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The crystal structure of  $\text{LiCuCl}_3 \cdot 2\text{H}_2\text{O}$ \*

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Abstract

$\text{LiCuCl}_3 \cdot 2\text{H}_2\text{O}$  forms garnet-red, monoclinic crystals,  $a = 6.078$ ,  $b = 11.145$ ,  $c = 9.145\text{\AA}$  (all  $\pm 0.003$ ),  $\beta = 108^\circ 50'$ , space group  $P2_1/c$ ,  $Z = 4$ . The structure contains planar  $\text{Cu}_2\text{Cl}_6^{2-}$  ions joined by longer  $\text{Cu} \cdots \text{Cl}$  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  $0.007\text{\AA}$  for oxygen parameters, less for others, while important interatomic distances have been determined with standard deviations of  $\sim 0.0025\text{\AA}$ .

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

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

#### Introduction

The garnet-red crystals of  $\text{LiCuCl}_3 \cdot 2\text{H}_2\text{O}$  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  $\text{Cu}_2\text{Cl}_6^{2-}$  ion, complete structural work was undertaken. Simultaneously this ion was found in  $\text{KCuCl}_3$  (Dwiggins, 1958).

#### Preparation and Properties

$\text{LiCuCl}_3 \cdot 2\text{H}_2\text{O}$  was prepared by the method of Getman (1922). The prismatic, monoclinic crystals are elongated along what we have chosen as the  $\underline{a}$ -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  $66^\circ$  to  $\underline{a}$ , 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:  $a = 6.078$ ,  $b = 11.145$ ,  $c = 9.145 \pm 0.0003 \text{ \AA}$ ,  $\beta = 108^\circ 50'$ . The X-ray density for  $Z = 4$  is  $2.39 \text{ g/cc}$ , in good agreement with the observed density, above.

Reflections  $\{h0\}$  were observed only with  $h$  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  $\text{MoK}\alpha$  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 anomalous dispersion were made, following Templeton and Dauben (1955).

#### Discussion of the Structure

General description— $\text{LiCuCl}_3 \cdot 2\text{H}_2\text{O}$  is made up of nearly planar  $\text{Cu}_2\text{Cl}_6^{2-}$  of approximately  $D_{2h}$  symmetry. The Cu-Cl distances within the ion are  $\sim 2.3\text{\AA}$ , and the ions are connected into  $(\text{Cu}_2\text{Cl}_6^{2-})_x$  chains through two  $\text{Cu} \cdots \text{Cl}$  links of about  $2.9\text{\AA}$ , 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  $2.9\text{\AA}$ , and a water molecule (O1) below at  $2.6\text{\AA}$ , 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  $\text{Cu}^{++}$  and  $\text{Li}^+$  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  $\text{Cu}_2\text{Cl}_6^{=}$  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  $\text{Cl}^-$  ions. If we let normals to the planes containing CII-Cu-Cu, CIII-Cu-Cu and CIII-Cu-Cu be denoted by  $N_1$ ,  $N_2$  and  $N_3$  the angle between  $N_1$  and  $N_2$  is  $1.7^\circ$ , that between  $N_1$  and  $N_3$  is  $5.05^\circ$  and that

between  $N_2$  and  $N_3$  is  $6.75^\circ$ . Cl I forms an external Cu-Cl bond of  $2.258\text{\AA}$  within the  $\text{Cu}_2\text{Cl}_6^{2-}$  ion and a weaker bond of  $2.922\text{\AA}$  to the copper of a neighboring  $\text{Cu}_2\text{Cl}_6^{2-}$ . Cl II forms an exterior Cu-Cl bond of  $2.284\text{\AA}$  with no further bond to copper. Standard deviations of  $0.0025\text{\AA}$  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  $2.306\text{\AA}$ . 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  $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$  (Peterson and Levy, 1957) for non-bridged Cu-Cl bonds ( $2.275\text{\AA}$ ) and bridges in  $\text{CuCl}_2$  (Wells, 1947a) ( $2.3\text{\AA}$ ).

