6.018
3	8	-4	18.260	20.223
3	8	-5	8.760	8.002
3	8	6	3.350	3.357
3	8	-6	5.290	5.886
3	8	-7	2.000	1.975
3	8	-8	7.910	-7.799
3	8	9	2.530	-1.933
3	8	10	2.380	-1.971
3	8	-10	9.260	-9.376
3	8	-13	2.380	-2.013
3	8	-14	4.940	4.445
3	8	-15	2.550	1.821
3	9	0	2.610	2.910
3	9	1	13.880	-13.803
3	9	-1	5.670	-5.340
3	9	2	5.940	5.928
3	9	-2	2.080	-2.687
3	9	3	2.530	-2.341
3	9	-3	5.060	4.849
3	9	4	1.850	.480
3	9	5	7.880	8.292
3	9	-5	13.820	14.762
3	9	6	6.350	-6.683
3	9	-6	3.380	4.143
3	9	7	2.110	-.973
3	9	-8	3.080	2.920
3	9	-9	11.170	-11.357
3	9	10	2.700	2.757
3	9	-10	4.640	-5.086
3	9	-13	3.410	3.151
3	9	-14	3.200	2.147
3	9	-15	2.550	1.528
3	10	0	9.910	-9.426
3	10	1	9.590	8.970
3	10	-2	2.880	2.661
3	10	3	2.380	2.196
3	10	-3	5.440	-5.142
3	10	4	3.000	2.974
3	10	-4	10.820	11.360
3	10	5	6.200	-6.475
3	10	6	3.790	4.024
3	10	7	3.080	-3.284
3	10	-7	1.940	2.242
3	10	-8	3.730	-3.501
3	10	-9	2.670	-1.980
3	10	10	3.470	-3.204
3	10	-10	3.290	-3.021
3	10	-11	3.140	-3.030
3	10	-12	2.380	-.503
3	10	-13	2.470	1.406
3	10	-14	3.580	3.074
3	10	-15	2.580	2.140
3	11	0	5.790	5.845
3	11	1	5.530	-5.327
3	11	2	4.260	4.699
3	11	-2	2.880	-3.569
3	11	4	3.910	-3.970
3	11	5	4.670	5.142
3	11	6	4.140	-3.878
3	11	-8	2.350	-1.444
3	11	9	2.970	-2.526
3	11	-9	3.080	-2.793
3	11	-11	2.350	1.739
3	11	-13	2.790	2.062
3	11	-14	2.550	1.762
3	12	1	2.410	-1.929
3	12	-2	2.140	.146
3	12	3	3.610	3.602
3	12	4	2.970	2.901
3	12	-5	3.080	-2.784
3	12	6	2.730	2.082
3	12	-6	2.050	-2.026
3	12	7	2.320	-2.328
3	12	-7	2.110	2.124
3	12	-8	2.170	-1.571
3	12	9	3.140	2.356
3	12	-9	3.080	-2.299
3	12	-10	2.320	1.747
3	12	-13	2.530	2.059
3	13	-1	3.350	-2.462
3	13	2	2.080	.799
3	13	-2	3.970	-3.896
3	13	3	3.030	2.996
3	13	-3	2.790	2.079
3	13	-4	4.760	4.244
3	13	-8	2.260	-1.373
3	14	0	2.910	-2.549
3	14	1	3.380	-3.227
3	14	-1	3.170	-2.814
3	14	2	2.170	-1.858
3	14	-2	2.110	-1.600
3	14	3	2.470	2.473
3	14	4	3.200	3.435
3	14	5	2.320	1.983
3	14	-6	3.350	3.176
3	14	7	2.010	2.723
3	14	-8	2.970	-3.069
3	15	1	2.850	-2.265
3	15	-1	5.000	-4.951
3	15	2	2.260	1.609
3	15	-2	3.580	-3.488
3	15	3	2.160	2.880
3	15	-3	4.380	4.448

H	K	L	OBSERVED	CALCULATED
3	15	4	2.610	1.909
3	15	5	2.410	1.191
3	15	-5	5.080	4.690
3	15	-6	3.260	3.273
3	15	-7	2.350	-1.603
3	15	-8	2.410	1.582
3	15	-9	3.140	-2.552
3	16	0	4.410	-4.001
3	16	1	3.670	3.425
3	16	-1	3.470	-3.164
3	16	2	3.230	-2.797
3	16	-2	2.290	-.040
3	16	-3	3.470	-3.418