Lithium position and hydrogen bonding—Two  $\text{O}_{\text{II}}$  oxygens are separated by only  $2.8\text{\AA}$ , 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 chlorine $\text{s}$  about these holes lead us to expect that each  $\text{O}_{\text{II}}$  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,  $\text{LiCuCl}_3 \cdot 2\text{H}_2\text{O}$  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  $\text{Cu}-\text{Cl}-\text{Cu}$  bridges where the bridge angle is  $\sim 90^\circ$  and where both bridge bonds are  $\sim 2.3\text{\AA}$ . These include  $\text{CuCl}_2$  (anhyd.) (Wells, 1947a),  $\text{Ca}_2\text{CuCl}_3$  (Wells, 1947b),  $\text{KCuCl}_3$  (Dwiggins, 1958).  $\text{NH}_4\text{CuCl}_3$  appears to be isomorphous with  $\text{KCuCl}_3$  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  $\text{Cu}-\text{Cl}-\text{Cu}$  bridges, there is one long bond  $\sim 2.9\text{\AA}$ , 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  $\text{LiCuCl}_3 \cdot 2\text{H}_2\text{O}$  and  $\text{CuCl}_2$  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— $\text{LiCuCl}_3 \cdot 2\text{H}_2\text{O}$  remains paramagnetic to about  $5.9^\circ\text{K}$ , where magnetic ordering, presumably antiferromagnetic, takes place (Vossos, Jennings and Rundle, 1960). The ground state for the  $\text{Cu}_2\text{Cl}_6^{2-}$  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*	$\sigma$	IBM 704 without unobserved F**	$\sigma$
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	$\sigma$
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	$\beta_{11}$	$\beta_{22}$	$\beta_{33}$	$\beta_{12}$	$\beta_{13}$	$\beta_{23}$
Cu	0.01402	0.00342	0.00607	0.00170	0.00512	0.00110
$\sigma$	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
$\sigma$	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
$\sigma$	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
$\sigma$	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
$\sigma$	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
$\sigma$	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	H	K	L	OBSERVED	CALCULATED	H	K	L	OBSERVED	CALCULATED
0	0	2	4.920	4.913	0	14	4	4.690	-3.964	1	5	3	7.650	7.581
0	0	4	24.930	-30.261	0	14	8	4.880	4.094	1	5	-3	24.750	-32.524
0	0	6	7.410	-7.468	0	15	1	6.980	6.641	1	5	4	2.540	-9.066
0	0	8	5.390	7.617	0	15	2	3.440	-3.782	1	5	-4	2.540	7.506
0	0	10	9.710	9.328	0	15	3	4.830	-4.163	1	5	-5	6.310	-6.413
0	0	12	3.490	-1.857	0	15	4	3.580	-2.366	1	5	6	6.310	5.783
0	0	14	3.920	-3.903	0	15	5	4.060	-3.251	1	5	-6	2.470	-2.154
0	1	2	8.180	-7.964	0	16	0	3.980	5.767	1	5	7	7.270	-7.027
0	1	3	6.220	-7.501	0	16	1	3.350	-4.937	1	5	-7	16.350	17.841
0	1	4	4.970	3.256	0	16	4	4.730	-4.559	1	5	8	2.670	7.816
0	1	5	27.900	-34.165	0	17	6	3.500	4.695	1	5	9	4.560	4.795
0	1	6	3.010	3.440	1	0	2	11.250	10.141	1	5	-9	3.600	3.917
0	1	7	2.440	2.318	1	0	4	3.050	4.089	1	5	-10	2.670	2.540
0	1	8	4.160	-4.665	1	0	6	15.490	-15.408	1	5	11	3.000	2.767
0	1	9	13.440	12.472	1	0	8	7.270	-7.411	1	5	-11	4.560	-4.168
0	1	10	3.920	-4.306	1	0	-8	2.240	-1.342	1	5	-13	3.990	-3.816
0	2	2	3.390	3.782	1	1	2	7.300	-6.920	1	6	0	4.620	4.833
0	2	3	4.350	3.470	1	1	3	23.190	26.080	1	6	1	12.290	-17.662
0	2	4	17.510	-17.941	1	1	4	12.350	14.330	1	6	-1	4.980	5.814
0	2	5	10.330	8.768	1	1	-3	4.260	-3.740	1	6	2	17.970	21.419
0	2	6	4.590	-5.629	1	1	4	4.320	3.473	1	6	-2	16.290	-17.272
0	2	7	9.710	8.858	1	1	-4	9.740	-9.545	1	6	3	5.880	-4.833
0	2	8	6.410	3.907	1	1	5	16.060	-19.068	1	6	-3	15.020	18.844
0	2	9	7.080	-6.816	1	1	-5	4.890	4.150	1	6	4	4.390	-3.817
0	2	10	4.880	3.097	1	1	6	8.720	-8.214	1	6	-4	1.520	-1.881
0	2	11	4.940	-4.321	1	1	6	4.980	-4.381	1	6	-5	5.180	-4.853
0	3	1	9.140	9.643	1	1	7	8.620	-8.964	1	6	6	8.720	-8.366
0	3	2	10.530	-10.797	1	1	-7	6.310	5.410	1	6	-6	3.840	5.393
0	3	3	10.050	-10.916	1	1	8	7.460	6.715	1	6	7	10.540	9.985
0	3	4	7.610	7.811	1	1	9	2.040	1.075	1	6	-7	2.910	-1.763
0	3	5	2.100	-1.365	1	1	-9	1.910	1.785	1	6	-8	8.360	8.106
0	3	6	4.780	-4.622	1	1	-10	2.640	-2.753	1	6	9	2.940	2.891
0	3	7	3.830	4.791	1	1	-11	3.250	-4.620	1	6	11	3.630	-3.673
0	3	8	3.110	-2.774	1	1	-12	2.910	-2.874	1	6	-11	3.100	-2.659
0	3	9	4.590	-4.129	1	1	-13	2.770	2.792	1	6	-12	6.170	-6.012
0	3	10	20.100	-20.366	1	2	2	16.520	17.030	1	7	0	4.820	4.682
0	4	0	6.650	6.095	1	2	3	4.620	-4.459	1	7	1	8.390	7.974
0	4	1	2.530	3.082	1	2	-3	24.710	-24.926	1	7	-1	3.070	-2.891
0	4	2	6.740	-6.510	1	2	-4	14.700	-14.971	1	7	2	16.450	-17.659
0	4	3	4.020	-4.541	1	2	5	1.480	-1.569	1	7	-2	1.980	1.075
0	4	4	4.060	4.566	1	2	-5	3.550	4.726	1	7	3	10.730	10.829
0	4	5	11.100	10.633	1	2	6	12.950	-12.375	1	7	-3	9.680	-9.715
0	4	6	12.490	12.633	1	2	-6	7.600	8.902	1	7	4	7.500	-8.455
0	4	7	11.530	-12.469	1	2	7	9.050	-9.056	1	7	-4	3.990	4.260
0	4	8	3.580	3.130	1	2	-7	2.240	1.946	1	7	5	6.170	-6.165
0	4	9	3.350	-7.961	1	2	8	1.910	-1.520	1	7	6	8.260	8.591
0	4	10	2.630	2.599	1	2	-8	9.610	9.406	1	7	-6	2.540	2.524
0	4	11	2.820	1.625	1	2	9	3.270	-3.014	1	7	7	9.740	-9.989
0	4	12	3.010	2.370	1	2	-9	1.910	1.675	1	7	-7	7.730	7.097
0	4	13	5.740	-4.981	1	2	10	6.640	6.274	1	7	-8	4.520	-4.353
0	5	0	8.850	8.849	1	2	-10	2.540	-2.753	1	7	-9	3.130	-2.509
0	5	1	4.690	-4.817	1	2	11	3.760	3.840	1	7	10	2.410	1.193
0	5	2	3.300	3.311	1	2	-11	3.410	4.850	1	7	-10	3.330	3.142
0	5	3	5.740	-5.891	1	2	-12	4.290	-3.699	1	7	11	4.820	4.890
0	5	4	13.300	-13.271	1	2	-13	2.770	2.852	1	7	-11	3.600	-2.953
0	5	5	3.870	-4.408	1	3	1	18.010	27.802	1	8	0	6.010	5.451
0	5	6	7.170	-7.351	1	3	-1	3.710	-4.851	1	8	-1	4.620	4.602
0	5	7	3.490	-2.663	1	3	2	19.100	24.198	1	8	2	9.940	9.197
0	5	8	9.230	9.483	1	3	-2	5.180	3.960	1	8	-2	8.290	-7.864
0	5	9	4.400	4.235	1	3	3	4.260	5.186	1	8	3	2.340	2.047
0	5	10	18.710	19.675	1	3	-3	28.120	-32.866	1	8	-3	4.320	4.053
0	5	11	9.710	-9.334	1	3	4	3.410	4.497	1	8	-4	3.600	-3.215
0	5	12	9.420	-7.750	1	3	-4	10.240	-11.401	1	8	5	3.330	-2.736
0	6	0	15.360	-16.436	1	3	5	6.140	-6.553	1	8	-5	5.280	-6.130
0	6	1	4.300	4.040	1	3	-5	3.850	-5.663	1	8	6	10.310	-9.948
0	6	2	3.400	4.769	1	3	6	9.250	-8.980	1	8	-6	4.360	3.923
0	6	3	6.840	6.321	1	3	-6	7.170	-7.303	1	8	7	3.460	7.786
0	6	4	29.480	27.355	1	3	7	4.690	-4.611	1	8	8	4.290	-4.674
0	6	5	13.110	-11.936	1	3	-7	16.020	16.058	1	8	-8	2.080	-1.301
0	6	6	3.920	3.583	1	3	8	9.150	8.468	1	8	9	3.500	4.204
0	6	7	5.790	-5.550	1	3	9	4.260	4.468	1	8	10	6.110	6.002
0	6	8	16.030	-16.609	1	3	-9	7.270	7.642	1	8	-10	3.600	-3.354
0	6	9	2.190	3.773	1	3	-10	2.110	-1.946	1	8	11	3.300	-2.883
0	6	10	6.940	-7.398	1	3	11	2.670	2.449	1	8	-11	3.370	-3.046
0	6	11	4.490	3.275	1	3	-11	3.410	-5.038	1	9	0	4.340	7.072
0	6	12	5.880	6.115	1	3	-12	3.750	-4.821	1	9	1	13.020	13.340
0	7	0	12.490	11.474	1	4	0	2.670	1.056	1	9	-1	3.230	-2.965
0	7	1	3.250	-4.140	1	4	1	8.420	9.056	1	9	2	4.790	4.851
0	7	2	2.820	-2.904	1	4	2	3.380	3.328	1	9	-2	4.820	-4.984
0	7	3	2.630	-2.185	1	4	-1	2.440	3.209	1	9	3	5.020	4.606
0	7	4	16.560	-17.950	1	4	2	20.150	25.534	1	9	-3	1.750	-1.568
0	7	5	8.900	9.240	1	4	-2	16.650	-19.796	1	9	4	4.420	-5.003
0	7	6	8.080	7.243	1	4	3	8.920	-8.483	1	9	-4	6.270	-5.767
0	7	7	5.880	-5.529	1	4	-3	3.710	-4.820	1	9	5	11.070	-10.745
0	7	8	16.360	16.256	1	4	4	6.440	-6.592	1	9	-5	1.880	1.322
0	7	9	3.920	-4.768	1	4	-4	12.850	-15.309	1	9	7	4.850	-4.318
0	7	10	6.840	-7.109	1	4	5	8.550	-7.993	1	9	-8	2.970	2.200
0	7	11	7.510	6.781	1	4	-5	7.460	8.166	1	9	-9	2.280	1.750
0	7	12	3.150	3.945	1	4	6	3.370	3.464	1	9	-11	3.100	-2.835
0	8	0	3.780	-3.793	1	4	-6	18.070	18.870	1	10	0	7.830	7.244
0	8	1	3.390	4.014	1	4	7	2.370	-1.708	1	10	1	10.010	8.983
0	8	2	4.540	-4.764	1	4	-7	3.200	2.657	1	10	-1	2.870	3.261
0	8	3	3.730	4.010	1	4	8	2.410	2.797	1	10	2	2.800	2.673
0	8	4	4.160	-3.936	1	4	-8	3.100	2.640	1	10	-2	4.030	-3.426
0	8	5	3.540	7.404	1	4	-9	9.510	-8.495	1	10	-3	10.900	-9.865
0	8	6	4.390	3.937	1	4	-10	3.300	-2.065	1	10	-4	13.440	-13.103
0	8	7	3.730	-3.071	1	5	0	1.680	1.809	1	10	5	2.310	-2.875
0	8	8	3.730	3.490	1	5	1	11.030	11.394	1	10	-5	3.960	-4.424
0	8	9	4.350	3.896	1	5	-1	2.140	-2.638	1	10	6	6.770	-6.731
0	8	10	4.300	-3.752	1	5	2	16.350	-16.615	1	10	-6	4.260	4.139
0	8	11	3.190	-2.721	1	5	-2	10.040	9.727	1	10	7	3.270	-3.385



H	K	L	OBSERVED	CALCULATED	H	K	L	OBSERVED	CALCULATED	H	K	L	OBSERVED	CALCULATED
1	10	-9	3.430	3.310	2	1	-9	7.960	-8.407	2	6	-3	5.170	-5.851
1	10	10	5.780	5.543	2	1	10	2.790	-2.622	2	6	4	7.120	7.154
1	10	-10	2.470	-2.289	2	1	-10	4.180	3.767	2	6	-4	3.630	3.623
1	11	0	4.090	4.199	2	1	11	3.830	4.166	2	6	5	6.420	-7.452
1	11	1	11.660	11.872	2	1	-11	4.210	-4.217	2	6	-5	1.420	1.636
1	11	2	7.600	6.819	2	1	-12	2.700	2.018	2	6	-6	11.240	11.364
1	11	-1	3.270	-2.926	2	1	-15	4.590	4.257	2	6	7	3.570	4.218
1	11	-2	2.640	2.106	2	2	1	4.530	4.237	2	6	-7	9.940	10.028
1	11	-3	8.060	-8.077	2	2	2	10.230	11.697	2	6	8	6.710	-6.336
1	11	-4	8.160	-7.884	2	2	3	5.980	-3.286	2	6	-8	1.710	-1.671
1	11	5	7.130	-6.430	2	2	4	11.850	12.325	2	6	9	3.540	3.656
1	11	-5	2.080	-2.005	2	2	-4	4.760	5.862	2	6	-9	3.160	2.860
1	11	6	3.800	-3.617	2	2	5	6.450	6.863	2	6	-10	3.950	-3.463
1	11	-6	4.720	-4.618	2	2	-5	4.500	-3.712	2	6	-11	8.020	-7.409
1	11	-7	4.360	4.343	2	2	6	5.900	-6.246	2	6	12	3.480	3.351
1	11	-7	5.550	4.968	2	2	-6	15.110	15.088	2	6	-12	2.960	-2.908
1	11	-9	6.870	6.804	2	2	7	6.010	-6.289	2	6	-13	2.260	-1.859
1	11	-11	2.640	-2.585	2	2	-7	6.830	-7.116	2	6	-15	2.470	1.829
1	11	-13	3.600	-3.428	2	2	8	5.900	-5.956	2	7	0	7.490	6.545
1	12	0	4.130	3.587	2	2	-8	2.060	1.486	2	7	-1	3.540	-3.271
1	12	1	2.970	3.196	2	2	9	2.130	-2.250	2	7	2	2.670	-2.648
1	12	-1	3.860	4.213	2	2	-9	2.870	-2.879	2	7	-2	5.080	-4.356
1	12	2	5.250	5.151	2	2	-10	9.180	-8.600	2	7	3	5.310	5.223
1	12	-2	6.930	-6.275	2	2	-11	8.160	7.457	2	7	-3	3.800	-3.895
1	12	3	6.600	-6.760	2	2	12	2.580	2.248	2	7	4	2.170	2.658
1	12	-3	3.760	-3.587	2	2	-14	3.740	3.467	2	7	-4	5.020	-4.980
1	12	-4	9.780	-9.615	2	2	-15	2.700	-2.024	2	7	-5	5.900	5.365
1	12	-5	2.180	-2.119	2	3	0	5.110	-4.581	2	7	-6	12.990	13.230
1	12	6	2.870	-2.445	2	3	2	7.260	6.682	2	7	7	4.880	-4.615
1	12	-6	3.660	3.651	2	3	-2	4.650	3.822	2	7	-7	7.030	6.728
1	12	-7	2.340	-1.713	2	3	3	21.240	25.666	2	7	-8	2.670	3.394
1	12	-8	8.170	8.231	2	3	-3	6.450	-6.499	2	7	-9	3.690	-3.204
1	12	-9	3.200	3.311	2	3	4	7.260	-7.345	2	7	10	3.220	3.043
1	12	-11	3.330	2.895	2	3	5	4.650	5.029	2	7	-10	4.560	-4.164
1	12	-12	3.560	-3.071	2	3	-5	13.680	15.285	2	7	11	2.290	1.375
1	12	-13	2.870	-2.057	2	3	6	2.840	-2.407	2	7	-11	5.460	-3.147
1	13	1	3.890	3.366	2	3	-6	14.240	-15.335	2	7	12	2.700	-2.571
1	13	-1	2.940	-2.431	2	3	7	9.470	-9.911	2	7	-12	3.020	-2.571
1	13	2	4.590	-4.405	2	3	-7	10.920	11.481	2	7	-15	2.790	2.609
1	13	-2	8.590	7.909	2	3	8	2.580	2.393	2	8	0	7.720	-3.402
1	13	3	4.030	4.006	2	3	9	3.340	-5.610	2	8	1	2.150	7.504
1	13	-3	9.310	-9.277	2	3	-9	4.730	-4.586	2	8	-1	6.680	-6.995
1	13	-5	2.280	-1.325	2	3	10	2.730	-2.359	2	8	2	3.250	2.904
1	13	-6	4.890	-4.682	2	3	-10	5.050	4.623	2	8	4	2.760	-2.108
1	13	7	2.510	-2.415	2	3	11	2.170	1.798	2	8	-4	3.400	3.184
1	13	-7	5.780	6.339	2	3	-11	5.750	-5.622	2	8	5	3.740	-3.925
1	13	8	3.430	3.554	2	3	12	2.580	2.120	2	8	-5	1.590	-0.983
1	13	-8	2.510	2.024	2	3	-12	2.060	0.762	2	8	6	4.500	-4.278
1	13	-9	2.610	2.579	2	3	-13	3.570	3.330	2	8	-6	5.200	4.560
1	14	1	3.100	-2.848	2	3	-14	2.320	1.630	2	8	7	3.480	3.630
1	14	-1	3.830	3.886	2	3	-15	2.410	1.440	2	8	-8	2.520	2.367
1	14	2	7.730	7.333	2	4	0	12.350	-12.689	2	8	-9	4.760	4.335
1	14	-2	6.670	-6.318	2	4	1	3.340	4.303	2	8	-10	6.590	-6.420
1	14	3	7.860	-7.388	2	4	-1	9.620	9.288	2	8	-11	2.930	-2.606
1	14	-3	3.730	3.340	2	4	2	14.530	17.658	2	8	-12	3.080	-2.205
1	14	4	2.510	-2.049	2	4	-2	27.780	-36.843	2	8	-14	3.100	2.757
1	14	7	5.280	4.871	2	4	-3	5.430	-5.882	2	9	0	5.170	4.696
1	15	1	2.370	-1.148	2	4	4	19.640	22.486	2	9	1	4.240	3.989
1	15	2	5.150	-5.146	2	4	-4	3.920	4.569	2	9	-1	4.270	-4.368
1	15	-2	3.270	2.779	2	4	-5	2.230	-1.652	2	9	2	2.060	-1.436
1	15	3	4.590	4.261	2	4	6	1.800	1.138	2	9	-2	5.720	5.718
1	15	-3	3.830	-3.721	2	4	-6	16.820	20.393	2	9	-3	4.150	-3.615
1	15	4	3.300	-3.286	2	4	7	3.130	-2.599	2	9	-4	4.350	-5.120
1	15	6	2.610	2.299	2	4	-7	5.170	4.609	2	9	5	2.050	1.321
1	15	7	4.750	-4.879	2	4	8	11.530	-12.085	2	9	-5	9.760	9.651
1	15	-7	3.330	3.166	2	4	-8	4.990	-4.956	2	9	-6	1.940	-2.114
1	15	8	2.740	2.788	2	4	9	2.700	1.573	2	9	7	1.970	-1.034
1	16	-1	2.470	2.018	2	4	-9	1.740	-1.490	2	9	-9	5.350	-5.236
1	16	2	4.190	4.215	2	4	-10	4.850	-3.887	2	9	11	3.050	3.111
1	16	-2	3.300	-2.083	2	5	0	4.040	3.945	2	9	-11	2.900	-2.754
1	16	6	3.330	-2.968	2	5	1	6.500	5.079	2	9	-12	2.290	1.552
1	17	0	3.430	3.406	2	5	1	6.360	-5.699	2	9	-15	3.480	3.151
1	17	1	3.200	2.291	2	5	-1	19.900	-26.769	2	10	0	10.230	-10.275
1	17	-2	2.900	-2.067	2	5	2	3.570	2.910	2	10	1	3.950	4.377
1	17	4	2.700	-2.663	2	5	-2	11.650	-11.006	2	10	-1	7.260	7.240
1	18	0	2.700	2.316	2	5	3	24.930	25.283	2	10	2	3.800	3.406
1	18	1	2.700	2.104	2	5	-3	4.350	-4.337	2	10	-2	2.410	-1.858
1	19	0	2.800	2.717	2	5	4	3.830	-2.840	2	10	3	2.230	-1.965
1	19	1	3.560	3.044	2	5	-4	2.550	-2.492	2	10	4	6.910	6.914
1	19	-4	3.460	-2.584	2	5	5	2.470	2.931	2	10	-4	3.310	2.995
1	19	-5	3.200	-1.7072	2	5	-5	8.570	8.474	2	10	-5	4.880	-4.466
1	20	-4	2.900	-3.068	2	5	6	1.860	-1.784	2	10	6	5.840	-5.674
1	21	-3	1.020	-1.314	2	5	-6	9.320	8.811	2	10	-6	7.120	6.702
2	0	2	4.650	5.411	2	5	7	10.020	-11.085	2	10	7	2.060	-1.800
2	0	4	2.410	-1.697	2	5	-7	13.660	14.885	2	10	-7	4.850	-4.127
2	0	6	9.180	-10.784	2	5	8	2.760	2.191	2	10	8	2.410	-2.224
2	0	-8	8.390	7.584	2	5	-8	4.120	4.436	2	10	-8	2.200	1.786
2	0	10	2.790	2.067	2	5	9	4.210	-4.248	2	10	-10	6.970	-6.437
2	0	-10	13.310	-11.478	2	5	-9	2.170	-1.925	2	10	-11	3.080	2.661
2	0	-12	2.900	-2.670	2	5	10	2.810	2.786	2	10	-14	2.810	2.891
2	0	-14	5.690	5.138	2	5	-10	2.780	-2.043	2	11	0	4.170	3.877
2	1	1	10.520	8.659	2	5	-11	6.300	-6.400	2	11	1	2.700	2.233
2	1	2	4.010	3.419	2	5	12	2.350	-1.359	2	11	-1	12.750	-13.642
2	1	4	2.030	3.169	2	5	-12	4.120	-4.113	2	11	2	4.760	4.575
2	1	5	4.010	-3.846	2	5	-13	3.370	3.641	2	11	3	7.990	7.998
2	1	5	2.040	2.700	2	6	0	3.050	-3.357	2	11	-3	5.020	-4.564
2	1	-5	14.730	17.095	2	6	1	1.910	2.613	2	11	4	5.520	-5.464
2	1	-6	13.980	-13.954	2	6	-1	12.750	-13.368	2	11	-4	3.600	-3.404
2	1	7	3.220	-2.821	2	6	2	10.630	11.224	2	11	5	4.940	4.854
2	1	-7	1.420	2.250	2	6	-2	17.580	-20.769	2	11	-5	10.110	9.651
2	1	-8	1.540	-1.214	2	6	3	3.						