3	16	-4	3.970	4.521
3	16	-5	3.320	3.082
3	16	-6	3.580	3.729
3	16	-7	2.440	2.417
3	16	-8	2.470	-2.991
3	16	-9	2.530	.387
3	16	-10	3.610	-3.292
3	17	1	3.610	-3.736
3	17	2	3.110	3.120
3	17	-3	3.380	3.036
3	17	4	2.500	1.082
3	17	-4	3.610	-3.155
3	17	5	2.530	1.711
3	17	-5	3.670	3.626
3	17	6	3.260	-3.133
3	17	-6	2.760	2.477
3	17	-8	2.530	1.902
3	17	-9	2.880	-2.621
3	17	-10	2.910	-2.958
3	18	1	3.940	4.184
3	18	-1	2.470	-.913
3	18	-2	2.470	1.230
3	18	-3	2.760	-2.401
3	18	-4	3.170	2.588
3	18	0	3.140	-1.890
4	0	2	16.500	-17.765
4	0	4	6.430	-7.009
4	0	6	10.550	12.560
4	0	-6	11.680	-10.890
4	0	-8	8.000	-7.955
4	0	-10	7.030	6.852
4	0	-14	2.730	-2.623
4	1	1	15.630	-17.120
4	1	2	8.380	-7.564
4	1	3	8.900	-9.357
4	1	4	1.700	1.987
4	1	5	6.050	6.631
4	1	6	2.350	2.259
4	1	7	5.490	5.335
4	1	-7	5.080	-6.187
4	1	-8	11.280	-11.128
4	1	-9	2.290	-1.823
4	1	-11	4.080	3.348
4	1	-12	3.970	3.375
4	1	-13	2.020	1.448
4	1	-15	3.540	-3.574
4	2	1	8.540	-7.824
4	2	2	11.330	-10.442
4	2	3	1.830	-1.382
4	2	5	4.570	-5.093
4	2	6	5.090	6.713
4	2	-6	9.060	-8.702
4	2	-7	9.600	-8.802
4	2	-8	9.250	-9.395
4	2	-10	3.920	3.939
4	2	-12	4.950	4.536
4	2	-13	5.140	4.984
4	3	0	5.890	5.016
4	3	1	6.890	-6.481
4	3	2	8.620	-7.829
4	3	3	1.650	-1.653
4	3	4	2.460	2.417
4	3	-4	5.510	3.674
4	3	5	2.590	2.941
4	3	6	2.810	2.974
4	3	-6	3.650	3.013
4	3	-7	11.820	-12.774
4	3	-8	11.470	-12.797
4	3	-9	4.350	-4.394
4	3	-10	2.240	-1.819
4	3	-11	7.570	6.921
4	3	-12	4.270	4.024
4	3	-13	4.840	4.641
4	3	-16	3.080	.943
4	4	1	1.890	-1.477
4	4	-1	4.590	-3.805
4	4	2	4.400	-3.946
4	4	-2	14.170	12.572
4	4	3	2.780	1.794
4	4	-3	5.110	3.764
4	4	4	5.430	5.304
4	4	-4	5.870	5.365
4	4	5	2.700	-2.526
4	4	-5	3.970	.968
4	4	6	1.750	-.456
4	4	-6	6.730	-6.475
4	4	-8	8.250	-8.676
4	4	-12	8.520	9.045
4	5	1	2.130	-1.849
4	5	-1	2.110	-1.543
4	5	2	6.680	6.135
4	5	-2	9.000	-7.673
4	5	3	4.590	-4.375
4	5	-3	8.440	7.945
4	5	-4	3.780	-2.819
4	5	-6	4.350	3.289
4	5	7	3.130	3.241
4	5	-7	14.520	-15.943
4	5	-8	5.730	5.617
4	5	-11	7.760	7.845
4	5	-13	2.890	2.891
4	5	-16	3.000	-.458
4	6	0	2.210	-1.481
4	6	1	5.300	4.863
4	6	-1	2.700	-2.362
4	6	2	10.030	-9.764
4	6	-2	15.980	16.921
4	6	3	5.190	4.596
4	6	-3	14.310	-15.355
4	6	4	1.670	1.766
4	6	-4	2.620	2.295
4	6	5	3.460	3.783
4	6	-5	2.920	3.457
4	6	6	2.510	2.310
4	6	-6	7.220	-6.955
4	6	7	3.130	-2.445
4	6	-7	7.140	7.397
4	6	-8	4.240	-4.187
4	6	-12	5.950	5.891
4	6	-13	2.920	-2.591
4	7	0	6.760	-7.757
4	7	1	7.870	-7.631
4	7	-1	6.240	5.406
4	7	2	8.600	8.232
4	7	-2	7.380	-6.634
4	7	3	9.520	-10.204
4	7	-3	10.840	10.947
4	7	5	2.840	3.140
4	7	6	2.890	-3.073
4	7	7	6.050	6.448
4	7	-7	9.190	-9.377
4	7	-8	7.890	8.177
4	7	-11	4.650	4.308
4	7	-12	2.080	-2.142
4	8	0	4.130	-3.528
4	8	-1	1.730	-1.581
4	8	2	11.090	-11.940
4	8	-2	9.460	9.701
4	8	3	2.620	2.337
4	8	-3	4.190	-4.181
4	8	4	3.480	-3.632
4	8	-4	6.220	5.868
4	8	5	4.080	4.787
4	8	-5	4.320	4.678
4	8	6	6.840	7.343
4	8	-6	5.700	-5.924
4	8	7	2.000	-2.066
4	8	8	3.650	4.015
4	8	-8	3.670	-3.475
4	8	-9	4.050	-4.278
4	8	-10	2.650	2.969
4	8	-14	2.270	-1.681
4	9	0	5.380	-5.516
4	9	1	10.140	-10.506
4	9	-1	6.730	6.354
4	9	2	1.700	-.763
4	9	3	4.220	-4.633
4	9	-3	9.520	9.906
4	9	4	2.510	2.543
4	9	-4	6.870	6.969
4	9	5	3.700	3.673
4	9	7	3.430	3.472
4	9	-8	4.320	-4.467
4	9	-9	2.130	-2.182
4	9	-12	2.160	1.512
4	9	-13	3.700	1.184
4	10	0	3.270	-3.000
4	10	1	4.000	-3.748
4	10	-1	1.890	-1.728
4	10	2	4.320	-4.068
4	10	-3	8.460	8.437
4	10	4	1.890	-2.267
4	10	-4	7.300	7.929
4	10	-5	2.890	3.367
4	10	6	5.000	5.273
4	10	-6	3.240	-3.373
4	10	-7	5.460	-4.752
4	10	-8	6.190	-6.325
4	10	-9	4.540	-4.672
4	10	-10	2.810	2.686
4	10	-12	2.810	1.266
4	10	-13	3.860	3.427
4	11	1	5.000	-4.941
4	11	-1	3.000	2.247
4	11	2	3.890	-3.006
4	11	-2	2.240	1.781
4	11	3	1.890	1.664
4	11	-3	5.190	5.035
4	11	-4	3.480	4.144
4	11	5	2.020	2.097
4	11	-8	6.380	-7.139
4	11	-9	4.430	-4.175
4	11	-11	2.160	2.024
4	11	-12	3.730	2.198
4	12	-1	3.460	-3.518
4	12	3	1.970	1.604
4	12	-3	3.350	3.295
4	12	-4	3.380	3.188
4	12	5	2.670	-2.388
4	12	-6	3.000	-3.049
4	12	-8	5.270	-5.155
4	12	-11	2.840	-1.956
4	12	-12	2.570	3.689
4	13	2	2.000	1.540
4	13	-2	4.840	-4.653
4	13	3	2.290	-1.637
4	13	-3	3.050	2.750
4	13	-4	2.480	-1.386
4	13	-6	4.510	4.314
4	13	-7	5.570	-5.742
4	14	0	2.020	.725
4	14	-1	3.480	-4.223
4	14	2	3.460	-3.489
4	14	-2	6.700	7.069
4	14	3	3.620	3.852
4	14	-3	3.350	-3.120
4	14	-6	3.050	-3.093
4	14	-7	3.110	2.969
4	15	0	2.700	-2.608
4	15	1	2.130	-.844
4	15	-1	2.350	1.576
4	15	2	2.970	2.779
4	15	-2	3.920	-3.892
4	15	3	4.920	-5.030
4	15	-3	2.970	2.873
4	15	-7	5.000	-4.639
4	16	2	3.700	-4.310
4	16	-2	4.920	4.792
4	16	-5	2.210	2.457
4	17	0	2.890	-3.327
4	17	1	2.270	-2.187
4	17	-1	2.240	.538
4	17	-3	2.240	2.279
4	17	-4	3.190	3.060
5	0	0	7.390	5.708
5	0	2	6.490	-6.960
5	0	4	1.960	-1.924