H	K	L	OBSERVED	CALCULATED	H	K	L	OBSERVED	CALCULATED	H	K	L	OBSERVED	CALCULATED
2	11	-6	6.620	-4.393	3	2	-14	3.300	4.602	3	8	6	3.350	3.357
2	11	7	2.900	-2.655	3	2	-15	2.440	1.987	3	8	-6	3.290	3.286
2	11	-7	1.970	1.530	3	3	0	14.700	14.535	3	8	-7	2.000	1.975
2	11	8	2.200	1.354	3	3	1	8.350	-7.177	3	8	-8	2.910	-7.799
2	11	9	4.090	-4.212	3	3	2	6.580	6.192	3	8	9	2.530	-1.933
2	11	-9	4.010	-3.672	3	3	3	6.730	6.739	3	8	10	2.380	-1.971
2	11	-10	2.490	1.998	3	3	-3	12.970	12.324	3	8	-10	9.260	-9.376
2	11	-13	2.470	.722	3	3	4	8.640	-8.924	3	8	-13	2.380	-2.013
2	12	0	8.080	-8.113	3	3	-4	2.440	2.095	3	8	-14	4.940	4.443
2	12	1	4.300	4.928	3	3	5	6.940	6.214	3	8	-15	2.440	1.821
2	12	-1	6.910	6.890	3	3	-5	1.520	1.117	3	9	0	2.610	2.910
2	12	2	6.270	5.876	3	3	6	4.230	-4.192	3	9	1	13.880	-11.803
2	12	-2	9.320	-9.501	3	3	-6	3.050	3.509	3	9	-1	3.670	-3.340
2	12	3	9.920	-6.455	3	3	7	2.050	2.296	3	9	2	3.940	3.928
2	12	-3	9.880	10.461	3	3	-7	4.730	-4.996	3	9	-2	2.080	-2.687
2	12	4	2.060	-2.513	3	3	8	1.970	-1.576	3	9	3	2.530	-2.341
2	12	-4	2.950	-2.715	3	3	-8	3.760	-3.561	3	9	-3	3.060	4.849
2	12	5	7.320	7.114	3	3	9	4.670	-4.987	3	9	4	1.890	.480
2	12	-5	3.020	-2.859	3	3	-9	2.470	-1.916	3	9	5	2.880	8.292
2	12	6	4.670	4.536	3	3	-10	2.080	1.409	3	9	-5	13.820	14.762
2	12	-6	5.050	-5.133	3	3	-13	3.760	3.702	3	9	6	6.550	-6.683
2	12	7	3.250	2.510	3	4	0	1.820	-1.113	3	9	-6	3.380	4.143
2	12	-7	3.940	-2.726	3	4	1	3.000	-2.927	3	9	7	2.110	-2.973
2	12	8	7.900	-8.359	3	4	-1	1.730	.776	3	9	-8	3.080	2.920
2	12	-8	5.260	5.159	3	4	2	10.590	-10.977	3	9	-9	11.170	-11.357
2	12	9	6.130	-6.167	3	4	-2	4.380	-3.417	3	9	10	2.700	2.757
2	12	-9	8.280	8.625	3	4	3	3.350	3.821	3	9	-10	4.640	-5.086
2	12	10	3.720	-3.593	3	4	-3	1.820	-1.817	3	9	-13	3.410	3.151
2	12	-10	9.310	-9.097	3	4	4	8.330	8.781	3	9	-14	3.200	2.147
2	12	11	1.970	-1.763	3	4	-4	2.980	-2.033	3	9	-15	2.590	1.528
2	12	-11	2.810	2.551	3	4	5	3.730	-3.692	3	10	0	9.910	-9.426
2	12	12	2.960	2.848	3	4	6	4.610	4.897	3	10	1	9.390	8.970
2	12	-12	2.470	-2.708	3	4	-6	3.640	3.405	3	10	-2	2.880	2.661
2	12	13	3.600	-3.518	3	4	7	1.880	-1.995	3	10	3	2.380	2.196
2	12	-13	5.780	5.503	3	4	-7	2.350	2.475	3	10	-3	9.440	-9.142
2	12	14	2.610	2.992	3	4	8	5.900	-6.321	3	10	4	3.000	2.974
2	12	-14	3.830	4.233	3	4	-8	6.970	-7.210	3	10	-4	10.820	11.360
2	12	15	3.310	-2.984	3	4	9	2.110	2.266	3	10	5	6.200	-6.473
2	12	-15	2.440	-2.059	3	4	-9	2.440	-1.805	3	10	6	3.790	4.024
2	13	0	3.630	-3.524	3	4	10	2.230	-2.057	3	10	7	3.080	-3.284
2	13	1	2.490	2.307	3	4	-10	3.550	3.239	3	10	-7	1.940	2.242
2	13	-1	3.890	3.419	3	4	12	5.580	5.770	3	10	-8	3.730	-4.501
2	13	2	7.140	-7.097	3	4	-13	2.500	1.924	3	10	-9	2.670	-1.980
2	13	-2	4.880	-5.309	3	5	0	7.790	-6.558	3	10	10	3.470	-3.204
2	13	3	2.150	2.363	3	5	1	2.820	-2.081	3	10	-10	3.290	-4.021
2	13	-3	2.200	-2.143	3	5	-1	10.760	-10.006	3	10	-11	3.140	-3.030
2	13	4	3.080	3.320	3	5	2	3.440	-3.700	3	10	-12	2.980	-2.503
2	13	-4	6.420	6.617	3	5	3	10.500	10.407	3	10	-13	2.470	1.406
2	13	5	3.080	-2.973	3	5	-3	12.820	13.378	3	10	-14	3.580	3.074
2	13	-5	2.760	2.446	3	5	4	3.290	3.039	3	10	-15	2.580	2.140
2	13	6	3.630	-3.047	3	5	-4	4.850	4.460	3	11	0	5.790	5.849
2	13	-6	2.520	-2.151	3	5	5	3.410	3.145	3	11	1	5.530	-5.327
2	13	7	3.100	-2.582	3	5	6	3.050	3.295	3	11	2	4.260	4.699
2	13	-7	4.380	3.688	3	5	7	2.440	2.398	3	11	-2	2.880	-3.569
2	13	8	4.620	3.959	3	5	-7	6.060	-6.469	3	11	4	3.910	-3.970
2	13	-8	2.640	2.613	3	5	8	4.350	-4.645	3	11	5	4.670	5.142
2	13	9	2.760	-2.930	3	5	-13	3.200	3.189	3	11	6	4.140	-3.878
2	13	-9	3.220	-2.536	3	6	0	11.350	-10.573	3	11	-8	2.350	-1.444
3	0	2	6.560	4.677	3	6	1	4.320	-4.452	3	11	9	2.970	-2.526
3	0	4	9.970	10.143	3	6	-1	7.230	-6.811	3	11	-9	3.060	-2.793
3	0	6	4.030	4.300	3	6	2	6.410	-6.889	3	11	-11	2.350	1.739
3	0	-6	5.200	4.544	3	6	-2	3.170	-2.527	3	11	-13	2.790	2.062
3	0	8	12.620	-11.183	3	6	4	8.670	8.531	3	11	-14	2.530	1.752
3	0	-8	13.000	-13.529	3	6	-4	8.290	8.113	3	12	1	2.410	-1.929
3	0	10	2.050	.557	3	6	5	5.610	5.545	3	12	-2	2.140	.146
3	0	-10	6.700	7.268	3	6	-5	8.350	8.540	3	12	3	3.610	3.602
3	1	1	10.130	-24.537	3	6	6	2.850	3.124	3	12	4	2.970	2.601
3	1	2	5.230	5.150	3	6	-6	7.610	7.778	3	12	-5	3.080	-2.784
3	1	3	1.970	-1.416	3	6	7	1.970	1.577	3	12	6	2.730	2.082
3	1	4	7.350	-6.919	3	6	8	4.700	-4.416	3	12	-6	2.050	-2.026
3	1	5	12.940	14.064	3	6	-8	7.760	-8.467	3	12	7	2.320	-2.328
3	1	-5	21.910	28.229	3	6	9	3.000	-2.995	3	12	-7	2.110	2.124
3	1	6	4.640	4.625	3	6	-10	3.500	-3.882	3	12	8	2.170	-1.571
3	1	-6	2.880	2.999	3	6	12	5.080	5.364	3	12	9	3.140	2.956
3	1	7	3.030	-3.326	3	6	-13	2.940	-2.536	3	12	-9	3.080	-2.299
3	1	-7	1.910	-2.189	3	7	0	9.910	-9.603	3	12	-10	2.320	1.747
3	1	8	1.940	-2.817	3	7	1	11.590	-11.496	3	12	-13	2.530	2.059
3	1	-8	2.410	-2.159	3	7	-1	12.320	-12.151	3	13	-1	3.350	-2.462
3	1	9	3.640	-3.297	3	7	3	4.380	4.557	3	13	2	2.080	.799
3	1	-9	17.560	-18.529	3	7	-3	10.090	10.099	3	13	-2	3.970	-1.896
3	1	10	9.560	9.318	3	7	4	7.230	7.755	3	13	3	3.030	2.996
3	2	1	10.170	8.004	3	7	-4	4.380	-3.426	3	13	-3	2.790	2.079
3	2	2	2.700	-3.106	3	7	5	6.670	6.763	3	13	4	4.760	4.244
3	2	3	3.700	4.018	3	7	-5	14.700	16.999	3	13	-8	2.260	-1.373
3	2	4	8.850	9.967	3	7	6	1.910	.287	3	14	0	2.910	-2.349
3	2	-4	17.760	19.277	3	7	-6	1.850	2.830	3	14	1	3.380	-3.227
3	2	5	8.730	-8.421	3	7	7	3.640	-3.918	3	14	-1	3.170	-2.814
3	2	-5	11.380	-11.043	3	7	-8	4.540	4.613	3	14	2	2.170	-1.858
3	2	6	4.480	5.109	3	7	9	2.820	-2.397	3	14	-2	2.110	-1.600
3	2	-6	2.790	2.840	3	7	-9	9.440	-10.175	3	14	3	2.470	2.473
3	2	7	4.260	-4.378	3	7	10	4.110	-4.083	3	14	4	3.200	3.435
3	2	-7	2.970	2.577	3	7	-13	3.610	3.681	3	14	5	2.320	1.983
3	2	8	1.940	-2.354	3	8	0	17.620	-18.406	3	14	-6	3.350	3.176
3	2	-8	9.620	-9.178	3	8	1	8.610	8.399	3	14	-7	2.910	2.723
3	2	9	3.140	3.407	3	8	-1	5.880	-5.940	3	14	8	2.970	-3.069
3	2	-9	3.410	-2.783	3	8	2	1.640	-1.427	3	15	1	2.850	-2.265
3	2	10	3.200	-3.436	3	8	-2	1.550	1.312	3	15	-1	5.000	-4.951
3	2	-10	4.670	-4.917	3	8	3	6.320	-5.549	3	15	2	2.260	1.609
3	2	11	4.440	-4.920	3	8	4	5.970	6.018	3	15	-2	3.580	-3.488
3	2	-11	2.850	2.547	3	8	-4	18.260	10.223	3	15	3	3.260	2.880
3	2	12	4.350	4.318	3	8	5	8.760	8.0					

H	K	L	OBSERVED	CALCULATED	H	K	L	OBSERVED	CALCULATED	H	K	L	OBSERVED	CALCULATED
3	15	4	2.610	1.909	4	5	1	2.180	-1.849	4	11	5	2.020	2.097
3	15	5	2.410	1.191	4	5	-1	2.110	-1.563	4	11	-8	4.380	-7.139
3	15	-5	5.080	4.690	4	5	2	6.660	6.135	4	11	-9	4.430	-4.175
3	15	-6	3.760	3.273	4	5	-2	9.000	-7.673	4	11	-11	2.160	2.024
3	15	-7	2.550	-1.603	4	5	3	4.590	-4.373	4	11	-12	3.730	2.198
3	15	-8	2.410	1.582	4	5	-3	8.440	7.945	4	12	-1	3.460	-3.518
3	15	-9	3.140	-2.452	4	5	-4	3.780	-2.819	4	12	3	1.970	1.604
3	16	0	4.410	-4.001	4	5	-6	4.350	3.289	4	12	-3	3.350	3.293
3	16	1	3.670	3.425	4	5	7	3.130	3.241	4	12	-4	3.380	3.188
3	16	-1	3.470	-3.164	4	5	-7	14.520	-15.943	4	12	5	2.670	-2.388
3	16	2	3.230	-2.797	4	5	-8	5.730	5.617	4	12	-6	3.000	-3.049
3	16	-2	2.290	-0.040	4	5	-11	7.760	7.845	4	12	-8	5.270	-5.155
3	16	-3	3.470	-3.418	4	5	-13	2.890	2.891	4	12	-11	2.840	-1.956
3	16	-4	3.970	4.521	4	5	-16	3.000	-4.458	4	12	-12	2.570	3.689
3	16	-5	3.520	3.082	4	6	0	2.210	-1.481	4	13	2	2.000	1.540
3	16	-6	3.580	3.729	4	6	1	5.300	4.863	4	13	-2	4.840	-4.853
3	16	-7	2.440	2.417	4	6	-1	2.700	-2.362	4	13	3	2.290	-1.637
3	16	-8	2.470	-2.991	4	6	2	10.030	-9.764	4	13	-3	3.050	2.750
3	16	-9	2.530	.387	4	6	-2	15.980	16.921	4	13	-4	2.480	-1.386
3	16	-10	3.610	-3.292	4	6	3	5.190	4.596	4	13	-6	4.510	4.314
3	17	1	3.610	-3.786	4	6	-3	14.310	-15.355	4	13	-7	5.570	-5.742
3	17	2	3.110	3.120	4	6	4	1.670	1.766	4	14	0	2.020	.725
3	17	-3	3.380	3.036	4	6	-4	2.620	2.299	4	14	-1	3.480	-4.223
3	17	4	2.500	1.082	4	6	5	3.460	3.783	4	14	2	3.460	-3.489
3	17	-4	3.610	-3.155	4	6	-5	2.920	3.457	4	14	-2	6.700	7.069
3	17	5	2.530	1.711	4	6	6	2.510	2.510	4	14	3	3.620	3.852
3	17	-5	3.670	3.626	4	6	-6	7.220	-6.955	4	14	-3	3.330	-3.120
3	17	6	3.260	-3.133	4	6	7	3.130	-2.445	4	14	-6	3.050	-3.093
3	17	-6	2.760	2.477	4	6	-7	7.140	7.397	4	14	-7	3.110	2.969
3	17	-8	2.530	1.902	4	6	-8	4.240	-4.187	4	15	0	2.700	-2.608
3	17	-9	2.480	-2.621	4	6	-12	5.950	5.891	4	15	1	2.130	-1.844
3	17	-10	2.910	-2.958	4	6	-13	2.920	-2.591	4	15	-1	2.550	1.576
3	18	1	3.940	4.184	4	7	0	6.760	-7.757	4	15	2	2.970	2.779
3	18	-1	2.470	-2.913	4	7	1	7.870	-7.631	4	15	-2	3.920	-3.892
3	18	-2	2.470	1.230	4	7	-1	6.240	5.406	4	15	3	4.920	-5.030
3	18	-3	2.760	-2.401	4	7	2	8.600	8.232	4	15	-3	2.970	2.473
3	18	-4	3.170	2.588	4	7	-2	7.380	-6.834	4	15	-7	5.000	-4.639
3	18	0	3.140	-1.890	4	7	3	9.520	-10.204	4	16	2	3.700	-4.310
4	0	2	16.500	-17.765	4	7	-3	10.840	10.947	4	16	-2	4.920	4.792
4	0	4	6.430	-7.009	4	7	5	2.840	3.140	4	16	-9	2.210	2.457
4	0	6	10.550	12.560	4	7	6	2.890	-3.073	4	17	0	2.890	-3.327
4	0	-6	11.680	-10.890	4	7	7	6.050	6.448	4	17	1	2.270	-2.187
4	0	-8	8.000	-7.955	4	7	-7	9.190	-9.377	4	17	-1	2.240	.538
4	0	-10	7.030	6.852	4	7	-8	7.890	8.177	4	17	-3	2.240	2.279
4	0	-14	2.730	-2.623	4	7	-11	4.650	4.308	4	17	-4	3.190	3.060
4	1	1	15.630	-17.120	4	7	-12	2.080	-2.142	5	0	0	7.390	7.708
4	1	2	8.980	-7.564	4	8	0	4.130	-3.528	5	0	2	6.490	-6.960
4	1	3	8.900	-9.357	4	8	-1	1.730	-1.581	5	0	4	1.960	-1.924
4	1	4	1.700	1.987	4	8	2	11.090	-11.940	5	0	-6	8.510	6.712
4	1	5	6.050	6.631	4	8	-2	9.460	9.701	5	0	-10	5.770	5.194
4	1	6	2.350	2.259	4	8	3	2.620	2.337	5	0	-14	5.870	-5.630
4	1	7	5.490	5.335	4	8	-3	4.190	-4.181	5	1	0	2.240	1.593
4	1	-7	5.080	-6.187	4	8	4	3.480	-3.632	5	1	1	2.160	-1.243
4	1	-8	11.280	-11.128	4	8	-4	6.220	5.868	5	1	2	4.580	-4.508
4	1	-9	2.290	-1.823	4	8	5	4.080	4.787	5	1	4	2.080	-1.615
4	1	-11	4.080	3.348	4	8	-5	4.320	4.678	5	1	5	2.160	-1.721
4	1	-12	3.970	3.375	4	8	6	6.840	7.343	5	1	-5	10.450	-9.422
4	1	-13	2.020	1.448	4	8	-6	5.700	-5.924	5	1	-6	4.920	4.173
4	1	-15	3.540	-3.574	4	8	7	2.000	-2.066	5	1	7	3.260	4.030
4	2	1	8.540	-7.824	4	8	8	3.650	4.015	5	1	8	1.890	1.103
4	2	2	11.330	-10.442	4	8	-8	3.670	-3.475	5	1	-9	7.270	-6.989
4	2	3	1.830	-1.382	4	8	-9	4.050	-4.278	5	1	-10	4.250	-3.766
4	2	5	4.570	-3.093	4	8	-10	2.650	2.969	5	1	-14	1.990	.579
4	2	6	5.890	6.715	4	8	-14	2.270	-1.681	5	1	-15	2.830	-2.509
4	2	-6	9.060	-8.702	4	9	0	5.380	-5.516	5	1	-16	2.140	1.367
4	2	-7	9.600	-8.802	4	9	1	10.140	-10.506	5	2	0	10.200	8.330
4	2	-8	9.250	-9.395	4	9	-1	6.730	6.354	5	2	1	5.900	5.643
4	2	-10	3.920	3.939	4	9	2	1.700	-1.763	5	2	2	6.050	-5.551
4	2	-12	4.950	4.596	4	9	3	4.220	-4.633	5	2	3	3.080	-2.740
4	2	-13	5.140	4.984	4	9	-3	9.520	9.906	5	2	4	5.800	-5.627
4	3	0	5.890	5.016	4	9	4	2.510	2.543	5	2	-4	5.500	-4.876
4	3	1	6.890	-6.481	4	9	-4	6.870	6.969	5	2	5	3.980	-4.191
4	3	2	8.620	-7.829	4	9	5	3.700	3.673	5	2	-5	4.500	3.936
4	3	3	1.650	-1.653	4	9	7	3.430	3.472	5	2	6	2.290	1.819
4	3	4	2.460	2.417	4	9	-8	4.320	-4.467	5	2	-6	8.960	-8.430
4	3	-4	5.510	3.674	4	9	-9	2.130	-2.182	5	2	7	2.930	3.460
4	3	5	2.590	2.941	4	9	-12	2.160	1.512	5	2	8	2.410	2.105
4	3	6	2.810	2.974	4	9	-13	3.700	1.184	5	2	-10	7.170	7.431
4	3	-6	3.650	3.013	4	10	0	3.270	-3.000	5	2	-11	5.570	-5.342
4	3	-7	11.620	-12.774	4	10	1	4.000	-3.748	5	2	-12	1.810	1.148
4	3	-8	11.470	-12.797	4	10	-1	1.890	-1.728	5	2	-13	2.140	-2.172
4	3	-9	4.350	-4.394	4	10	2	4.320	-4.068	5	2	-14	4.130	-4.099
4	3	-10	2.240	-1.619	4	10	-3	8.460	8.437	5	2	-15	3.280	5.020
4	3	-11	7.570	6.921	4	10	4	1.890	-2.267	5	2	-16	2.140	-1.980
4	3	-12	4.270	4.024	4	10	-4	7.300	7.929	5	3	0	1.340	-1.820
4	3	-13	4.840	4.641	4	10	-5	2.890	3.367	5	3	1	1.910	1.593
4	3	-16	3.080	.943	4	10	6	5.000	5.273	5	3	-1	21.380	19.034
4	4	1	1.890	-1.477	4	10	-6	3.240	-3.373	5	3	2	6.340	-6.584
4	4	-1	4.590	-3.803	4	10	-7	5.460	-4.752	5	3	-2	3.950	2.898
4	4	2	4.400	-3.946	4	10	-8	6.190	-6.325	5	3	3	10.280	-10.570
4	4	-2	14.170	12.572	4	10	-9	4.540	-4.672	5	3	-3	3.930	2.729
4	4	3	2.780	1.794	4	10	-10	2.810	2.686	5	3	-4	3.860	-3.085
4	4	-3	5.110	3.764	4	10	-12	2.810	1.266	5	3	5	2.560	-2.571
4	4	4	5.430	5.304	4	10	-13	3.860	3.427	5	3	-5	13.320	-13.315
4	4	-4	5.870	5.365	4	11	1	5.000	-4.941	5	3	6	2.310	-1.504
4	4	5	2.700	-2.526	4	11	-1	3.000	2.247	5	3	-6	4.880	4.752
4	4	-5	3.970	.968	4	11	2	3.890	-3.006	5	3	7	2.510	2.228
4	4	6	1.750	-1.456	4	11	-2	2.240	1.781	5	3	-7	8.310	-8.669
4	4	-6	6.730	-6.475	4	11	3	1.890	1.664	5	3	-9	5.870	5.765
4	4	-8	8.250	-8.676	4	11	-3	5.190	5.035	5	3	-10	4.800	-4.935
4	4	-12	8.520	9.045	4	11	-4	3.480	4.144	5	3	-11	7.610	8.646