5	0	-6	8.510	6.712
5	0	-10	5.770	5.194
5	0	-14	5.870	-5.830
5	1	0	2.240	1.593
5	1	1	2.160	-1.243
5	1	2	4.580	-4.508
5	1	4	2.060	-1.615
5	1	5	2.160	-1.721
5	1	-5	10.450	-9.422
5	1	-6	4.920	4.173
5	1	7	3.260	4.030
5	1	8	1.890	1.103
5	1	-9	7.270	6.989
5	1	-10	4.250	-3.766
5	1	-14	1.990	.579
5	1	-15	2.830	-2.509
5	1	-16	2.140	1.367
5	2	0	10.200	8.330
5	2	1	5.900	5.645
5	2	2	6.050	-5.551
5	2	3	3.080	-2.740
5	2	4	5.800	-5.627
5	2	-4	5.500	-4.876
5	2	5	3.980	-4.191
5	2	-5	4.500	3.936
5	2	6	2.290	1.819
5	2	-6	8.960	-8.430
5	2	7	2.930	3.460
5	2	8	2.410	2.105
5	2	-10	7.170	7.431
5	2	-11	5.570	-5.342
5	2	-12	1.810	1.148
5	2	-13	2.140	-2.172
5	2	-14	4.130	-4.099
5	2	-15	3.280	3.020
5	2	-16	2.140	-.980
5	3	0	1.340	-.820
5	3	1	1.910	1.593
5	3	-1	21.380	19.034
5	3	2	6.340	-6.584
5	3	-2	3.950	2.898
5	3	3	10.280	-10.570
5	3	-3	3.950	2.729
5	3	-4	3.660	-3.085
5	3	5	2.560	-2.571
5	3	-5	13.320	-13.315
5	3	6	2.310	-1.504
5	3	-6	4.880	4.752
5	3	7	2.510	2.228
5	3	-7	8.310	-8.669
5	3	-9	5.870	5.765
5	3	-10	4.800	-4.935
5	3	-11	7.610	8.646

H	K	L	OBSERVED	CALCULATED
5	3	-12	1.840	.733
5	3	-13	2.560	-2.600
5	3	-14	2.010	.658
5	3	-15	3.380	-3.081
5	3	-16	2.160	.875
5	4	0	9.680	8.909
5	4	-1	3.330	-2.757
5	4	2	2.760	-2.597
5	4	-2	16.750	17.244
5	4	-3	4.150	4.008
5	4	4	8.610	-8.572
5	4	-4	6.990	-6.772
5	4	5	1.860	.958
5	4	-5	4.500	3.858
5	4	6	1.760	.100
5	4	-6	19.890	-23.394
5	4	7	1.840	1.300
5	4	-7	4.150	-4.427
5	4	8	4.150	4.921
5	4	-8	1.960	2.118
5	4	-10	7.640	8.150
5	4	-12	1.860	1.582
5	4	-15	2.090	.576
5	4	-16	2.410	-2.493
5	5	0	6.290	-5.162
5	5	1	3.660	3.516
5	5	-1	17.170	18.591
5	5	3	11.300	-12.114
5	5	4	4.330	4.086
5	5	-4	3.780	3.262
5	5	5	2.260	-2.495
5	5	-5	9.030	-8.456
5	5	6	1.790	1.665
5	5	-6	3.210	-2.731
5	5	7	1.860	1.165
5	5	-7	7.840	-8.203
5	5	8	1.940	-1.711
5	5	-8	2.560	-2.427
5	5	-9	3.410	3.435
5	5	-10	2.360	1.674
5	5	-11	8.240	9.906
5	5	-12	3.060	3.491
5	5	-13	1.960	-2.458
5	5	-15	3.260	-2.908
5	5	-16	2.160	-2.170
5	6	0	3.680	3.181
5	6	1	6.020	-5.990
5	6	-1	1.440	-1.405
5	6	2	1.740	-1.261
5	6	-2	9.210	8.766
5	6	3	3.010	3.008
5	6	4	4.150	-4.148
5	6	-4	4.280	-4.333
5	6	5	4.500	4.972
5	6	-6	10.180	-11.143
5	6	7	2.510	-2.287
5	6	-7	2.510	-2.752
5	6	8	3.580	3.973
5	6	-8	2.210	2.106
5	6	-10	4.030	4.054
5	6	-11	5.220	5.723
5	6	-13	2.210	2.253
5	6	-15	3.280	-2.776
5	6	-16	2.190	-1.912
5	7	0	2.390	-1.721
5	7	-1	2.530	2.106
5	7	2	4.100	4.077
5	7	-2	2.090	-1.636
5	7	3	3.700	-3.620
5	7	4	1.910	1.714
5	7	-4	5.850	5.443
5	7	-5	1.940	-1.771
5	7	-6	4.920	-4.617
5	7	-8	2.480	-2.584
5	7	-9	2.660	2.702
5	7	-10	4.880	4.524
5	7	-11	1.860	1.861
5	7	-13	2.010	-1.307
5	7	-15	2.730	-2.235
5	7	-16	2.460	-1.719
5	8	1	3.980	-4.225
5	8	-1	2.510	1.809
5	8	2	2.960	-2.995
5	8	-2	2.090	-.573
5	8	-3	1.540	-.808
5	8	-4	2.190	-1.558
5	8	-5	2.660	-2.637
5	8	-6	3.010	2.683
5	8	-7	2.860	2.289
5	8	-9	1.960	-1.681
5	8	-10	2.760	2.720
5	8	-13	2.290	1.986
5	8	-14	3.180	-3.117
5	8	-15	2.160	-1.757
5	9	1	1.840	-1.368
5	9	-1	1.590	-.722
5	9	-3	2.980	2.238
5	9	4	2.010	-1.880
5	9	-4	2.960	2.984
5	9	-5	4.780	-5.167
5	9	-9	3.950	4.285
5	9	-10	1.860	.250
5	10	0	5.870	5.744
5	10	2	4.080	-4.222
5	10	-2	2.810	2.340
5	10	3	1.790	-1.577
5	10	-3	2.760	2.984
5	10	4	2.710	-3.074
5	10	-4	2.360	-2.353
5	10	-5	1.890	1.817
5	10	-6	1.910	-1.819
5	10	-9	2.090	-1.741
5	10	-10	4.830	5.197
5	10	-11	2.630	-2.177
5	11	0	2.760	-2.675
5	11	-1	7.320	7.162
5	11	2	3.410	-3.900
5	11	-2	2.360	2.506
5	11	3	2.460	-2.645
5	11	-3	2.980	2.997
5	11	-4	2.290	1.675
5	11	-5	8.680	-9.314
5	11	-7	4.180	-4.037
5	11	-9	4.200	4.369
5	11	-10	2.710	-2.620
5	11	-11	2.040	2.457
5	11	-12	2.090	1.315
5	12	0	6.120	6.499
5	12	-1	2.910	-2.934
5	12	2	2.580	-1.915
5	12	-2	5.800	6.157
5	12	-3	4.180	4.862
5	12	4	4.580	-4.677
5	12	-4	3.060	-3.263
5	12	-5	4.280	4.332
5	12	-6	7.120	-7.795
5	12	-7	4.330	-4.800
5	12	-10	3.880	4.978
5	13	0	4.880	-4.699
5	13	-1	6.890	6.904
5	13	2	2.660	-2.840
5	13	-2	2.780	2.386
5	13	3	3.850	-4.093
5	13	4	3.510	3.765
5	13	-5	3.850	-4.291
5	13	-7	3.310	-3.794
5	13	-11	3.430	3.713
5	13	-12	3.510	3.713
5	14	0	2.190	1.392
5	14	1	2.610	-1.765
5	14	-1	2.660	-2.237
5	14	-2	3.280	3.122
5	14	-3	1.940	2.090
5	14	-4	1.940	-1.641
5	14	-6	4.280	-4.218
5	14	-7	3.410	-3.717
5	14	-11	3.060	2.831
6	0	0	9.140	9.307
6	0	2	1.680	-1.226
6	0	-8	10.450	9.242
6	0	-10	5.950	5.437
6	0	-12	3.430	-2.634
6	0	-14	6.990	-7.538
6	1	0	6.640	-5.897
6	1	1	7.070	6.448
6	1	2	1.900	-1.739
6	1	3	1.980	-1.956
6	1	5	3.960	-4.385
6	1	-5	9.750	-8.686
6	1	-6	1.600	.133
6	1	-7	2.760	2.685
6	1	-9	12.460	13.720
6	1	-10	2.780	-2.475
6	1	-13	5.920	-6.476
6	1	-14	5.090	1.037
6	2	0	7.550	7.416
6	2	1	6.640	-6.158
6	2	-1	3.770	-2.858
6	2	2	2.780	2.711
6	2	3	3.210	-3.322
6	2	4	1.840	-2.344
6	2	-4	12.920	-10.346
6	2	5	3.800	4.274
6	2	-5	10.370	8.564