H	K	L	OBSERVED	CALCULATED	H	K	L	OBSERVED	CALCULATED	H	K	L	OBSERVED	CALCULATED
5	3	-12	1.840	2.733	5	10	0	5.870	5.744	6	3	-13	2.110	-2.332
5	3	-13	2.560	-2.600	5	10	2	4.080	-4.222	6	3	-14	2.460	1.189
5	3	-14	2.010	4.858	5	10	-2	2.810	2.340	6	4	0	5.570	4.897
5	3	-15	3.380	-3.081	5	10	3	1.790	-1.577	6	4	2	5.680	5.994
5	3	-16	2.160	4.879	5	10	-3	2.760	2.984	6	4	-2	3.320	-3.160
5	4	0	9.680	8.905	5	10	4	2.710	-3.074	6	4	3	1.820	-2.532
5	4	-1	3.330	-2.797	5	10	-4	2.360	-2.953	6	4	4	7.640	-7.156
5	4	2	2.760	-2.597	5	10	-5	1.890	1.817	6	4	-4	2.270	-1.744
5	4	-7	16.750	17.244	5	10	-6	1.910	-1.819	6	4	6	5.090	-4.310
5	4	-3	4.150	4.008	5	10	-9	2.090	-1.741	6	4	-6	3.240	-2.363
5	4	4	8.610	-8.572	5	10	-10	4.830	5.197	6	4	-7	2.190	-1.821
5	4	-4	6.990	-6.772	5	10	-11	2.630	-2.177	6	4	-8	4.390	4.336
5	4	5	1.860	4.958	5	11	0	2.760	-2.675	6	4	-11	1.980	1.639
5	4	-5	4.300	3.858	5	11	-1	7.320	7.162	6	4	-12	3.640	-4.108
5	4	6	1.760	4.100	5	11	2	3.410	-3.900	6	5	0	4.120	3.548
5	4	-6	19.890	-23.394	5	11	-2	2.360	2.506	6	5	1	4.450	4.416
5	4	7	1.840	1.300	5	11	3	2.460	-2.644	6	5	-1	9.160	8.496
5	4	-7	4.150	-4.627	5	11	-3	2.980	2.997	6	5	-2	2.330	4.968
5	4	8	4.150	4.921	5	11	-4	2.290	1.675	6	5	-3	7.370	-6.545
5	4	-8	1.960	2.118	5	11	-5	8.680	-9.314	6	5	-4	6.380	-5.523
5	4	-10	7.640	8.150	5	11	-7	4.180	-4.737	6	5	-5	4.710	-4.550
5	4	-12	1.860	1.582	5	11	-9	4.200	4.369	6	5	-6	2.700	-2.456
5	4	-15	2.090	4.574	5	11	-10	2.710	-2.620	6	5	-7	4.500	4.749
5	4	-16	2.410	-2.493	5	11	-11	2.040	2.457	6	5	-8	2.380	1.842
5	5	0	6.290	-5.162	5	11	-12	2.090	1.315	6	5	-9	1.840	-1.710
5	5	1	3.660	3.516	5	12	0	6.120	6.499	6	5	-10	2.170	2.175
5	5	-1	17.170	18.591	5	12	-1	2.910	-2.934	6	6	0	4.530	4.295
5	5	3	11.300	-12.114	5	12	2	2.380	-1.915	6	6	1	4.230	3.944
5	5	4	4.330	4.086	5	12	-2	5.800	6.147	6	6	-1	3.910	3.558
5	5	-4	3.780	3.262	5	12	-3	4.180	4.862	6	6	2	2.030	2.314
5	5	5	2.260	-2.495	5	12	4	4.380	-4.677	6	6	3	4.310	-3.118
5	5	-5	9.030	-8.456	5	12	-4	3.060	-3.263	6	6	-4	3.830	-3.347
5	5	6	1.790	1.685	5	12	-5	4.280	4.332	6	6	-5	8.230	-7.528
5	5	-6	3.210	-2.731	5	12	-6	7.120	-7.798	6	6	-6	3.910	-3.319
5	5	7	1.860	1.185	5	12	-7	4.330	-4.800	6	6	-8	4.740	4.093
5	5	-7	7.840	-8.203	5	12	-10	3.880	4.378	6	6	-9	5.380	5.250
5	5	8	1.940	-1.711	5	13	0	4.880	-4.699	6	6	-10	4.340	4.510
5	5	-8	2.560	-2.427	5	13	-1	6.890	6.904	6	6	-12	3.510	-4.056
5	5	-9	3.410	3.435	5	13	2	2.660	-2.840	6	7	0	5.760	5.345
5	5	-10	2.360	1.674	5	13	-2	2.780	2.386	6	7	1	2.890	2.704
5	5	-11	8.240	9.906	5	13	3	3.840	-4.093	6	7	-1	3.830	3.799
5	5	-12	3.060	3.491	5	13	4	3.510	3.765	6	7	-2	1.930	-1.992
5	5	-13	1.960	-2.458	5	13	-5	3.740	-4.291	6	7	-3	4.340	-4.149
5	5	-15	3.260	-2.908	5	13	-7	3.310	-3.794	6	7	-4	4.930	-4.644
5	5	-16	2.160	-2.170	5	13	-11	3.430	3.713	6	7	-5	7.900	-7.625
5	6	1	3.680	3.181	5	13	-12	3.510	4.713	6	7	-6	1.790	-2.387
5	6	0	6.020	-5.990	5	14	0	2.190	1.392	6	7	-7	3.100	3.327
5	6	-1	1.440	-1.405	5	14	1	2.610	-1.765	6	7	-8	2.090	-2.310
5	6	2	1.740	-1.261	5	14	-1	2.660	-2.237	6	7	-9	6.880	6.990
5	6	-2	9.210	8.766	5	14	2	3.780	3.172	6	7	-10	3.750	4.507
5	6	3	3.010	3.008	5	14	-3	1.940	2.090	6	7	-13	3.240	-3.813
5	6	4	4.130	-4.148	5	14	-4	1.940	-1.641	6	8	0	4.310	4.867
5	6	-4	4.280	-4.333	5	14	-6	4.280	-4.218	6	8	1	2.090	-2.160
5	6	5	4.300	4.972	5	14	-7	3.410	-3.717	6	8	-1	3.220	3.117
5	6	-6	10.180	-11.149	5	14	-11	3.060	2.881	6	8	-4	4.520	-4.942
5	6	7	2.510	-2.287	6	0	0	9.140	9.307	6	8	-5	3.210	-3.537
5	6	-7	2.510	-2.737	6	0	2	1.680	-1.226	6	8	-6	6.080	6.348
5	6	8	3.980	3.973	6	0	-8	10.480	9.242	6	8	-10	4.710	4.968
5	6	-8	2.210	2.104	6	0	-10	5.950	5.437	6	8	-12	2.430	-2.586
5	6	-10	4.030	4.034	6	0	-12	3.430	-2.634	6	8	-14	4.470	-4.955
5	6	-11	5.220	5.723	6	0	-14	6.990	-7.538	6	9	0	1.870	-1.764
5	6	-13	2.210	2.233	6	1	0	6.640	-5.897	6	9	1	4.310	4.534
5	6	-15	3.280	-2.776	6	1	1	7.070	6.448	6	9	2	3.190	-3.444
5	6	-16	2.140	-1.912	6	1	2	1.900	-1.739	6	9	-3	4.390	-4.154
5	7	0	2.390	-1.721	6	1	3	1.980	-1.956	6	9	-4	4.730	4.739
5	7	-1	2.530	2.106	6	1	5	3.960	-4.383	6	9	5	2.140	-2.748
5	7	2	4.100	4.077	6	1	-5	9.750	-8.686	6	9	-5	4.390	-4.519
5	7	-2	2.090	-1.636	6	1	-6	1.600	4.133	6	9	6	2.190	2.436
5	7	3	3.700	-3.620	6	1	-7	2.760	2.684	6	9	-7	2.170	2.072
5	7	4	1.910	1.714	6	1	-9	12.460	13.720	6	9	-8	3.830	-4.224
5	7	-4	5.850	5.443	6	1	-10	2.780	-2.475	6	9	-9	7.580	8.819
5	7	-5	1.940	-1.771	6	1	-13	5.920	-6.476	6	9	-13	3.430	-4.270
5	7	-6	4.920	-4.617	6	1	-14	5.790	1.037	6	10	0	4.100	4.380
5	7	-8	2.480	-2.584	6	2	0	7.550	7.416	6	10	1	4.930	-5.409
5	7	-9	2.660	2.702	6	2	1	6.640	-6.158	6	10	-3	4.740	4.918
5	7	-10	4.880	4.924	6	2	-1	3.770	-2.858	6	10	-4	7.100	-7.874
5	7	-11	1.860	1.861	6	2	2	2.780	2.711	6	10	-5	3.050	2.650
5	7	-13	2.010	-1.307	6	2	3	3.210	-3.322	6	10	-6	1.950	1.916
5	7	-15	2.730	-2.235	6	2	4	1.840	-2.344	6	10	-7	2.220	-2.547
5	7	-16	2.460	-1.719	6	2	-4	12.920	-10.346	6	10	-8	3.600	4.471
5	8	1	3.980	-4.225	6	2	5	3.800	4.274	6	11	0	3.190	-3.496
5	8	-1	2.510	1.809	6	2	-5	10.370	8.564	6	11	1	4.530	4.051
5	8	2	2.960	-2.995	6	2	6	2.250	-2.287	6	11	2	2.940	-2.812
5	8	-2	2.090	-4.573	6	2	-6	1.820	-4.430	6	11	-2	1.490	4.104
5	8	3	1.540	-4.808	6	2	-7	3.540	-3.197	6	11	-3	3.130	-3.405
5	8	-4	2.190	-1.558	6	2	-8	8.010	7.170	6	11	-4	3.350	3.797
5	8	-5	2.660	-2.637	6	2	-9	6.130	-6.131	6	12	0	2.740	2.920
5	8	-6	3.010	2.683	6	2	-11	2.170	2.432	6	12	2	2.380	2.380
5	8	-7	2.860	2.289	6	2	-12	3.370	-3.166	6	12	-2	2.030	-4.821
5	8	-9	1.960	-1.681	6	2	-14	2.460	-2.921	6	12	3	2.170	-2.941
5	8	-10	2.740	2.720	6	3	0	7.500	-6.748	6	12	-4	2.490	-2.460
5	8	-13	2.290	1.986	6	3	1	6.910	6.843	6	13	-1	3.330	2.714
5	8	-14	3.180	-3.117	6	3	-1	6.400	5.702	6	13	-2	2.970	2.972
5	8	-15	2.160	-1.757	6	3	2	1.930	-1.994	6	13	-4	3.350	-2.062
5	9	1	1.840	-1.368	6	3	-2	6.460	5.844	7	0	0	2.570	-2.292
5	9	-1	1.590	-4.722	6	3	-3	8.570	-7.651	7	0	2	6.770	7.313
5	9	3	2.980	2.238	6	3	-4	8.600	7.069	7	0	4	2.590	2.863
5	9	4	2.010	-1.880	6	3	5	3.430	-3.929	7	0	-6	8.420	6.433
5	9	-4	2.960	2.984	6	3	-5	3.940	-3.716	7	0	-8	9.670	9.573
5	9	-5	4.780	-5.167	6	3	-7	4.450	4.454	7	0	-10	4.420	-4.398
5	9	-9	3.990	4.289	6	3	-10	3.190	-2.911	7	0	-12	3.220	-3.634
5	9	-10	1											