6	2	6	2.250	-2.287
6	2	-6	1.820	-.430
6	2	-7	3.590	-3.197
6	2	-8	8.010	7.170
6	2	-9	6.130	-6.131
6	2	-11	2.170	2.432
6	2	-12	3.370	-3.166
6	2	-14	2.460	-2.921
6	3	0	7.500	-6.748
6	3	1	6.910	6.843
6	3	-1	6.400	5.702
6	3	2	1.930	-1.994
6	3	-2	6.640	5.844
6	3	-3	9.570	-7.651
6	3	-4	8.600	7.069
6	3	5	3.450	-3.929
6	3	-5	3.940	-3.716
6	3	-7	4.450	4.454
6	3	-10	3.190	-2.911
6	3	-13	2.110	-2.332
6	3	-14	2.460	1.189
6	4	0	5.570	4.697
6	4	2	5.680	5.994
6	4	-2	3.320	-3.160
6	4	3	1.820	-2.532
6	4	4	7.640	-7.156
6	4	-4	2.270	-1.744
6	4	6	5.090	-4.310
6	4	-6	3.240	-2.363
6	4	-7	2.190	-1.821
6	4	-8	4.390	4.336
6	4	-11	1.980	1.639
6	4	-12	3.640	-4.106
6	5	0	4.120	3.548
6	5	1	4.450	4.416
6	5	-1	9.160	8.496
6	5	-2	2.330	.968
6	5	-3	7.370	-6.545
6	5	-4	6.380	-5.523
6	5	-5	4.710	-4.550
6	5	-6	2.700	-2.456
6	5	-7	4.500	4.749
6	5	-8	2.380	1.842
6	5	-9	1.840	-1.710
6	5	-10	2.170	2.175
6	6	0	4.530	4.295
6	6	1	4.230	3.949
6	6	-1	3.910	3.558
6	6	2	2.030	2.314
6	6	4	4.310	-5.118
6	6	-4	3.830	-3.347
6	6	-5	8.230	-7.528
6	6	-6	3.910	-3.519
6	6	-8	4.740	4.993
6	6	-9	5.380	5.250
6	6	-10	4.340	4.510
6	6	-12	3.910	-4.056
6	7	0	5.760	5.345
6	7	1	2.890	2.704
6	7	-1	3.830	3.795
6	7	-2	1.930	-1.992
6	7	-3	4.340	-4.149
6	7	-4	4.930	-4.645
6	7	-5	7.500	-7.625
6	7	-6	1.790	-2.387
6	7	-7	3.100	3.327
6	7	-8	2.090	-2.310
6	7	-9	6.880	6.990
6	7	-10	3.750	4.507
6	7	-13	3.240	-3.813
6	8	0	4.310	4.867
6	8	1	2.090	-2.160
6	8	-3	5.220	5.117
6	8	-4	8.520	-8.942
6	8	-5	3.210	-3.537
6	8	-8	6.080	6.348
6	8	-10	4.710	4.968
6	8	-12	2.430	-2.586
6	8	-14	4.470	-4.955
6	9	0	1.870	-1.764
6	9	1	4.310	4.534
6	9	2	3.190	-3.444
6	9	-3	4.390	-4.156
6	9	-4	4.770	4.739
6	9	5	2.140	-2.748
6	9	-5	4.390	-4.519
6	9	6	2.190	2.426
6	9	-7	2.170	2.072
6	9	-8	3.830	-4.224
6	9	-9	7.580	8.819
6	9	-13	3.430	-4.270
6	10	0	4.100	4.380
6	10	1	4.930	-5.409
6	10	-3	4.740	4.918
6	10	-4	7.100	-7.826
6	10	-5	3.050	2.650
6	10	-6	1.950	1.916
6	10	-7	2.220	-2.547
6	10	-8	3.800	4.371
6	11	0	3.190	-3.496
6	11	1	4.590	4.951
6	11	2	2.940	-2.812
6	11	-2	3.690	4.105
6	11	-3	3.130	-3.405
6	11	-4	3.350	3.797
6	12	0	2.760	2.920
6	12	2	2.380	2.380
6	12	-2	2.030	-.821
6	12	3	2.170	-2.941
6	12	-4	2.490	-2.460
6	13	-1	3.350	2.714
6	13	-2	2.970	2.972
6	13	-4	3.350	-2.062
7	0	0	2.570	-2.292
7	0	2	6.770	7.313
7	0	4	2.590	2.863
7	0	-6	8.420	6.433
7	0	-8	9.670	9.573
7	0	-10	4.400	-4.398
7	0	-12	3.220	-3.634