H	K	L	OBSERVED	CALCULATED	H	K	L	OBSERVED	CALCULATED	H	K	L	OBSERVED	CALCULATED
7	0	-14	2.470	2.462	7	9	1	1.440	-1.324	7	10	-9	2.450	2.549
7	1	0	1.720	-0.626	7	9	-2	2.110	1.615	7	10	-10	2.740	-3.023
7	1	1	7.240	7.540	7	9	3	1.520	1.170	7	11	1	2.250	2.079
7	1	-1	6.000	-4.802	7	9	-5	1.460	-1.429	7	11	-2	1.880	-0.761
7	1	2	1.600	1.535	7	9	-6	1.960	-1.430	7	11	-3	1.580	-1.629
7	1	3	4.050	4.308	7	9	-7	4.890	4.764	7	11	-4	2.860	2.899
7	1	4	1.520	-1.355	7	9	-8	3.000	-2.799	7	11	-5	1.740	-0.792
7	1	-5	4.260	4.719	7	9	-11	4.910	-5.108	7	11	-6	3.180	-2.878
7	1	-7	4.980	-1.575	7	9	-12	2.040	2.226	7	11	-7	2.000	-2.057
7	1	-8	4.520	4.266	7	9	-15	1.980	2.024	7	12	-7	1.860	1.655
7	1	-9	1.440	0.912	7	9	-16	1.800	-1.185	7	12	-8	1.760	0.793
7	1	-11	3.340	-3.321	7	9	-17	1.800	1.480	7	12	-9	1.740	-1.558
7	1	-12	4.440	-4.318	7	6	0	2.350	2.338	7	13	-6	2.530	-2.395
7	1	-13	2.800	-2.839	7	6	1	1.640	1.655	7	13	-7	1.700	1.736
7	1	-15	2.230	2.196	7	6	2	3.200	3.401	7	13	-11	2.450	-2.212
7	1	-16	1.780	0.519	7	6	-2	6.440	-6.740	7	14	-1	1.920	1.786
7	2	1	2.150	-1.976	7	6	-3	3.890	3.774	7	14	-2	2.490	-2.725
7	2	-1	3.980	3.421	7	6	-5	2.480	-2.757	7	14	-5	1.720	-1.648
7	2	2	4.200	3.872	7	6	-6	5.420	5.803	7	14	-6	2.860	2.886
7	2	-2	4.580	-4.680	7	6	-7	4.260	-4.965	7	14	-7	1.940	-1.974
7	2	3	2.080	-2.356	7	6	-10	2.140	-1.747	7	14	-11	1.800	1.218
7	2	-6	5.110	4.938	7	6	-12	3.920	-3.643	7	14	-12	2.000	-1.811
7	2	-7	8.660	7.846	7	6	-15	2.930	1.064	7	15	-1	2.850	-2.217
7	2	-8	5.370	5.180	7	6	-16	2.840	2.837	7	15	-2	1.960	1.758
7	2	-10	3.160	-3.037	7	7	0	2.780	2.791	7	15	-3	1.640	-1.619
7	2	-12	3.140	-3.402	7	7	1	3.060	2.833	7	15	-4	1.740	-1.110
7	2	-13	3.360	-3.327	7	7	-1	4.640	-4.799	7	15	-6	1.960	-1.754
7	2	-14	1.700	0.961	7	7	2	2.490	-2.709	7	15	-7	3.000	3.607
7	2	-16	1.980	1.891	7	7	-2	3.890	3.520	7	15	-11	2.470	-2.281
7	2	-17	2.000	2.368	7	7	3	4.070	3.311	7	16	-1	1.980	1.543
7	3	0	1.370	-1.141	7	7	-3	6.590	-6.468	7	16	-2	2.880	-3.368
7	3	1	1.400	0.845	7	7	-4	2.310	-2.364	7	16	-3	1.780	-2.103
7	3	-1	1.530	-0.785	7	7	-7	2.000	2.615	7	16	-4	1.980	2.338
7	3	2	2.550	2.223	7	7	-8	2.850	-2.354	7	8	-7	2.510	-2.640
7	3	-2	2.840	-2.154	7	7	-11	4.090	-4.304	7	8	-8	4.640	5.164
7	3	-3	2.150	-1.858	7	7	-12	3.400	3.627	7	8	-9	2.850	3.010
7	3	4	1.720	-1.397	7	7	-15	1.780	1.727	7	8	-10	2.480	-2.372
7	3	-5	2.430	-2.305	7	8	1	2.110	1.687	7	8	-12	2.780	-2.630
7	3	-7	3.970	3.422	7	8	2	4.740	5.331	7	8	-15	1.740	-1.174
7	3	-8	4.540	4.425	7	8	-2	7.260	-7.761	7	9	0	2.190	2.424
7	3	-11	3.970	-4.127	7	8	3	1.400	-0.980	7	9	1	4.000	4.774
7	3	-12	4.720	-5.077	7	8	-3	1.460	1.357	7	9	-1	2.960	-3.101
7	3	-15	2.230	2.119	7	8	4	2.110	1.934	7	9	2	1.780	-1.653
7	3	-17	2.000	1.709	7	8	-4	4.170	-4.150	7	9	3	2.970	2.961
7	4	0	3.490	2.929	7	8	-5	2.000	-2.061	7	9	-3	6.370	-6.364
7	4	1	1.940	-0.634	7	8	-6	4.860	5.083	7	9	4	1.860	-1.833
7	4	-1	2.170	1.634	7	10	-1	1.980	1.706	7	9	-4	2.710	-2.952
7	4	-3	1.840	-1.088	7	10	2	2.460	2.207	7	9	-5	2.450	2.701
7	4	4	1.560	-1.444	7	10	-2	1.720	-1.547	7	9	-7	4.030	4.067
7	4	-4	1.500	1.987	7	10	3	1.860	-1.681	7	9	-8	2.900	3.262
7	4	-6	3.420	3.276	7	10	-3	2.310	-2.020	7	9	-12	1.720	-1.634
7	4	-7	2.310	1.734	7	10	-4	3.140	-3.287	7	9	-13	1.960	-2.214
7	4	-9	1.880	-0.405	7	10	-5	1.540	-1.353	7	9	-14	1.980	-1.548
7	4	-12	3.240	-3.463	7	10	-7	3.280	2.918	7	10	0	1.740	-1.636
7	4	-16	3.160	3.420	7	10	-8	3.090	4.264					

Table V: Interatomic distances  $\leq 3.5\text{\AA}$ 

Bond (1) (2)	Distance $\text{\AA}$	$\sigma$ ( $\text{\AA}$ )
Cu-Cl I	2.259 2.922	0.0025
Cu-Cl II	2.285	0.0025
Cu-Cl III	2.301 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)	$\sigma$ (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  $\text{Cu}_2\text{Cl}_6^{2-}$  ion in perspective drawing.
- b) The complete structure model. The labeled atoms belong to the O II set.



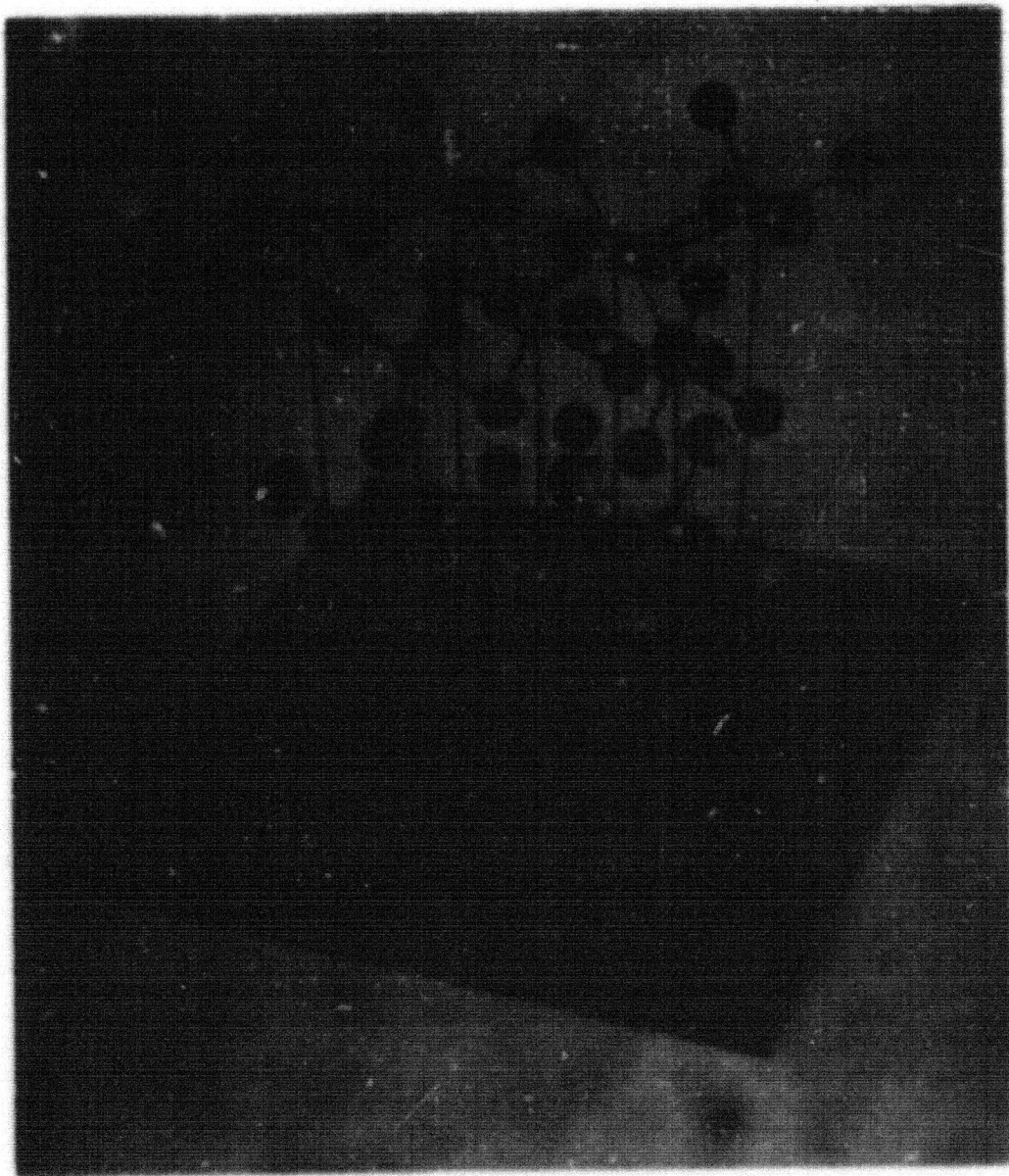


Figure 1 b)



**END**