H	K	L	OBSERVED	CALCULATED
7	0	-14	2.470	2.362
7	1	0	1.720	-.626
7	1	1	7.240	7.540
7	1	-1	6.000	-4.802
7	1	2	1.600	1.535
7	1	3	4.050	4.308
7	1	4	1.520	-1.355
7	1	-5	4.260	4.219
7	1	-7	8.380	7.575
7	1	-8	4.520	4.266
7	1	-9	1.440	.912
7	1	-11	3.340	-3.321
7	1	-12	4.440	-4.318
7	1	-13	2.800	-2.839
7	1	-15	2.230	2.196
7	1	-16	1.780	.519
7	2	1	2.150	-1.926
7	2	-1	3.950	3.421
7	2	2	4.200	3.872
7	2	-2	6.990	-4.880
7	2	3	2.080	-2.356
7	2	-6	5.110	4.338
7	2	-7	8.660	7.846
7	2	-8	5.370	5.180
7	2	-10	3.160	-3.037
7	2	-12	3.140	-3.402
7	2	-13	3.360	-3.327
7	2	-14	1.700	.961
7	2	-16	1.980	1.891
7	2	-17	2.000	2.368
7	3	0	1.370	-1.141
7	3	1	1.400	.845
7	3	-1	1.330	-.785
7	3	2	2.550	2.223
7	3	-2	2.840	-2.156
7	3	-3	2.150	-1.858
7	3	4	1.720	-1.397
7	3	-6	2.430	-2.308
7	3	-7	3.970	3.422
7	3	-8	4.540	4.426
7	3	-11	3.970	-4.127
7	3	-12	4.720	-5.077
7	3	-15	2.230	2.119
7	3	-17	2.000	1.709
7	4	0	3.490	2.999
7	4	1	1.940	-.834
7	4	-1	2.170	1.638
7	4	-3	1.840	-1.088
7	4	4	1.560	-1.445
7	4	-4	1.500	1.337
7	4	-6	3.420	3.276
7	4	-7	2.310	1.733
7	4	-9	1.880	-.405
7	4	-12	3.240	-3.463
7	4	-16	3.160	3.420
7	5	1	1.440	-1.324
7	5	-2	2.110	1.615
7	5	3	1.520	1.170
7	5	-5	1.880	-1.529
7	5	-6	1.960	-1.430
7	5	-7	4.890	4.764
7	5	-8	3.000	-2.799
7	5	-11	4.910	-5.328
7	5	-12	2.080	2.226
7	5	-15	1.980	2.024
7	5	-16	1.800	-.185
7	5	-17	1.800	1.480
7	6	0	2.330	2.338
7	6	1	1.640	1.555
7	6	2	3.200	3.401
7	6	-2	6.430	-6.240
7	6	-3	3.890	3.774
7	6	-5	2.490	-2.237
7	6	-6	5.820	5.803
7	6	-7	6.260	-5.965
7	6	-10	2.130	-1.747
7	6	-12	3.320	-3.643
7	6	-13	2.330	1.965
7	6	-16	2.860	2.832
7	7	0	2.750	2.791
7	7	1	3.060	2.833
7	7	-1	4.440	-4.298
7	7	2	2.490	-2.709
7	7	-2	3.030	3.520
7	7	3	4.070	4.311
7	7	-3	6.590	-6.468
7	7	-4	2.310	-2.364
7	7	-7	7.000	7.615
7	7	-8	2.450	-2.354
7	7	-11	4.090	-4.394
7	7	-12	3.400	3.527
7	7	-15	1.780	1.727
7	8	1	2.110	1.687
7	8	2	4.780	5.331
7	8	-2	7.260	-7.761
7	8	3	1.800	-.950
7	8	-3	1.460	1.337
7	8	4	2.110	1.936
7	8	-4	4.170	-4.150
7	8	-5	2.900	-3.061
7	8	-6	4.860	5.088
7	10	-1	1.980	1.706
7	10	2	2.450	2.207
7	10	-2	1.720	-1.547
7	10	3	1.860	-1.681
7	10	-3	2.310	-2.020
7	10	-4	3.140	-3.287
7	10	-5	1.540	-1.353
7	10	-7	3.280	2.918
7	10	-8	3.990	4.264
7	10	-9	2.650	2.549
7	10	-13	2.730	-3.023
7	11	1	2.250	2.079
7	11	-2	1.580	-.761
7	11	-3	1.580	-1.429
7	11	-8	2.860	2.899
7	11	-11	1.740	-.792
7	11	-12	3.180	-2.878
7	11	-13	2.000	-2.057
7	12	-7	1.860	1.655
7	12	-11	1.760	.793
7	12	-12	1.780	-1.538
7	13	-6	2.530	-2.395
7	13	-7	1.700	1.736
7	13	-11	2.450	-2.212
7	14	-1	1.920	1.786
7	14	-2	2.490	-2.725
7	14	-5	1.720	-1.448
7	14	-6	2.860	2.886
7	14	-7	1.940	-1.374
7	14	-11	1.800	1.218
7	14	-12	2.000	-1.811
7	15	-1	2.550	-2.217
7	15	-2	1.960	1.758
7	15	-3	1.940	-1.913
7	15	-4	1.740	-1.110
7	15	-6	1.960	-1.794
7	15	-7	3.000	3.407
7	15	-11	2.470	-2.281
7	16	-1	1.980	1.593
7	16	-2	2.880	-3.368
7	16	-5	1.780	-2.103
7	16	-6	1.980	2.338
7	8	-7	2.510	-2.642
7	8	-8	4.660	5.168
7	8	-9	2.550	3.010
7	8	-10	2.430	-2.372
7	8	-12	2.750	-2.630
7	8	-13	1.740	-1.178
7	9	0	2.190	2.428
7	9	1	4.090	4.779
7	9	-1	2.960	-3.101
7	9	2	1.780	-1.653
7	9	3	2.900	2.961
7	9	-3	6.370	-6.364
7	9	4	1.860	-1.833
7	9	-4	2.710	-2.952
7	9	-5	2.450	2.701
7	9	-7	4.030	4.067
7	9	-8	2.900	3.262
7	9	-12	1.720	-1.538
7	9	-13	1.960	-2.216
7	9	-14	1.980	-1.548
7	10	0	1.760	-1.636

Table V: Interatomic distances $\leq$ 3.5Å

Bond (1) (2)	Distance Å	σ (Å)
Cu-Cl I	2.259	0.0025
	2.922	
Cu-Cl II	2.285	0.0025
Cu-Cl III	2.301	0.0024
	2.307	0.0024
Cu-O I	2.600	0.0084
Cu-Cu	3.399	0.0029
O I-Cl I	3.261	0.0077
O I-Cl II	3.408	0.0084
O I-Cl II	3.396	0.0073
O I-Cl II	3.201	0.0083
O I-Cl III	3.375	0.0080
O I-Cl III	3.407	0.0082
O I-Cl III	3.539	0.0081
O I-O II	3.058	0.0105
O I-O II	3.066	0.0108
O II-Cl I	3.195	0.0075
O II-Cl II	3.365	0.0074
O II-Cl II	3.201	0.0069
O II-Cl II	3.365	0.0074
O II-Cl III	3.340	0.0077
O II-O II	2.876	
Cl II-Cl I	3.266	0.0035
Cl II-Cl III	3.294	0.0036
Cl III-Cl I	3.275	0.0037
Cl III-Cl III	3.112	0.0044

Table VI: Bond distances averaged over thermal motion

(1) Bond (2)	Atom (2) riding on atom (1). (Å)	Atom (1) riding on atom (2). (Å)	Independent motion (Å)	σ (Å)
Cu - Cl I	2.258	2.260	2.281	0.0025
Cu - Cl II	2.284	2.286	2.307	0.0025
Cu - Cl III	2.300	2.302	2.323	0.0024
Cu - Cl III	2.306	2.308	2.329	0.0024
Cu - O I	2.597	2.604	2.617	0.0084

FIGURE CAPTIONS

Figure 1: a) The $Cu_2Cl_6^{=}$ ion in perspective drawing.

b) The complete structure model. The labeled atoms belong to the O II set.

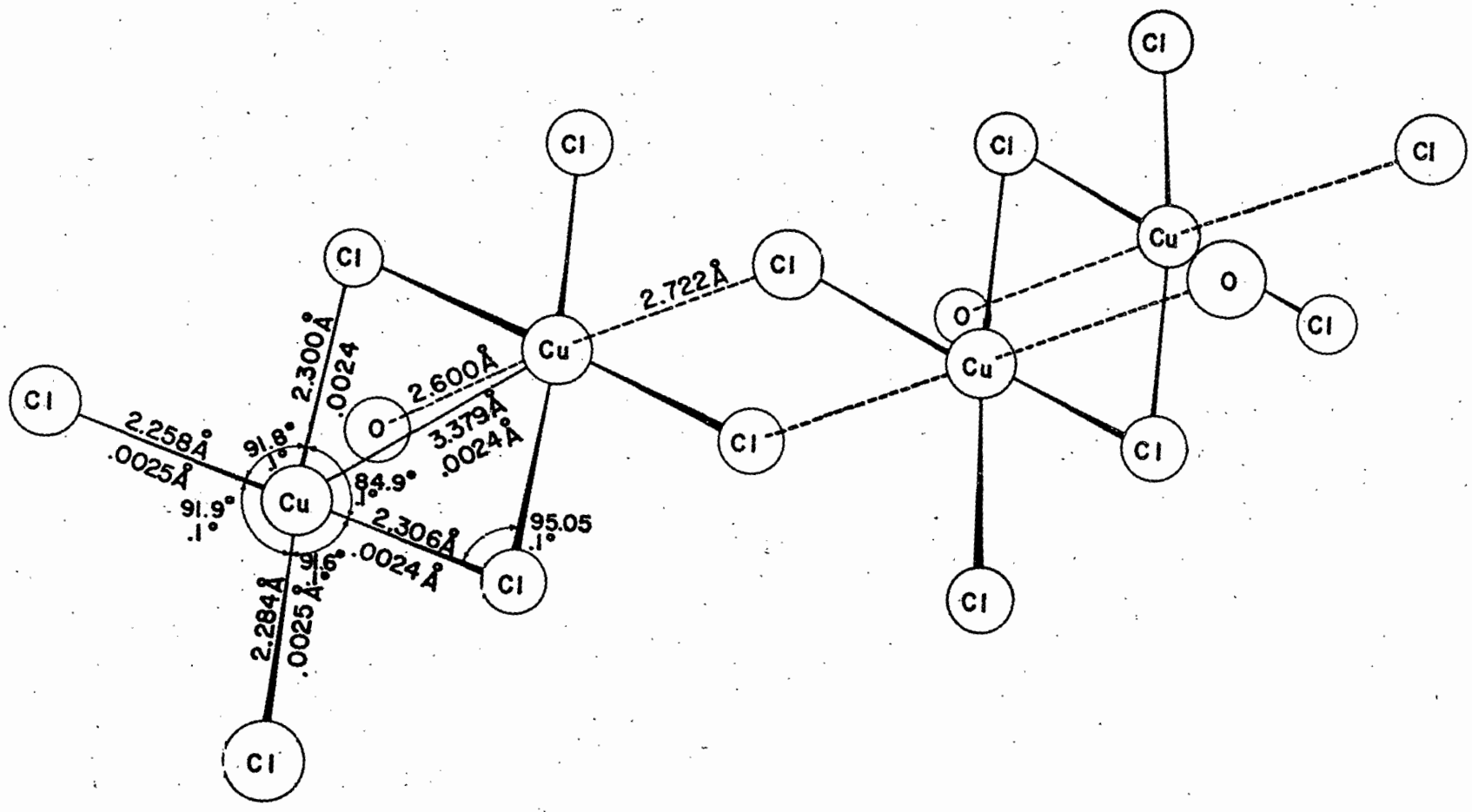
Cl
Cl
Cl
Cl
Cl
Cu
O
Cl
2.722Å
Cl
O
Cu
Cl
Cl
Cl
2.600Å
2.300Å
.0024
3.379Å
.0024Å
2.258Å
.0025Å
91.8°
.1°
84.9°
.1°
91.9°
.1°
Cu
2.306Å
95.05
.1°
.0024 Å
Cl
2.284Å
.0025 Å
Cl

Figure 1 a)

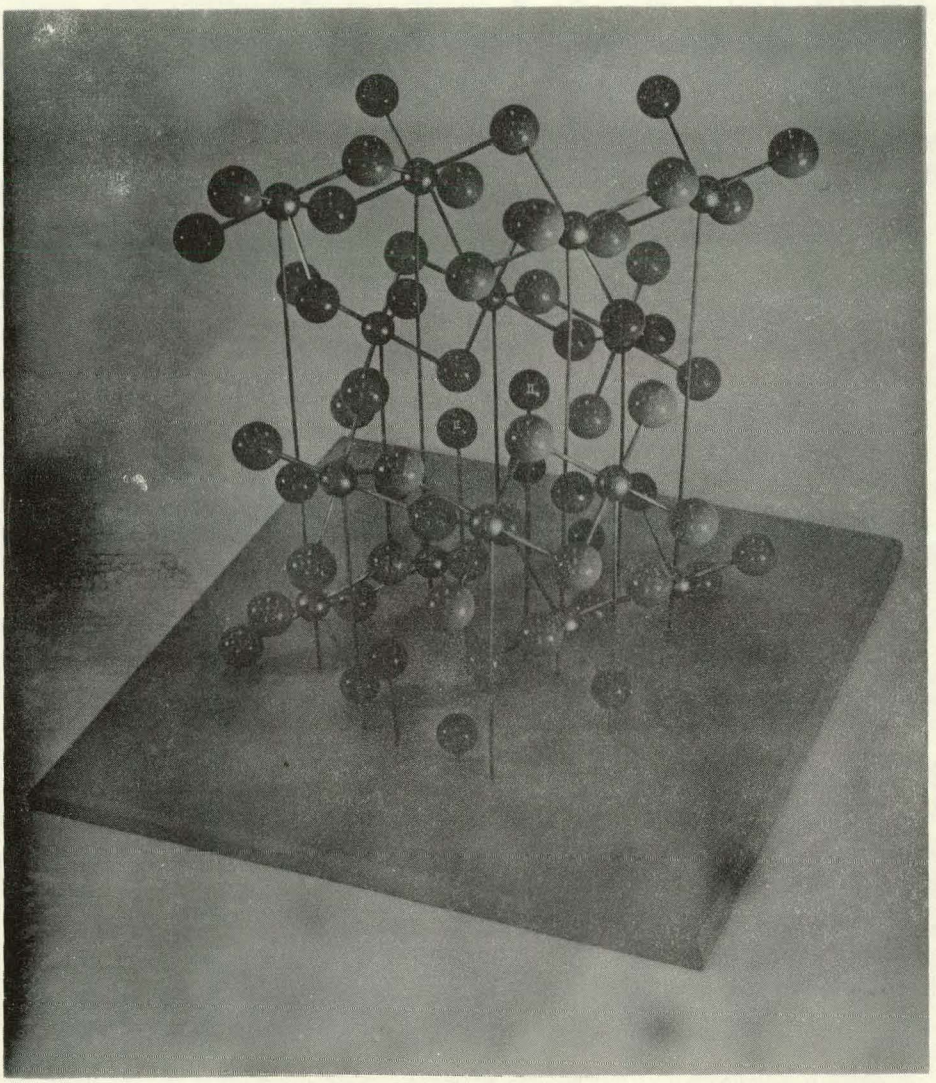

Figure 1 b)